

1 **Importance of isomerization reactions for the OH radical** 2 **regeneration from the photo-oxidation of isoprene investigated** 3 **in the atmospheric simulation chamber SAPHIR**

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34 A Theoretical work

35 A.1 Isoprene di-HPCARP-RO₂-I

36 A 1.1 Methodology

37 The reactants, transition states and products in the studied mechanistic branches of the isoprene chemistry
38 were characterized at the M06-2X and CCSD(T) levels of theory. A brute force search of the conformer
39 space for each of these structures was performed at the M06-2X/cc-pVDZ level of theory, (Dunning,
40 1989; Zhao and Truhlar, 2008; Alecu et al., 2010; Bao et al., 2017) starting from a systematic series of
41 starting geometries generated by orienting the internal rotors along a set of dihedral angles reasonable for
42 the type of rotor, and optimizing the geometry. While there is no guarantee that this approach yields all
43 stable conformers, it should provide a near-complete description of the rotameric space. For the case at
44 hand, ~24000 distinguishable structures were located from ~60000 starting geometries. The most relevant
45 conformers (~850 structures across all reactions examined) were then fully re-optimized at the M06-
46 2X/aug-cc-pVTZ level of theory. (Dunning, 1989) The number of conformers re-optimized at this higher
47 level of theory differs per structure (see Table S1), but enough were included to cover over ~80% of the
48 thermal population at 300K. Intrinsic reaction coordinate (IRC) calculations were performed on the
49 lowest transition states (TS) to verify the nature to the transition state; the end points of these trajectories
50 were further optimized and the energies used for determining an Eckart energy barrier shape. Finally,
51 single energy point calculations at the CCSD(T)/aug-cc-pVTZ level of theory (Purvis and Bartlett, 1982)
52 were performed on the energetically lowest-lying geometries of each structure, to further refine the
53 energy barrier estimates.

54 The rate coefficients are calculated using multi-conformer canonical transition state theory (MC-CTST),
55 where each structure is described as the ensemble of each of its conformers in a rigid rotor, harmonic
56 oscillator approximation (Vereecken and Peeters, 2003).

$$57 \quad k(T) = \frac{kT}{h} \frac{\kappa \cdot Q^\ddagger(T)}{Q_{\text{reactant}}(T)} \exp\left(\frac{-E_b}{kT}\right) \quad (\text{eq. S1})$$

58 The barrier height E_b is the ZPE-corrected energy difference between the lowest conformers of transition
59 state and reactant. The partition functions for each critical point is obtained from a Boltzmann-weighted
60 sum of the partition functions $Q_i(T)$ of the n_{conf} conformers constituting that critical point, with $E_i = 0$ for
61 the lowest-energy conformer:

$$62 \quad Q(T) = \sum_{i=1}^{n_{\text{conf}}} Q_i(T) \cdot \exp\left(\frac{-E_i}{kT}\right) \quad (\text{eq. S2})$$

63 This relies on a (near-)Boltzmann equilibrium population across all conformers, e.g. by internal rotation
64 being significantly faster than chemical transformation reactions, a condition easily fulfilled for the
65 reaction examined, given the much higher energy barriers for chemical reaction. To improve the
66 prediction of $k(T)$ and its temperature dependence, the partition functions $Q(T)^{\text{all}}$ are estimated for the
67 M06-2X/aug-cc-pVTZ level of theory by combining the high level M06-2X/aug-cc-pVTZ result,
68 available for the dominant conformers, with the low-level M06-2X/cc-pVDZ rovibrational characteristics,
69 available for all conformers, as follows:

70
$$Q(T)_{high}^{all} = Q(T)_{high}^{selected} \times \frac{Q(T)_{low}^{all}}{Q(T)_{low}^{selected}} \quad (\text{eq. S3})$$

71 i.e. the full partition function at the M06-2X/aug-cc-pVTZ level of theory is estimated by scaling the
 72 partition function for the dominant conformers to the total population, using the M06-2X/cc-pVDZ
 73 information of the minor conformers scaled to higher-level M06-2X/aug-cc-pVTZ. This procedure
 74 mitigates most of the impact of omitting the higher-energy conformers at the more costly levels of theory,
 75 and provides an approach that can be systematically improved to the limit of full characterization at the
 76 higher level of theory. Alternative additive schemes for merging of the high- and low levels of theory, e.g.
 77 the following:

78
$$Q(T)_{all} = Q(T)_{high}^{selected} + Q(T)_{low}^{all} - Q(T)_{low}^{selected} \quad (\text{eq. S4})$$

79 were not retained, as such additive schemes do not scale the low-level conformer partition functions to the
 80 high-level properties, and thus converge somewhat slower to the limit where all conformers are treated at
 81 the high level of theory. Tunneling, κ , is accounted for by asymmetric Eckart tunneling, where the
 82 conformer-specific reactant and product energies, and imaginary wavenumber, of the lowest-lying TS
 83 conformer are used in the calculation. As the modeling study shows that the chemistry is not overly
 84 sensitive to the exact rate coefficient, we saved some computational cost at this time by not implementing
 85 conformer-specific tunneling κ_i in $Q^\ddagger(T)$ (e.g. Ocana et al., 2019(Ocaña et al., 2019)) but applying the
 86 same tunneling correction κ to all conformers. Conformer-specific tunneling will be implemented later
 87 when merging the current data into a structure-activity relationship (SAR).

88 As shown below, the rates of fast H-scrambling exceed the rates of product formation by 3 to 4 orders of
 89 magnitude, instating a fast equilibrium between **di-HPCARP-RO₂-Ia**, **-Ib**, and **-Ic**. In the absence of
 90 other loss processes that approach the rate of H-scrambling (as would be the case in e.g. high
 91 concentrations of NO, HO₂ or RO₂ radicals), one can then calculate a bulk rate coefficient for aldehyde H-
 92 migration, forming the tri-hydroperoxy-acyl radical. Within the MC-TST paradigm, this involves
 93 calculating the partition functions in eq. S1 across all **di-HPCARP-RO₂-I** and all aldehyde-H-shift TS
 94 conformers, as follows:

95
$$Q_{reactant}(T) = \sum_{j=a,b,c} \sum_{i=1}^{n_{confj}} Q_{\text{di-HPCARP-RO}_2\text{-I}_{j,i}}(T) \cdot \exp\left(\frac{-E_{\text{di-HPCARP-RO}_2\text{-I}_{j,i}}}{kT}\right) \quad (\text{eq. S5})$$

96
$$Q^\ddagger(T) = \sum_{j=1,4;1,5;1,6} \sum_{i=1}^{n_{confj}} Q_{j\text{-aldehyde-H-shift},i}^\ddagger(T) \cdot \exp\left(\frac{-E_{\text{TS}_{j,i}}}{kT}\right) \quad (\text{eq. S6})$$

97 where $E_{\text{diHPCARP-I}_{j,i}}$ is the energy of the i -th conformer of **di-HPCARP-RO₂-I_j** ($j=a,b,c$) relative to the
 98 lowest **di-HPCARP-RO₂-I** conformer, and $E_{\text{TS}_{j,i}}$ the energy of the i -th conformer of the 1,4-, 1,5-, and
 99 1,6-aldehyde-H-shift relative to the lowest aldehyde-H-shift TS conformer, while $Q_{\text{di-HPCARP-RO}_2\text{-I}_{j,i}}(T)$ and
 100 $Q_{j\text{-aldehyde-H-shift},i}^\ddagger$ are the conformer-specific partition functions; n_{confj} signifies the number of conformers
 101 for structure j . The overall barrier E_b in eq. S1 is then the (ZPE-corrected) energy difference between the
 102 lowest **diHPCARP-RO₂-I** conformer and the lowest aldehyde-H-shift TS conformer (in this case, the
 103 lowest-energy **diHPCARP-RO₂-Ic** and 1,6-aldehyde-H-shift conformers). The rate coefficients
 104 calculated thus are included in Table 3. Note that H-scrambling does not alter the stereo-specificity, i.e.
 105 eq. S5 and S6 must be calculated for each stereo-specific pool of reactants/TS. In the current case, the

106 difference in reaction rate between the two isomeric pools is not overly large, and a generalized
107 expression can be obtained by averaging the two stereo-specific rate coefficients (see Table S1).

108

109 A 1.2 Reaction mechanism for di-HPCARP peroxy radicals

110 Table S1 shows a summary of the quantum chemical analysis of the **di-HPCARP-RO₂-I** system. These
111 molecules have 2 chiral carbon atoms, where (2R,3R) and (2S,3S) enantiomers have identical
112 rovibrational data, with a second distinct set of data for the (2R,3S) and (2S,3R) enantiomers. For some
113 reactions the energetic differences are slight, but barrier height differences of several kcal mol⁻¹ exist for
114 H-migration reactions spanning across both chiral atoms, owing to the impact on ring strain and
115 substituent interaction in the cyclic TS.

116 Formation of acyl radicals by migration of the aldehyde H-atom is an accessible channel for all **di-**
117 **HPCARP-RO₂-I** isomers; the barrier height depends strongly on the TS cycle size, and changes from
118 over 20 kcal mol⁻¹ for a 1,4-aldehyde-H-migration, to as low as 16.3 kcal mol⁻¹ for a 1,6-aldehyde-H-
119 migration. The energetically most favorable H-migrations, however, are those involving migration of H-
120 atoms of the hydroperoxide groups to the peroxy radical site, which allows rapid scrambling of the H-
121 atoms, thus allowing access to reaction channels inaccessible from **di-HPCARP-RO₂-Ia** formed initially
122 from **Z-δ-RO₂-I** (see main paper). The reactions of the **di-HPCARP-RO₂-II** isomers can be expected to
123 be similar, i.e. fast hydroperoxide H-scrambling with energy barriers several kcal mol⁻¹ below the
124 aldehyde-H-migration pathways. Our results are analogous to those of Møller et al. (2019) (see also
125 below).

126 HO₂ elimination is found to have too high barriers to compete (see Table S1 and 2), and is not studied in
127 great detail. HO₂ elimination with a -CH₃ H-atom is omitted as this is expected to be even less favorable
128 than those with aldehyde- or α-OOH H-atoms owing to the stronger C-H bond. 1,4- and 1,5-migration of
129 the H-atoms from an -OOH-substituted carbon in **di-HPCARP-RO₂-I** is found to be less favorable than
130 shifting the aldehyde-H-atom; while the energy barrier for the α-OOH 1,5-H-shift is only slightly higher
131 than for the 1,4-aldehyde-H-migration, the additional entropic disadvantage of losing an additional degree
132 of internal rotation in the TS lowers the rate coefficient significantly (see Table S1). While HO₂
133 elimination and α-OOH H-migrations were only examined for **di-HPCARP-RO₂-Ia**, the H-scrambled
134 forms **-Ib** and **-Ic** are not expected to present more favorable channels for these reaction classes, as no
135 pathways exist with more weakly bonded H-atoms, nor allowing for a TS with a lower ring strain.
136 Likewise, it is improbable that **di-HPCARP-RO₂-II** isomers, which differ only by the position of
137 the -CH₃ group, show channels that are competitive against the aldehyde- and hydroperoxide-H-
138 migrations discussed above.

139

140

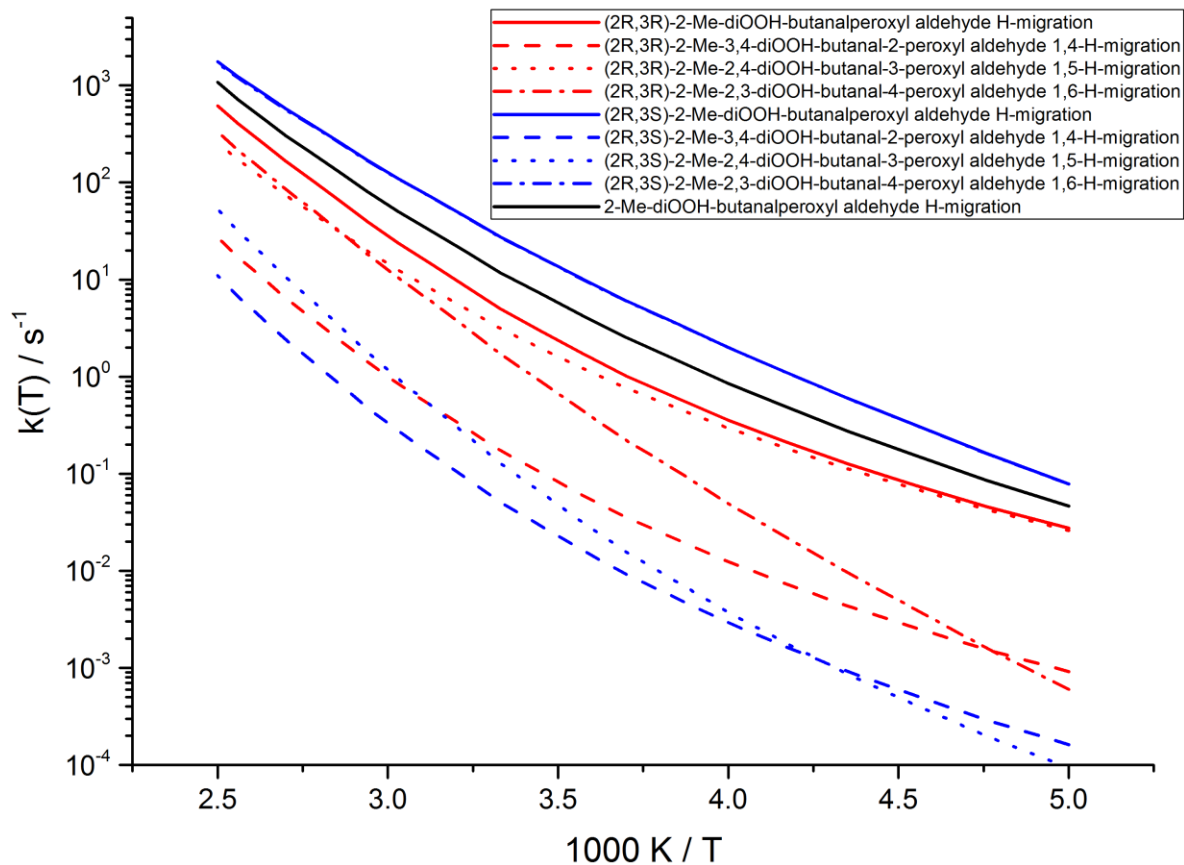
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143 **Table S1: Relative energies (kcal mol⁻¹) of the reactants and transition states for the stereo-specific chemistry of di-**
 144 **HPCARP-RO₂-I (2-Me-3,4-diOOH-butanal-2-peroxyl), at the CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ level of**
 145 **theory. Also indicated are the number of distinguishable conformers characterized at the different levels of theory, and**
 146 **the fraction of the population covered by the data at the highest level of theory.**

Reaction	E_{rel}	# Conformers^a	Pop. fraction^b
(2 <i>R</i> ,3 <i>R</i>)-2-Me-3,4-diOOH-butanal-2-peroxyl (A)	0.0	64 / 1470	0.91
1,4-aldehyde-H-migration	21.4	24 / 251	0.88
1,4- α -OOH-H-migration	28.6	6 / 125	0.98
1,5- α -OOH-H-migration	22.6	22 / 212	0.96
1,6-OOH-H-migration to B	19.3	6 / 100	0.88
1,7-OOH-H-migration to C	12.3	14 / 35	0.99
Aldehyde-HO ₂ -elimination	29.4 ^c	^d	
α -OOH-HO ₂ -elimination	31.9 ^c	^d	
(2 <i>R</i> ,3 <i>R</i>)-2-Me-2,4-diOOH-butanal-3-peroxyl (B)	0.6	47 / 1290	0.83
1,5-aldehyde-H-migration	18.5	18 / 146	0.95
1,6-OOH-H-migration to C	18.9	33 / 95	0.99
(2 <i>R</i> ,3 <i>R</i>)-2-Me-2,3-diOOH-butanal-4-peroxyl (C)	-1.2	39 / 1234	0.96
1,6-aldehyde-H-migration	17.6	27 / 157	0.97
(2 <i>R</i> ,3 <i>R</i>)-2-Me-2,3,4-diOOH-1-oxo-1-butyl (D)	3.4	82 / 2719	0.79
CO elimination	11.1	104 / 2335	0.83
(2 <i>R</i> ,3 <i>S</i>)-2-Me-3,4-diOOH-butanal-2-peroxyl (A')	0.0	26 / 1362	0.87
1,4-aldehyde-H-migration	20.6	25 / 253	0.96
1,4- α -OOH-H-migration	27.2	4 / 128	0.99
1,5- α -OOH-H-migration	23.0	27 / 215	0.98
1,6-OOH-H-migration to B'	16.4	9 / 74	0.99
1,7-OOH-H-migration to C'	14.2	14 / 60	0.99
Aldehyde-HO ₂ -elimination	29.3 ^c	^d	
α -OOH-HO ₂ -elimination	31.3 ^c	^d	
(2 <i>R</i> ,3 <i>S</i>)-2-Me-2,4-diOOH-butanal-3-peroxyl (B')	-1.5	40 / 1280	0.91
1,5-aldehyde-H-migration	19.4	24 / 157	0.93
1,6-OOH-H-migration to C'	18.9	17 / 99	0.96
(2 <i>R</i> ,3 <i>S</i>)-2-Me-2,3-diOOH-butanal-4-peroxyl (C')	-1.3	46 / 1172	0.94
1,6-aldehyde-H-migration	16.3	25 / 146	0.98
(2 <i>R</i> ,3 <i>S</i>)-2-Me-2,3,4-diOOH-1-oxo-1-butyl (D')	3.1	65 / 2904	0.83
CO elimination	10.8	68 / 2495	0.78
2,2,2-triMe-acetyl	0.00		
CO elimination	9.66		
O ₂ addition	0.47		
2,2,2-triMe-acetylperoxy	-32.80		
2,2-diMe-2-OOH-acetyl	0.00		
CO elimination	7.83		
O ₂ addition	0.63		
2,2-diMe-2-OOH-acetylperoxy	-31.31		

147 ^a Number of distinguishable conformers found, with the last number indicating all conformers characterized at the
 148 M06-2X/cc-pVDZ level of theory, and the number before the dividus the number of conformers re-optimized at the
 149 M06-2X/aug-cc-pVTZ level of theory. ^b Fraction of the population at 300K that is based on M06-2X/aug-cc-pVTZ
 150 rovibrational data. The remainder of the population is described by scaling the partition function at the M06-2X/cc-
 151 pVDZ level towards the aug-cc-pVTZ data (see methodology section). ^c Energy barrier at the M06-2X/aug-cc-pVTZ
 152 level of theory. ^d The conformational space is not examined in as much detail as the other structures; statistics are
 153 omitted.



154

155 **Figure S1: Temperature-dependent rate coefficients for the aldehyde H-shift in di-HPCARP-RO₂-I.**

156

157 **A 1.3 Comparison to literature theoretical data**

158 There are two recent theoretical kinetic studies available examining the di-HPCARP-RO₂-I chemical
 159 system. A detailed comparison of the methodological differences is technical, and outside the scope of the
 160 current paper. To assess the uncertainties of the predictions, however, it is useful to give a short
 161 comparison of the results. We limit ourselves here to a discussion of the (R,R)-conformers, though the
 162 comparison can be generalized.

163 The first study by Wang et al. (2018) identified 9 conformers for di-HPCARP-RO₂-Ia, and 9 conformers
 164 for the transition state for 1,4-aldehyde-H-migration, from an examination of a subset of the
 165 conformational space with a selection of conformers based on semi-empirical methods. Despite the
 166 limited set of conformers, the rate coefficient at 298K, 0.86 s⁻¹, is only a factor 1.3 below our predicted
 167 rate of 1.15 s⁻¹ based on all conformers. It is unclear whether this accuracy is due to fortuitous
 168 cancellation of error, or from judicious selection of the two (out of 8) degrees of freedom for internal
 169 rotation considered; note that the authors state that all 9 di-HPCARP-RO₂-Ia conformers can undergo the
 170 1,4-aldehyde-H-migration directly, which indicates they include some less stable conformers, as our set of
 171 9 energetically lowest conformers includes structures where the aldehyde H-atom and the radical oxygen

172 are not pointing towards each other. We optimized some of the provided conformers at the M06-2X/cc-
173 pVDZ level of theory, finding them to be up to 8.7 kcal mol⁻¹ above our most stable conformer, indicating
174 that at least some of the 9 conformers have a negligible contribution to the thermal population. For the
175 1,5- α -OOH-H-migration, this study finds a rate coefficient $9.2 \times 10^{-1} \text{ s}^{-1}$, over an order of magnitude higher
176 than our value of $5 \times 10^{-3} \text{ s}^{-1}$, mostly due to their reported barrier height being several kcal mol⁻¹ below our
177 value; these results are again likely distorted due to the strongly reduced conformer space missing low-
178 energy conformers. Wang et al. (2018) do not examine any of the other aldehyde H-migration pathways
179 to allow further comparison. The barrier for CO elimination after aldehyde H-migration, 8.5 kcal mol⁻¹,
180 somewhat higher than our value which, combined with the limited set of conformers considered, results in
181 a slower dissociation rate of $6.6 \times 10^6 \text{ s}^{-1}$ compared to our value of $2 \times 10^8 \text{ s}^{-1}$. For such low values of CO
182 elimination barrier heights, O₂ addition forming acylperoxy radicals would become competitive.

183 The methodology used by Møller et al. (2019) is more directly comparable to our methodology, and
184 includes an extensive search of the conformer space, while the ROCCSD(T)-F12a/cc-pVDZ-
185 F12// ω B97X-D/aug-cc-pVTZ level of theory used for the rovibrational and energetic parameters in the
186 multi-conformer kinetics is of a comparable class of methods as the methodology used in our work. In
187 most cases, we find strongly comparable barrier heights, with differences of a few tenths of a kcal mol⁻¹
188 only, as expected from the levels of theory applied. Despite these resemblances, the predicted rate
189 coefficients still differ by over an order of magnitude at room temperature. We surmise that these
190 differences are caused by the low-level methodology used to discover and screen the conformers as
191 outlined in Møller et al. (2016), which returns only a subset of the conformers. For example, Møller et al.
192 (2019) report finding over 600 conformers for R,R-di-HPCARP-RO₂-Ia, whereas we have characterized
193 almost 1500 conformers for this compound, over twice as many. Their semi-empirical screening might
194 hope to find predominantly the most important, lowest-energy conformers, where the ~800 missed
195 conformers would then be almost exclusively unstable, high-energy conformers with negligible
196 contribution to the population. However, Møller et al. (2019) found 11 conformers below a 2 kcal mol⁻¹
197 cutoff, whereas we found 27 conformers below 2 kcal mol⁻¹ (M06-2X/aug-cc-pVTZ level of theory),
198 indicating that low-energy conformers are missed in about equal proportion as for the total conformer
199 pool. The 11 lowest conformers in our subset of 27 contribute less than 50 % of the thermal population at
200 300K, thus not describing the population all that well; it is unclear if the 11 conformers of Møller et al.
201 (2019) actually correspond to our lowest 11. Furthermore, while the use of an energetic cut-off (typically
202 2 kcal mol⁻¹ for work based on Møller et al. (2016)) is likely a reasonable choice for aliphatic compounds,
203 it is less appropriate for work with oxygenated compounds. In particular, H-bonded conformers are
204 energetically more favorable, but tend to be more rigid, while higher-energy conformers with less or no
205 hydrogen bonds are more loose, i.e. more entropically favorable. Thus, as can be seen in the population
206 analysis (shown in the supporting information), conformers with energies above 2 kcal mol⁻¹ are still
207 contributing strongly to the population. In our analysis, enough conformers are included in our high-level
208 calculations to ascertain the bulk of the population, $\geq 80\%$, is covered, and all remaining conformers are
209 still included in the kinetic analysis using the data at the lower level of theory. Another drawback of using
210 an energetic cut-off in the population analysis is that, with hundreds to thousands of conformers, the high
211 number of conformers can overcome a Boltzmann weight disadvantage of one or two orders of magnitude
212 and still provide a non-negligible contribution to the population compared to the dozen lowest-energy
213 conformers. The impact of this can't be assessed properly without a more complete population analysis;
214 for the case at hand, we find that at 300K over 30% of the R,R-di-HPCARP-RO₂-Ia population is

215 contributed by conformers over the 2 kcal mol⁻¹ energy cut-off (over 50% when referenced to the 11
216 lowest conformers). Having most of the conformer population represented in the kinetic analysis is
217 especially important when the temperature-dependence is examined, e.g. the contribution of the 11 lowest
218 conformers decreases to less than 35% of the population at 400K (though obviously Møller et al. (2019)
219 would have used a higher energy cut-off value at this temperature). As described by Møller et al. (2019),
220 using semi-empirical methods for screening of conformers is significantly more problematic for transition
221 states than for reactants, spreading the conformer energy range (typically 10 to 20 kcal mol⁻¹ for the
222 multi-oxygenated compounds studied here) to over more than 1000 kcal mol⁻¹. It seems unlikely that the
223 recovered fraction of the conformers, or fraction of the population, is always sufficiently similar for
224 minima and TS to provide reliable cancellation of error, incurring a larger uncertainty on the rate
225 coefficient predictions and their temperature dependence. In the following section, we shortly discuss
226 technical aspects for further improvements in MC-TST methodologies building on the benefits of both
227 our and Møller et al. approach.

228 **A.2 Outlook for multi-conformer methodologies**

229 Based on the comparison between our theoretical results and that of other authors, we find that using
230 semi-empirical methods for screening the conformers relies more on cancellation of error than has been
231 assumed so far, at least for more complex molecules such as studied here. To our knowledge, this is the
232 first exploratory comparison for a complex reaction system between the Møller et al. (2016) methodology
233 based on semi-empirical screening with a kinetic analysis of a subset of the conformers on the one hand,
234 and the all-conformer MC-TST (Vereecken and Peeters, 2003) based on DFT screening as typically
235 performed by our research group. Hence, it is too early to properly assess the relative performance of the
236 two MC-TST approaches. An ineffective screening method can lead to larger *a priori* uncertainties of the
237 kinetic predictions, probably exceeding an order of magnitude when using semi-empirical methods,
238 though the statistical nature of the sampling prevents systematic under- or over-prediction across many
239 reactions. It is important to stress that the search of the conformer space remains a heuristic process in
240 practice, and all practical screening methods are likely to miss some conformer in complex cases, as well
241 as return structures that are non-existing at higher levels of theory. Furthermore, due to the large number
242 of structures involved, it becomes more likely that e.g. erroneous structures are not removed from the
243 populations, or that other flaws are missed by the scientist, despite extensive use of software in
244 generating, handling, and testing all structures. Our more rigorous screening is thus also likely both a
245 subset and superset of the true conformer pool. The larger number of conformers found, and the inclusion
246 of all conformers in the kinetic analysis, dampens the impact to a larger extent than in the methodology
247 of Møller et al. (2016), but this increased robustness comes at a considerable additional computational
248 cost. Note that applying higher levels of theory afterwards on the subset of conformers obtained can't
249 rectify shortcomings in the conformer screening.

250 For the reactions classes studied here, i.e. H-migration in RO₂ intermediates leading to poly-
251 functionalized species and HOMs, there is significant interest in the chemistry of larger terpenoids. The
252 increased computational cost of characterizing these molecules could become overwhelming, so
253 developing efficient and accurate screening methods are critical. Despite the challenges encountered
254 when using semi-empirical methods, the computationally more affordable methodology implemented by
255 Møller et al. (2016) has then many uses; in particular, it remains a cost-effective method for identifying
256 which reactions might be important or can be neglected (e.g. the α -OOH H-shift reactions or HO₂

257 eliminations given in Table S1), providing an order-of-magnitude estimate of the rate coefficient, and of
258 its temperature dependence over small temperature ranges. Future work should try to identify screening
259 methods that are computationally less costly than used in our work, yet are more reliable than semi-
260 empirical methods in returning most conformers, or returning all low-energy conformers. A detailed
261 numerical comparison between this work and the data in Møller et al. (2019) is outside the scope of this
262 paper, but would be an excellent starting point in the search for reliable yet affordable screening methods.
263 This method development would need to include quantum chemical methods such as semi-empirical,
264 molecular mechanics, DFT, and wavefunction-based methodologies, include sampling methods such as
265 explicit iteration over all variables, nearest-neighbor search, random walks, or Monte-Carlo sampling, and
266 include ensemble methods, asymptotic convergence, and other quality metrics to assess the completeness
267 of the sampling. Superimposed on this sampling problem, the traditional improvements on the prediction
268 of energetic and rovibrational characteristics of the molecules and on the theoretical kinetic analysis,
269 remain an important factor facing its own challenges when dealing with exceedingly large sets of
270 conformers.

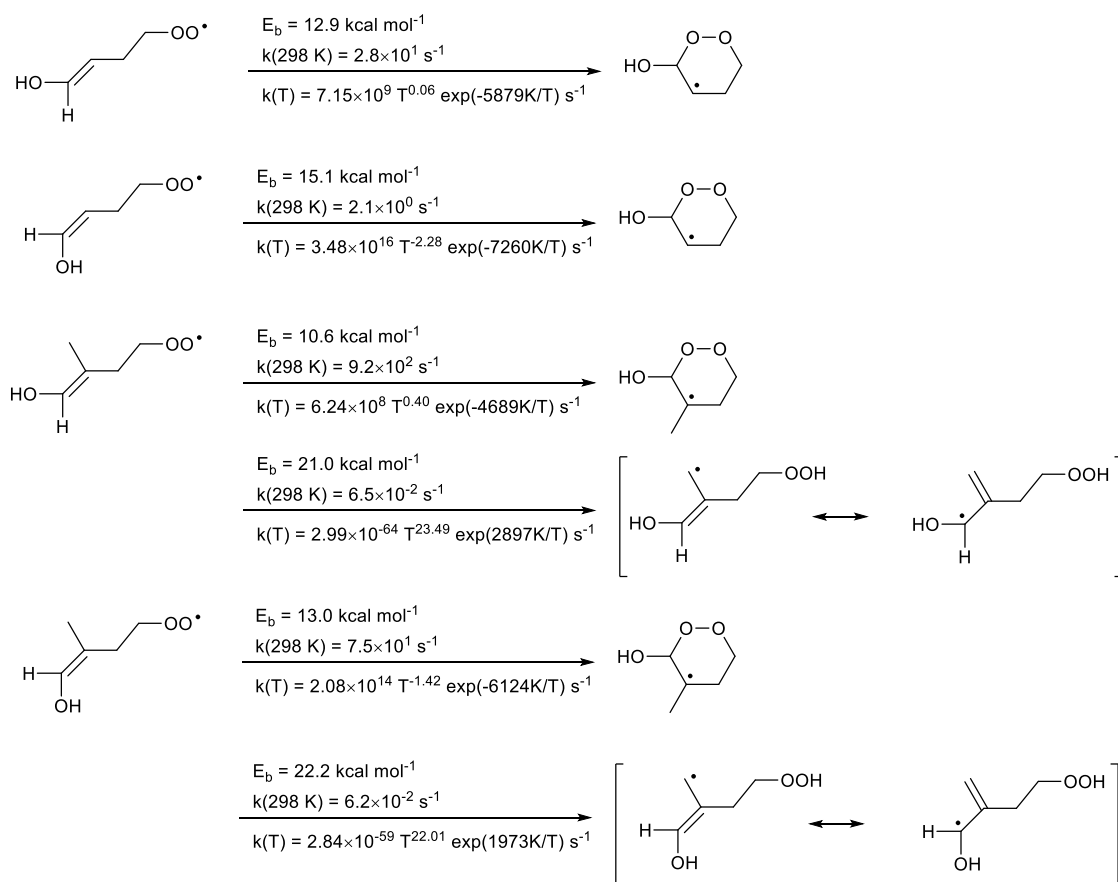
271 **A.3 Chemistry of enol-peroxy radicals**

272 Earlier studies have shown that unsaturated peroxy radicals can have fast ring closure reactions
273 (Vereecken and Peeters, 2004), and this reaction class has been invoked in atmospheric models such as
274 the OH-initiated β -pinene oxidation to explain experimentally observed nopinone and acetone yields
275 (Kaminski et al., 2017). Similarly, H-migrations accelerated by double bonds have been proposed
276 (Peeters et al., 2014). In contrast, the enol peroxy radicals, formed in the isoprene mechanism from Z,E'-
277 HOO-hydroxy-allyl radicals by O₂ addition (see figure S2), are thought by Müller et al. (2019) to have no
278 viable reaction channels competing with redissociation to an alkyl radical + O₂, implying that H-
279 migration and ring closure reactions are negligibly slow. In this section, we perform some exploratory
280 calculations on template enol-peroxy radicals to examine at the impact of unsaturated bonds and of -OH
281 substitution on these two reaction classes.

282 Figure S2 shows the barrier heights and rate coefficients obtained for 6-membered ring closure reactions
283 in enols. In our earlier work we only examined isoprene-derived unsaturated peroxy radicals where the -
284 OH substituent was not attached to the double-bonded carbons, finding ring closure rates of the order of
285 0.3 s⁻¹ at 303 K (Vereecken and Peeters, 2004). In this work, we find that the formation of α -OH cyclic
286 peroxides significantly lowers the barriers compared to aliphatic peroxide radicals with only a spectator -
287 OH substituent, thus increasing the reaction rates significantly (to ~ 10 s⁻¹). We also observe strong stereo-
288 specificity in the calculated rates, with the Z-enols reaction being slower than E-enols. The underlying
289 reason is the H-bond in the Z-enol reactant, which needs to break when performing the ring closure, and
290 thus leading to a higher effective reaction barrier. Still, the rate coefficient difference between Z- and E-
291 enols is not as large as would be expected from the difference in barrier height, as the dominant H-bonded
292 Z-enol conformer is also much more rigid than the E-enols, leading to a lower state density for the Z-enol
293 reactant and hence a more favorable entropic factor in the rate coefficient calculations. Figure S2 also
294 shows the impact of a methyl group on the double bond, where we find that formation of a tertiary
295 product radical further lowers the ring closure barrier height by 2 kcal mol⁻¹, again enhancing the reaction
296 rate. This result is expected, confirming a traditional Evans-Polanyi correlation. Combined, we find that
297 ring closure is accelerated by several orders of magnitude compared to the ring closure rates found in our
298 earlier work, with ring closure rate coefficients as high as 10³ s⁻¹.

299 Similar enhancement was found for H-migration reactions (see figure S2), where formation of an
 300 hydroxy-allyl-resonance stabilized radical product leads to H-migration reactions several orders of
 301 magnitude faster ($k \sim 6 \times 10^{-2} \text{ s}^{-1}$) than traditional, aliphatic methyl-H-abstractions which have rather slow
 302 reaction rates ($k \sim 10^{-4} \text{ s}^{-1}$) as predicted by theory and observed by experiment (Nozière and Vereecken;
 303 Sharma et al., 2010; Miyoshi, 2011; Otkjær et al., 2018). In this particular case, the H-migration rate
 304 coefficients are too low to compete against the ring closure reaction. However, the enhancement of the H-
 305 migration rates could be important for formation of oxygenates and highly oxygenated molecules
 306 (HOMs) from other compounds, where experimental evidence on HOM formation shows very high
 307 oxygen to carbon ratios, which can only be explained if all carbons in the reactant molecule are activated
 308 for oxidation. Allyl-resonance stabilization of the product radical, possibly aided by stabilizing
 309 substituents on the second radical site, could thus prove an important mechanism to enable oxygenation of
 310 otherwise mostly unreactive methyl groups in terpenoids and other atmospherically relevant compounds.

311 At this time, it is unclear whether the current results are directly applicable to the isoprene-derived
 312 intermediates discussed elsewhere in this work. The enol-peroxy radicals of interest there have additional
 313 oxygenated substituents, which may either enhance or reduce the reaction rate, or affect alternative loss
 314 processes such as loss of O_2 . Future work will examine reactions of a wider range of enol-peroxy radicals
 315 to investigate these effects.



316

317 **Figure S2: Barrier heights, room-temperature rate coefficients and temperature-dependent rate coefficients for ring**
 318 **closure and H-migration reactions in enol-peroxy radicals.**

319 B. Kinetic models

320 B.1 M0 model

321 The M0 model is the same as the MCM 3.3.1 model but with H-shift isomerization reactions removed. To
322 keep the number of changes as limited as possible, the removal of the isomerization reaction was
323 implemented by removing the OH-isoprene adducts CISOPA, CISOPC, TISOPA, TISOPC that were
324 introduced in the 2015 update to the MCM chemistry (Jenkin et al., 2015), and their equilibrium
325 reactions. The reactions with formation of either CISOPCO2 or CISOPAO2 were likewise removed, as
326 was the 1,5-H shift reaction as a loss path for ISOPBO2, ISOPDO2 and C524O2. To account for the
327 resulting removal of two of the RO₂ isomers formed after reaction of isoprene with OH radicals, the
328 yields for the remaining RO₂ radicals were scaled, accommodating the attack of the OH radicals on the
329 isoprene carbons C2 and C3 introduced in MCM 3.3.1 (Jenkin et al., 2015). Table S2 lists all reactions
330 affected.

331 **Table S2 Reactions removed (in red), or modified (black) within the M0 model, compared to th MCM v3.3.1. The names**
332 **of the compounds are as in the MCM v3.3.1.**

Model	Reaction	Partial rate coefficient (cm ³ s ⁻¹)
M0	OH + C5H8 -> CISOPA	
	OH + C5H8 -> CISOPC	
	OH + C5H8 -> TISOPA	
	OH + C5H8 -> TISOPC	
	ISOPAO2 -> TISOPA	
	ISOPBO2 -> CISOPA	
	ISOPBO2 -> TISOPA	
	ISOPCO2 -> TISOPC	
	ISOPDO2 -> CISOPC	
	ISOPDO2 -> TISOPC	
	OH + C5H8 -> ISOPAO2	$2.7 \times 10^{-11} \times \exp(390/T) \times 0.14$
	OH + C5H8 -> ISOPBO2	$2.7 \times 10^{-11} \times \exp(390/T) \times 0.41$
	OH + C5H8 -> ISOPCO2	$2.7 \times 10^{-11} \times \exp(390/T) \times 0.09$
	OH + C5H8 -> ISOPDO2	$2.7 \times 10^{-11} \times \exp(390/T) \times 0.28$
	ISOPBO2 -> MVK + HCHO + OH	
	ISOPDO2 -> MACR + HCHO + OH	
	C524O2 -> HMACR + HCHO + OH	

333

334 B.2 M1 model

335 The M1 model is based on the MCM 331 model but contains:

- 336 1- The equilibrium reactions between OH-isoprene adducts and isoprene-RO₂ conformers as
337 implemented in the Caltech mechanism (Wennberg et al., 2018).
- 338 2- A faster 1,6-H shift for the Z- δ -RO₂ combined with a higher yield of formation for di-HPCARP-
339 RO₂ (0.6), as suggested by experimental and theoretical results (Peeters et al., 2014; Teng et al.,
340 2017) and as described in the Caltech mechanism (Wennberg et al., 2018).
- 341 3- The rate coefficients for the aldehyde-H shift of di-HPCARP-RO₂ and product distribution as
342 calculated from theory within this study.

343 Table S3 lists all reactions affected.

344 **Table S3 Reactions modified within the M1 model, compared to th MCM v3.3.1. The names of the compounds are as in**
 345 **the MCM v3.3.1.**

Model	Reaction	Partial rate coefficients (cm ³ s ⁻¹ or s ⁻¹)
M1	TISOPA-->ISOPAO2	0.4×10 ⁻¹²
	TISOPA--> ISOPBO2	0.8×10 ⁻¹²
	CISOPA-->ISOPBO2	0.8×10 ⁻¹²
	CISOPA-->CISOPAO2	0.1×10 ⁻¹²
	CISOPC-->CISOPCO2	0.2×10 ⁻¹²
	CISOPC-->ISOPDO2	0.7×10 ⁻¹²
	TISOPC-->ISOPDO2	0.7×10 ⁻¹²
	TISOPC-->ISOPCO2	0.5×10 ⁻¹²
	ISOPAO2-->TISOPA	1.8×10 ¹⁴ ×exp(-8930/T)
	ISOPBO2-->TISOPA	2.2×10 ¹⁵ ×exp(-10355/T)
	ISOPBO2-->CISOPA	2.2×10 ¹⁵ ×exp(-10865/T)
	CISOPAO2-->CISOPA	1.8×10 ¹⁴ ×exp(-8830/T)
	CISOPCO2-->CISOPC	1.7×10 ¹⁴ ×exp(-9054/T)
	ISOPDO2-->CISOPC	2.5×10 ¹⁵ ×exp(-10890/T)
	ISOPDO2-->TISOPC	2.5×10 ¹⁵ ×exp(-11112/T)
	ISOPCO2-->TISOPC	2.1×10 ¹⁴ ×exp(-9400/T)
	CISOPAO2-->C5HPALD1+HO2	5.0×10 ¹⁵ ×exp(-12200/T)×exp(1×10 ⁸ /T ³)×0.4
	CISOPAO2-->C536O2	5.0×10 ¹⁵ ×exp(-12200/T)×exp(1×10 ⁸ /T ³)×0.6
	CISOPCO2-->C5HPALD2+HO2	2.2×10 ⁹ ×exp(-7160/T)×exp(1×10 ⁸ /T ³)×0.4
	CISOPCO2-->C537O2	2.2×10 ⁹ ×exp(-7160/T)×exp(1×10 ⁸ /T ³)×0.6
	C536O2-->DHPMEK+CO+OH	6.5×10 ⁻⁵³ ×T ^{20.52} ×exp(1669/T)
	C537O2-->DHPMPAL+CO+OH	6.5×10 ⁻⁵³ ×T ^{20.52} ×exp(1669/T)

346

347 B.3 M2 model

348 The M2 model is based on the MCM 331 model but contains:

- 349 1- A faster 1,6-H shift for the Z-δ-RO₂ combined with a higher yield of formation for di-HPCARP-
 350 RO₂ (0.6), as suggested by experimental and theoretical results (Peeters et al., 2014; Teng et al.,
 351 2017) and as described in the Caltech mechanism (Wennberg et al., 2018).
 352 2- The rate coefficients for the aldehyde-H shift of di-HPCARP-RO₂ and product distribution as
 353 calculated from theory within this study.

354 Table S4 lists all reactions affected.

355 **Table S4 Reactions modified within the M2 model, compared to th MCM v3.3.1. The names of the compounds are as in**
 356 **the MCM v3.3.1.**

Model	Reaction	Partial rate coefficients (s ⁻¹)
M2	CISOPAO2-->C5HPALD1+HO2	5.0×10 ¹⁵ ×exp(-12200/T)×exp(1×10 ⁸ /T ³)×0.4
	CISOPAO2-->C536O2	5.0×10 ¹⁵ ×exp(-12200/T)×exp(1×10 ⁸ /T ³)×0.6
	CISOPCO2-->C5HPALD2+HO2	2.2×10 ⁹ ×exp(-7160/T)×exp(1×10 ⁸ /T ³)×0.4
	CISOPCO2-->C537O2	2.2×10 ⁹ ×exp(-7160/T)×exp(1×10 ⁸ /T ³)×0.6
	C536O2-->DHPMEK+CO+OH	6.5×10 ⁻⁵³ ×T ^{20.52} ×exp(1669/T)
	C537O2-->DHPMPAL+CO+OH	6.5×10 ⁻⁵³ ×T ^{20.52} ×exp(1669/T)

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359 **B.4 M3 model**

360 The M3 model is based on the MCM 331 model but contains:

- 361 1- A faster 1,6-H shift for the Z- δ -RO₂ as suggested by experimental and theoretical results (Peeters
 362 et al., 2014; Teng et al., 2017) and as described in the Caltech mechanism (Wennberg et al.,
 363 2018).
 364 2- A larger yield for HPALD as described in the study by Berndt et al. (2019)
 365 3- The rate coefficients for the aldehyde-H shift of di-HPCARP-RO₂ and product distribution as
 366 calculated from theory within this study.

367 Table S5 lists all reactions affected.

368 **Table S5 Reactions modified within the M3 model, compared to th MCM v3.3.1. The names of the compounds are as in**
 369 **the MCM v3.3.1.**

Model	Reaction	Partial rate coefficients (s ⁻¹)
M3	CISOPAO2-->C5HPALD1+HO2	$5.0 \times 10^{15} \times \exp(-12200/T) \times \exp(1 \times 10^8/T^3) \times 0.75$
	CISOPAO2-->C536O2	$5.0 \times 10^{15} \times \exp(-12200/T) \times \exp(1 \times 10^8/T^3) \times 0.25$
	CISOPCO2-->C5HPALD2+HO2	$2.2 \times 10^9 \times \exp(-7160/T) \times \exp(1 \times 10^8/T^3) \times 0.75$
	CISOPCO2-->C537O2	$2.2 \times 10^9 \times \exp(-7160/T) \times \exp(1 \times 10^8/T^3) \times 0.25$
	C536O2-->DHPMEK+CO+OH	$6.5 \times 10^{-53} \times T^{20.52} \times \exp(1669/T)$
	C537O2-->DHPMPAL+CO+OH	$6.5 \times 10^{-53} \times T^{20.52} \times \exp(1669/T)$

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373 **C. Modelled OH regeneration efficiency (RE)**

374 The aldehyde-H shift includes the isomerization reaction of the di-HPCARP-RO₂ (C536O2 and C537O2)
 375 formed after the isomerization of the Z- δ -RO₂, combined with the OH radical which is directly recycled
 376 from the products of the aldehyde-H shift (dihydroperoxy carbonyl compounds, DHPMEK and
 377 DHPMPAL). In addition, the isomerization of the RO₂ which originates from OH reaction with MACR
 378 (MACRO2) is included (Table S6).

379 **Table S6. Reaction paths forming OH radicals included in the modelled OH regeneration efficiency, with their label as**
 380 **used in figure 7. The names of the compounds are as in the MCM v3.3.1.**

Reaction label	Reaction paths included
HONO + <i>hν</i>	HONO + <i>hν</i>
O ₃ + <i>hν</i>	O ₃ + <i>hν</i>
HO ₂ + O ₃	HO ₂ + O ₃
HO ₂ + NO	HO ₂ + NO
1,5-H shift	ISOPBO2 and ISOPDO2
HPALD + <i>hν</i>	C5HPALD1+ C5HPALD2+ C5PACALD1+ C5PACALD2 + <i>hν</i>
Aldehyde-H shift	C536O2, C537O2, DHPMEK, DHPMPAL, MACRO2

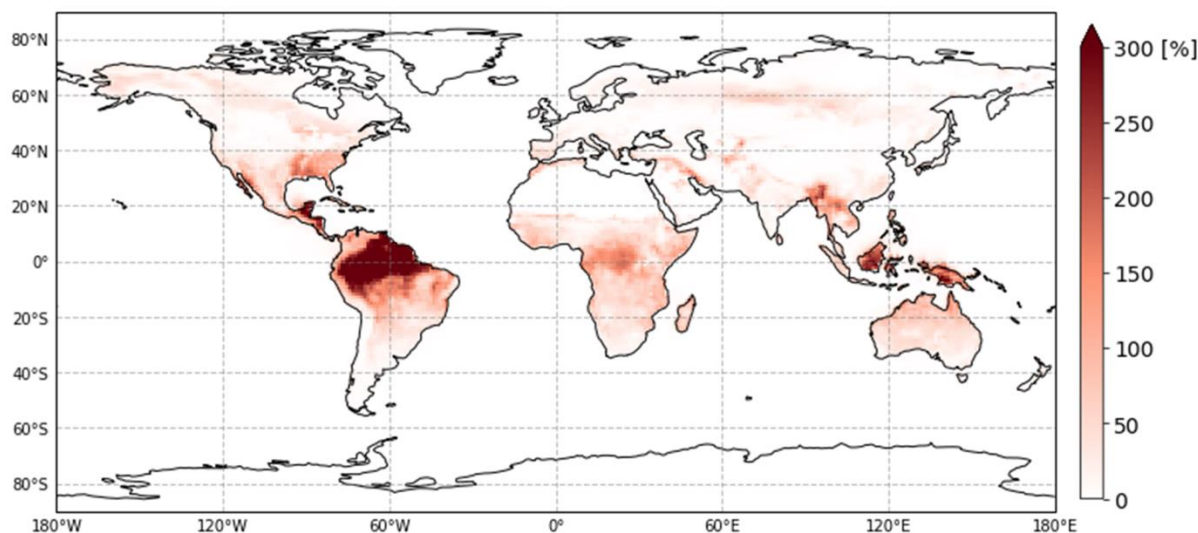
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383 **D. Global model**

384 The ECHAM/MESSy Atmospheric Chemistry (EMAC) (Jöckel et al., 2010) model was used to
385 investigate the global impact of changes in the isomerization of the isoprene chemistry. In this study, two
386 simulations were performed using the Mainz Organic Mechanism (MOM) (Sander et al., 2019). The first
387 simulation served as a reference and the second one included changes as discussed in this study. In the
388 reference simulation, no 1,6-H shift and aldehyde-H shift isomerization in the isoprene chemistry were
389 included (comparable to the no-H shift model). The second simulation is comparable to the M2 model
390 and includes isomerization reactions (1,5-, 1,6- and aldehyde –H shift) using a 0.4 yield for HPALD and
391 0.6 yield for di-HPCARP-RO₂ from the 1,6-H shift. In addition, traditional RO₂ chemistry was included
392 for HPALD and di-HPCARP as used in the MCM v3.3.1. For both simulations, the reaction rates adapted
393 from LIM1 (Peeters et al., 2014) for the equilibrium reactions between OH-isoprene adducts and
394 isoprene-RO₂ conformers were used. Finally, a third simulation was run where the yield of HPALD was
395 set to 0.75, comparable to model M3. The relevant reactions are listed in table S7, while the impact on the
396 OH concentrations is illustrated in figure S3.

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399 **Figure S3. Relative increase of the global ground-level concentration of OH radicals. The implementation of a fast rate**
400 **coefficient for the 1,6-H shift together with the inclusion of the aldehyde-H shift results in an increase of more than a**
401 **factor of 3 for the OH radical concentrations in regions with large concentrations of isoprene and low NO, when**
402 **compared to a model without isomerization reactions.**

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409 **Table S7. Changes to the MOM mechanism used in this study to assess the global impact of isomerisation reaction in the**
 410 **isoprene chemistry. The names of the compounds are as in the original MOM mechanism, whereas newly added**
 411 **compounds are labeled as in the MCM v3.3.1.**

Reaction	(Partial) Rate coefficients (cm ³ s ⁻¹ or s ⁻¹)
LISOPACO2-->C536O2	5.47 x 10 ¹⁵ x EXP(-12200/T) x EXP(1.D8/T ³) x 0.6
LISOPACO2-->ZCODC23DBCOOH+HO2	5.47 x 10 ¹⁵ x EXP(-12200/T) x EXP(1.D8/T ³)x 0.4
LDISOPACO2-->C537O2	5.47 x 10 ¹⁵ x EXP(-12200/T) x EXP(1.D8/T ³) x 0.6
LDISOPACO2-->ZCODC23DBCOOH+HO2	5.47 x 10 ¹⁵ x EXP(-12200/T) x EXP(1.D8/T ³) x 0.4
C536O2+HO2-->C536OOH+O2	2.91 x 10 ⁻¹³ x EXP(1300/T)*0.706
C536O2+NO-->C536O+NO2	2.54 x 10 ⁻¹² x EXP(360./T)
C536O2+NO3-->C536O+NO2	2.50 x 10 ⁻¹²
C536O2-->C536O	9.20 x 10 ⁻¹⁴ x RO2
C536O2-->DHPMEK+CO+OH	6.52x10 ⁻⁵³ xT ^{20.52} xexp(1669/T)
C537O2+HO2-->C537OOH+O2	2.91 x 10 ⁻¹³ x EXP(1300/T)*0.706
C537O2+NO-->C537O+NO2	2.54 x 10 ⁻¹² x EXP(360./T)
C537O2+NO3-->C537O+NO2	2.50 x 10 ⁻¹²
C537O2-->C537O	8.80 x 10 ⁻¹³ x RO2
C537O2-->DHPMPAL+CO+OH	6.52x10 ⁻⁵³ xT ^{20.52} xexp(1669/T)
C536OOH+OH-->DHPMEK+CO+OH	6.60 x 10 ⁻¹¹
C536O-->MGLYOX+HOOCH2CHO+OH	1.00 x 10 ⁶
C537OOH+OH-->DHPMPAL+CO+OH	5.64 x 10 ⁻¹¹
C537O-->GLYOX+HYPERACET+OH	1.00 x 10 ⁶
DHPMEK+OH-->BIACETOOH+OH+H2O	2.92 x 10 ⁻¹¹ x 0.56
DHPMEK+OH-->C4CO2OOH+OH+H2O	2.92 x 10 ⁻¹¹ x 0.44
DHPMPAL+OH-->C3MDIALOOH+OH+H2O	3.77 x 10 ⁻¹¹ x 0.32
DHPMPAL+OH-->HYPERACET+CO+OH+ H2O	3.77 x 10 ⁻¹¹ x 0.68
C3MDIALOOH+OH-->C3MDIALO2+H2O	1.35 x 10 ⁻¹⁰
C4CO2OOH+OH-->CO23C3CHO+OH+H2O	7.83 x 10 ⁻¹¹
C4CO2O+O2-->GLYOX+CH3CO3	1.00 x 10 ⁶ x 0.5
C4CO2O+O2-->MGLYOX+HO2+CO	1.00 x 10 ⁶ x 0.5
C3MDIALO+O2-->MGLYOX+CO+HO2	1.00 x 10 ⁶
C536OOH+hv-->C3MDIALOOH+HCHO+OH+OH	jx(ip_CH3OOH)
C536OOH+hv-->DHPMEK+CO+OH+HO2	jx(ip_IPRCHO2HCO)
C536OOH+hv-->MGLYOX+HOOCH2CHO+OH+OH	jx(ip_CH3OOH)*2
C537OOH+hv-->C4CO2OOH+HCHO+OH+OH	jx(ip_CH3OOH)
C537OOH+hv-->DHPMPAL+CO+OH+HO2	jx(ip_IPRCHO2HCO)
C537OOH+hv-->GLYOX+HYPERACET+OH+OH	jx(ip_CH3OOH)*2
DHPMEK+hv-->CH3CO3+HOOCH2CHO+OH	jx(ip_CH3OOH)+ jx(ip_CHOH)* 0.42
DHPMEK+hv-->MGLYOX+HCHO+OH+OH	jx(ip_CH3OOH)
DHPMPAL+hv-->C3MDIALOOH+OH	jx(ip_CH3OOH)
DHPMPAL+hv-->HYPERACET+OH+CO+HO2	jx(ip_C3H7CHO2HCO)
DHPMPAL+hv-->MGLYOX+OH+HCHO+OH	jx(ip_CH3OOH)
C3MDIALOOH+hv-->C3MDIALO+OH	jx(ip_CH3OOH)
C3MDIALOOH+hv-->MGLYOX+OH+HO2+CO	jx(ip_IPRCHO2HCO)*2
C4CO2OOH+hv-->C4CO2O+OH	jx(ip_CH3OOH)
C4CO2OOH+hv-->CH3CO3+GLYOX+OH	jx(ip_CHOH)* 0.42
C4CO2OOH+hv-->HO2+CO+MGLYOX+OH	jx(ip_IPRCHO2HCO)

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417 **D. Additional tables and figures**

418 **Table S8. Rate coefficients for the addition of O₂ to OH-isoprene adducts, and for re-dissociation of isoprene-RO₂ (Fig. 1).**
 419 **The rate coefficients for the oxygen additions (kf) are in cm³ s⁻¹ and are typically temperature independent. The rate**
 420 **coefficient for the re-dissociations (kr) are in s⁻¹.**

	LIM1(Peeters et al., 2014)	MCM v3.3.1.(Jenkin et al., 2015)	Caltech (Wennberg et al., 2018)
kf1	$0.5 \times 10^{-12} \times \exp(-480/T)$	$2.5 \times 10^{-12} \times \exp(-480/T)$	0.4×10^{-12}
kf2	0.6×10^{-12}	3.0×10^{-12}	0.8×10^{-12}
kf3	0.6×10^{-12}	3.0×10^{-12}	0.8×10^{-12}
kf4	0.7×10^{-12}	3.5×10^{-12}	0.1×10^{-12}
kf5	0.4×10^{-12}	2.0×10^{-12}	0.2×10^{-12}
kf6	0.7×10^{-12}	3.5×10^{-12}	0.7×10^{-12}
kf7	0.7×10^{-12}	3.5×10^{-12}	0.7×10^{-12}
kf8	$0.5 \times 10^{-12} \times \exp(-480/T)$	$2.5 \times 10^{-12} \times \exp(-480/T)$	0.5×10^{-12}
kr1	$5.7 \times 10^{13} \times \exp(-9028/T)$	$2.9 \times 10^{14} \times \exp(-9028/T)$	$1.8 \times 10^{14} \times \exp(-8930/T)$
kr2	$1.7 \times 10^{15} \times \exp(-10743/T)$	$8.5 \times 10^{15} \times \exp(-10743/T)$	$2.2 \times 10^{15} \times \exp(-10355/T)$
kr3	$1.7 \times 10^{15} \times \exp(-11322/T)$	$8.6 \times 10^{15} \times \exp(-11322/T)$	$2.2 \times 10^{15} \times \exp(-10865/T)$
kr4	$1.0 \times 10^{15} \times \exp(-9838/T)$	$5.2 \times 10^{15} \times \exp(-9838/T)$	$1.8 \times 10^{14} \times \exp(-8830/T)$
kr5	$6.1 \times 10^{14} \times \exp(-10254/T)$	$3.1 \times 10^{15} \times \exp(-10254/T)$	$1.7 \times 10^{14} \times \exp(-9054/T)$
kr6	$2.1 \times 10^{15} \times \exp(-11075/T)$	$1.1 \times 10^{16} \times \exp(-11075/T)$	$2.5 \times 10^{15} \times \exp(-11112/T)$
kr7	$2.1 \times 10^{15} \times \exp(-11565/T)$	$1.1 \times 10^{16} \times \exp(-11569/T)$	$2.5 \times 10^{15} \times \exp(-10890/T)$
kr8	$4.2 \times 10^{13} \times \exp(-9984/T)$	$2.1 \times 10^{14} \times \exp(-9984/T)$	$2.1 \times 10^{14} \times \exp(-9400/T)$

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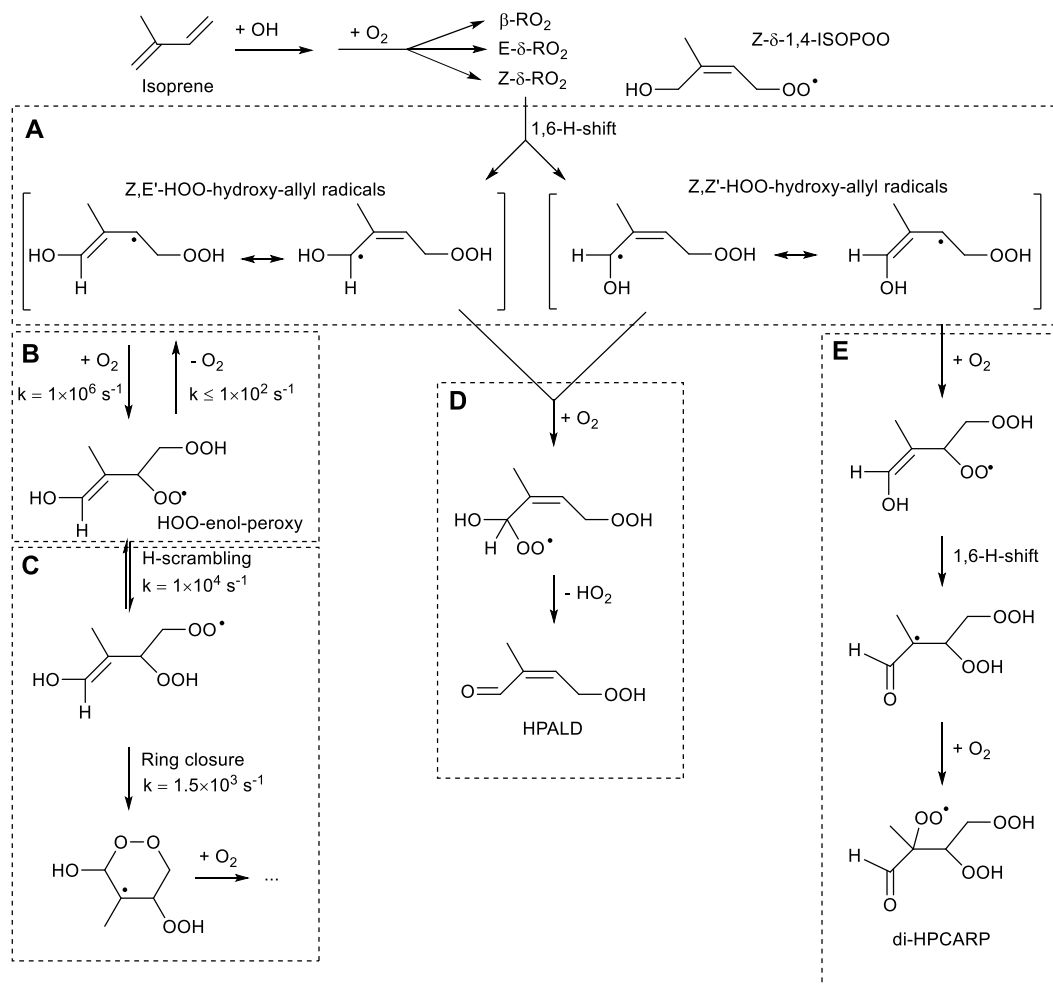
425 **Table S9: Instrumentation for radical and trace-gas quantification during the oxidation experiment.**

	Technique	Time resolution	1σ precision	1σ accuracy
OH	LIF	47 s	$0.3 \times 10^6 \text{ cm}^{-3}$	13%
OH	DOAS	200 s	$0.8 \times 10^6 \text{ cm}^{-3}$	6.5%
HO₂*, RO₂*	LIF	47 s	$1.5 \times 10^7 \text{ cm}^{-3}$	16%
k_{OH}	Laser-photolysis + LIF	180 s	0.3 s^{-1}	10%
NO	Chemiluminescence	180 s	4 pptv	5%
NO₂	Chemiluminescence	180 s	2 pptv	5%
O₃	UV-absorption	10 s	1 ppbv	5%
Isoprene, MVK+MACR	PTR-TOF-MS	30 s	> 15 pptv	< 14%
Isoprene, MVK+MACR	GC	30 min	4 – 8 %	5%
CO	CRDS	60 s	1.5 ppbv	1%
Photolysis frequencies	Spectroradiometer	60 s	10 %	10 %

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430 **Figure S4: Reaction scheme detailing the reaction steps affecting the HPALD vs. di-HPCARP yields. The submechanism**
 431 **in the labeled boxes A through E are discussed in the text.**

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554 **Raw quantum chemical and theoretical kinetic data**
 555 #####
 556 M06-2X/cc-pVDZ data for di-HPCARP-I
 557 #####
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559 Due to the large number of total structures, we only provide
 560 the population analysis across the conformers, for each of the critical
 561 points on the potential energy surface. For handling reasons, the R,R
 562 stereoisomers can also contain S,S enantiomers, while the R,S and R,S
 563 can also be mixed. HO2-elimination TS are not included in this supporting
 564 information.

565
 566 (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
 567 =====

568
 569 Population analysis at 300K. Vibrational scaling: 0.971.
 570 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 571 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 572 %: contribution to the population (with current data set assumed 100%)

573 Compound	Qtot	Erel	Erel2	n*Q*MB	%
574 -----					
575 diHPCARP_I.tmmmpmtmd	3.063e+43	0.08	0.08	2.673e+43	14.6
576 diHPCARP_I.mmmmpmtmpd	1.977e+43	0.09	0.09	1.702e+43	9.27
577 diHPCARP_I.tmmmpmtmpd	1.682e+43	0.00	0.00	1.682e+43	9.16
578 diHPCARP_I.pmtmpmtmd	1.746e+43	0.30	0.30	1.063e+43	5.79
579 diHPCARP_I.pmmmpmtmd	3.236e+43	0.80	0.80	8.432e+42	4.59
580 diHPCARP_I.pppmpmtmpd	1.103e+43	0.18	0.18	8.116e+42	4.42
581 diHPCARP_I.pmmmpmtmpd	1.468e+43	0.66	0.66	4.836e+42	2.63
582 diHPCARP_I.tmtmpmtmd	2.801e+43	1.07	1.07	4.617e+42	2.52
583 diHPCARP_I.tmmmptttd	4.269e+43	1.35	1.35	4.417e+42	2.41
584 diHPCARP_I.ttpmtttd	9.240e+42	0.52	0.52	3.863e+42	2.1
585 diHPCARP_I.tmmmpptpd	2.696e+43	1.16	1.16	3.846e+42	2.1
586 diHPCARP_I.tpmmpmtmpd	1.034e+43	0.68	0.68	3.286e+42	1.79
587 diHPCARP_I.tmmmpttmd	3.799e+43	1.58	1.58	2.703e+42	1.47
588 diHPCARP_I.mmmmpmtmd	1.027e+44	2.18	2.18	2.650e+42	1.44
589 diHPCARP_I.ttpmttmd	4.988e+42	0.38	0.38	2.632e+42	1.43
590 diHPCARP_I.ptmmmtmpd	2.828e+43	1.48	1.48	2.378e+42	1.3
591 diHPCARP_I.pppmtmpd	9.232e+42	0.85	0.85	2.208e+42	1.2
592 diHPCARP_I.pmtmttmd	2.764e+43	1.55	1.55	2.069e+42	1.13
593 diHPCARP_I.tmmmttmd	2.544e+44	2.87	2.87	2.058e+42	1.12
594 diHPCARP_I.tttptmmd	1.243e+43	1.07	1.07	2.053e+42	1.12
595 diHPCARP_I.mttmpmtmd	1.881e+43	1.40	1.40	1.783e+42	0.971
596 diHPCARP_I.tttptmmd	1.371e+43	1.28	1.28	1.608e+42	0.876
597 diHPCARP_I.ttppttmd	4.881e+42	0.67	0.67	1.579e+42	0.86
598 diHPCARP_I.mtppmttmd	8.112e+42	1.01	1.01	1.488e+42	0.811
599 diHPCARP_I.mtppmttmd	5.530e+42	0.80	0.80	1.453e+42	0.792
600 diHPCARP_I.mmmmpptpd	1.130e+44	2.60	2.60	1.450e+42	0.79
601 diHPCARP_I.tmmmttmd	1.324e+44	2.72	2.72	1.391e+42	0.758
602 diHPCARP_I.mttptmmd	1.963e+43	1.60	1.60	1.330e+42	0.725
603 diHPCARP_I.tmppttmd	2.513e+43	1.77	1.77	1.296e+42	0.706
604 diHPCARP_I.pppmpmtmd	5.361e+43	2.23	2.23	1.268e+42	0.691
605 diHPCARP_I.pmmmptttd	5.382e+43	2.26	2.26	1.209e+42	0.659
606 diHPCARP_I.mtppmttmd	5.742e+42	0.99	0.99	1.089e+42	0.594
607 diHPCARP_I.pmmmpptpd	2.695e+43	1.97	1.97	9.853e+41	0.537
608 diHPCARP_I.mmmmpmtmd	6.414e+43	2.50	2.50	9.689e+41	0.528
609 diHPCARP_I.mmmmptttd	6.409e+43	2.51	2.51	9.498e+41	0.517
610 diHPCARP_I.pmtptmmd	2.225e+43	1.88	1.88	9.485e+41	0.517
611 diHPCARP_I.mmmmpptpd	6.076e+43	2.50	2.50	9.095e+41	0.496
612 diHPCARP_I.pppmpmtmd	4.229e+43	2.32	2.32	8.623e+41	0.47
613 diHPCARP_I.pppmtttd	4.028e+43	2.30	2.30	8.526e+41	0.465
614 diHPCARP_I.tmppttmd	1.950e+43	1.92	1.92	7.801e+41	0.425
615 diHPCARP_I.mtmmmtmd	7.789e+44	4.17	4.17	7.086e+41	0.386
616 diHPCARP_I.tppmpmtmd	1.136e+43	1.68	1.68	6.736e+41	0.367
617 diHPCARP_I.tmtmttmd	4.412e+43	2.50	2.50	6.673e+41	0.364
618 diHPCARP_I.pppmpmtmd	1.881e+43	2.01	2.01	6.443e+41	0.351
619 diHPCARP_I.tmmmttmd	1.794e+44	3.38	3.38	6.209e+41	0.338
620 diHPCARP_I.tmtptmmd	3.606e+43	2.44	2.44	6.028e+41	0.328
621 diHPCARP_I.pmmmpttmd	4.762e+43	2.61	2.61	6.023e+41	0.328
622 diHPCARP_I.tmpptmmd	2.112e+43	2.14	2.14	5.848e+41	0.319
623 diHPCARP_I.tmtpttmd	5.527e+43	2.80	2.80	5.016e+41	0.273
624 diHPCARP_I.mmmmpttmd	7.070e+43	2.95	2.95	4.977e+41	0.271
625 diHPCARP_I.pttpttmd	5.501e+43	2.83	2.83	4.761e+41	0.259

626	diHPCARP_I.pmtptmtpd	2.822e+43	2.46	2.46	4.528e+41	0.247
627	diHPCARP_I.pttpptmtd	6.872e+43	3.01	3.01	4.427e+41	0.241
628	diHPCARP_I.pmtppmtmd	8.032e+43	3.10	3.10	4.408e+41	0.24
629	diHPCARP_I.pmtppttpd	6.265e+43	2.96	2.96	4.363e+41	0.238
630	diHPCARP_I.pptmptmpd	1.450e+43	2.10	2.10	4.275e+41	0.233
631	diHPCARP_I.tttmmtmmd	1.753e+43	2.23	2.23	4.169e+41	0.227
632	diHPCARP_I.ttmptmpd	1.222e+43	2.04	2.04	3.999e+41	0.218
633	diHPCARP_I.pmtmtttd	6.835e+43	3.10	3.10	3.798e+41	0.207
634	diHPCARP_I.pppmtpd	6.251e+43	3.06	3.06	3.716e+41	0.202
635	diHPCARP_I.ptppmtpd	7.779e+42	1.83	1.83	3.598e+41	0.196
636	diHPCARP_I.pptptmpd	1.002e+45	4.76	4.76	3.420e+41	0.186
637	diHPCARP_I.pptmptmmd	5.366e+43	3.04	3.04	3.269e+41	0.178
638	diHPCARP_I.mttmmtmmd	2.730e+43	2.67	2.67	3.124e+41	0.17
639	diHPCARP_I.pptmptmpd	6.827e+43	3.22	3.22	3.060e+41	0.167
640	diHPCARP_I.pptptmpd	6.426e+43	3.21	3.21	2.929e+41	0.16
641	diHPCARP_I.ttpmtpd	1.026e+43	2.13	2.13	2.857e+41	0.156
642	diHPCARP_I.tppmtpd	2.579e+43	2.75	2.75	2.557e+41	0.139
643	diHPCARP_I.mppmtpd	1.353e+43	2.37	2.37	2.523e+41	0.137
644	diHPCARP_I.tptmtpd	1.868e+43	2.58	2.58	2.454e+41	0.134
645	diHPCARP_I.ttmpttd	1.936e+43	2.61	2.61	2.414e+41	0.132
646	diHPCARP_I.tppmtpd	9.629e+42	2.21	2.21	2.377e+41	0.13
647	diHPCARP_I.tppmtpd	6.801e+43	3.39	3.39	2.302e+41	0.125
648	diHPCARP_I.mtppmtpd	1.028e+43	2.29	2.29	2.198e+41	0.12
649	diHPCARP_I.mtppmtpd	1.198e+43	2.39	2.39	2.163e+41	0.118
650	diHPCARP_I.ptmtmtpd	1.108e+43	2.36	2.36	2.118e+41	0.115
651	diHPCARP_I.pptmtpd	3.613e+43	3.08	3.08	2.056e+41	0.112
652	diHPCARP_I.tmtpttd	1.110e+44	3.75	3.75	2.055e+41	0.112
653	diHPCARP_I.pmptmtpd	1.609e+43	2.61	2.61	2.024e+41	0.11
654	diHPCARP_I.mtmmtmtpd	9.446e+43	3.67	3.67	1.999e+41	0.109
655	diHPCARP_I.mmmtpmtpd	1.384e+43	2.54	2.54	1.951e+41	0.106
656	diHPCARP_I.tmtptmtpd	1.342e+44	3.90	3.90	1.938e+41	0.106
657	diHPCARP_I.ttpptmtpd	3.152e+43	3.04	3.04	1.930e+41	0.105
658	diHPCARP_I.tptptmtpd	1.054e+44	3.77	3.77	1.882e+41	0.103
659	diHPCARP_I.tppmtpd	2.671e+43	2.97	2.97	1.828e+41	0.0996
660	diHPCARP_I.pmpmtpd	2.321e+43	2.89	2.89	1.816e+41	0.0989
661	diHPCARP_I.mpmmtmtpd	1.416e+43	2.62	2.62	1.741e+41	0.0949
662	diHPCARP_I.mtmmtmtpd	3.951e+44	4.61	4.61	1.726e+41	0.0941
663	diHPCARP_I.tptmtpmtpd	7.880e+43	3.65	3.65	1.718e+41	0.0936
664	diHPCARP_I.tmtmtttd	1.039e+44	3.82	3.82	1.711e+41	0.0932
665	diHPCARP_I.tmmmttttd	2.948e+44	4.46	4.46	1.652e+41	0.09
666	diHPCARP_I.tttptmtpd	1.645e+44	4.14	4.14	1.578e+41	0.086
667	diHPCARP_I.pppmtpmtpd	1.395e+43	2.70	2.70	1.509e+41	0.0822
668	diHPCARP_I.mtppmtpd	1.086e+43	2.57	2.57	1.452e+41	0.0791
669	diHPCARP_I.ttpmtpmtpd	2.932e+43	3.17	3.17	1.449e+41	0.079
670	diHPCARP_I.tppmtpmtpd	1.028e+43	2.54	2.54	1.446e+41	0.0788
671	diHPCARP_I.tptmtpmtpd	1.363e+44	4.10	4.10	1.399e+41	0.0762
672	diHPCARP_I.pptmtpmtpd	4.085e+43	3.41	3.41	1.340e+41	0.073
673	diHPCARP_I.ppppttd	9.426e+43	3.94	3.94	1.281e+41	0.0698
674	diHPCARP_I.tmmmtmtpd	9.720e+43	3.96	3.96	1.263e+41	0.0688
675	diHPCARP_I.mttptmtpd	2.994e+43	3.27	3.27	1.240e+41	0.0676
676	diHPCARP_I.tmmmtmtpd	1.759e+44	4.33	4.33	1.237e+41	0.0674
677	diHPCARP_I.ttpmtpmtpd	1.514e+43	2.87	2.87	1.221e+41	0.0665
678	diHPCARP_I.tppmtpmtpd	1.737e+43	2.98	2.98	1.164e+41	0.0634
679	diHPCARP_I.mttptmtpd	1.680e+44	4.35	4.35	1.145e+41	0.0624
680	diHPCARP_I.pptmtpd	1.230e+44	4.17	4.17	1.126e+41	0.0613
681	diHPCARP_I.ttmptmtpd	4.883e+43	3.64	3.64	1.094e+41	0.0596
682	diHPCARP_I.ptmptmtpd	9.589e+42	2.67	2.67	1.085e+41	0.0591
683	diHPCARP_I.pttpmtpd	1.405e+43	2.90	2.90	1.078e+41	0.0588
684	diHPCARP_I.mppmtpmtpd	1.371e+43	2.90	2.90	1.066e+41	0.0581
685	diHPCARP_I.pptmtpd	2.308e+44	4.59	4.59	1.052e+41	0.0573
686	diHPCARP_I.tmmmtmtpd	1.151e+44	4.17	4.17	1.049e+41	0.0572
687	diHPCARP_I.pmpptmtpd	1.685e+43	3.05	3.05	1.018e+41	0.0555
688	diHPCARP_I.pptmtpmtpd	5.316e+43	3.74	3.74	9.976e+40	0.0543
689	diHPCARP_I.ptmptmtpd	4.378e+42	2.26	2.26	9.960e+40	0.0543
690	diHPCARP_I.pptptmtpd	5.253e+43	3.75	3.75	9.755e+40	0.0531
691	diHPCARP_I.tppmtpmtpd	4.357e+43	3.65	3.65	9.631e+40	0.0525
692	diHPCARP_I.tttptmtpd	1.359e+44	4.33	4.33	9.566e+40	0.0521
693	diHPCARP_I.tmmmtmtpd	1.950e+44	4.56	4.56	9.319e+40	0.0508
694	diHPCARP_I.ttpmtpmtpd	2.570e+43	3.35	3.35	9.294e+40	0.0506
695	diHPCARP_I.pmtptmtpd	2.282e+44	4.67	4.67	8.991e+40	0.049
696	diHPCARP_I.tmptmtpd	1.327e+44	4.36	4.36	8.871e+40	0.0483
697	diHPCARP_I.mppmtpmtpd	1.498e+43	3.06	3.06	8.834e+40	0.0481

698	diHPCARP_I.tptmptpmd	1.122e+44	4.26	4.26	8.825e+40	0.0481
699	diHPCARP_I.pptmttmd	1.038e+44	4.23	4.23	8.560e+40	0.0466
700	diHPCARP_I.tmpmptpmd	1.165e+44	4.32	4.32	8.280e+40	0.0451
701	diHPCARP_I.ptppmmmpd	1.120e+43	2.93	2.93	8.230e+40	0.0448
702	diHPCARP_I.pttpmtmmd	1.040e+43	2.93	2.93	7.680e+40	0.0418
703	diHPCARP_I.tttptttd	4.936e+43	3.87	3.87	7.433e+40	0.0405
704	diHPCARP_I.tppppttd	1.027e+44	4.32	4.32	7.261e+40	0.0396
705	diHPCARP_I.tpmptpmd	3.115e+43	3.61	3.61	7.256e+40	0.0395
706	diHPCARP_I.mttptmmd	3.649e+43	3.72	3.72	7.154e+40	0.039
707	diHPCARP_I.mptmptpmd	2.072e+43	3.39	3.39	7.044e+40	0.0384
708	diHPCARP_I.tmpmptmmd	3.938e+43	3.78	3.78	6.936e+40	0.0378
709	diHPCARP_I.mmtptmtd	3.648e+43	3.74	3.74	6.875e+40	0.0375
710	diHPCARP_I.mttmptpmd	4.717e+43	3.90	3.90	6.812e+40	0.0371
711	diHPCARP_I.ptmmmtmmd	1.038e+44	4.39	4.39	6.584e+40	0.0359
712	diHPCARP_I.ptpmtmmd	4.217e+42	2.50	2.50	6.326e+40	0.0345
713	diHPCARP_I.pptpmttd	2.545e+44	4.95	4.95	6.258e+40	0.0341
714	diHPCARP_I.tmmptmtd	9.316e+43	4.38	4.38	6.034e+40	0.0329
715	diHPCARP_I.mmtmmttd	1.839e+44	4.79	4.79	5.981e+40	0.0326
716	diHPCARP_I.tmtmtmtd	1.684e+43	3.41	3.41	5.513e+40	0.03
717	diHPCARP_I.pmtmptpmd	5.901e+43	4.17	4.17	5.397e+40	0.0294
718	diHPCARP_I.mttptpmd	1.325e+44	4.66	4.66	5.358e+40	0.0292
719	diHPCARP_I.pmtmttd	8.883e+43	4.44	4.44	5.183e+40	0.0282
720	diHPCARP_I.tmtmptpmd	1.367e+44	4.70	4.70	5.113e+40	0.0279
721	diHPCARP_I.ppmptpmd	4.566e+43	4.05	4.05	5.112e+40	0.0279
722	diHPCARP_I.ttpmmttd	3.610e+43	3.92	3.92	5.039e+40	0.0275
723	diHPCARP_I.tttmttd	4.408e+43	4.04	4.04	5.015e+40	0.0273
724	diHPCARP_I.tptpmtpmd	2.376e+44	5.05	5.05	4.945e+40	0.0269
725	diHPCARP_I.ptppmtpmd	1.678e+43	3.48	3.48	4.927e+40	0.0268
726	diHPCARP_I.ptppmpmd	1.779e+43	3.51	3.51	4.911e+40	0.0268
727	diHPCARP_I.tptmttd	2.071e+44	4.98	4.98	4.897e+40	0.0267
728	diHPCARP_I.pmpmptpmd	7.348e+42	2.99	2.99	4.848e+40	0.0264
729	diHPCARP_I.pptpmttd	3.270e+44	5.26	5.26	4.811e+40	0.0262
730	diHPCARP_I.mmmptpmd	7.963e+43	4.42	4.42	4.809e+40	0.0262
731	diHPCARP_I.ppppmtpmd	3.692e+43	3.96	3.96	4.795e+40	0.0261
732	diHPCARP_I.tmtpmttd	2.869e+44	5.19	5.19	4.735e+40	0.0258
733	diHPCARP_I.mtmtmtd	1.598e+43	3.49	3.49	4.558e+40	0.0248
734	diHPCARP_I.mppmmttd	7.806e+43	4.45	4.45	4.481e+40	0.0244
735	diHPCARP_I.ttmmmttd	1.876e+44	4.97	4.97	4.458e+40	0.0243
736	diHPCARP_I.tttptmtd	3.584e+43	3.99	3.99	4.447e+40	0.0242
737	diHPCARP_I.tptmptpmd	3.960e+43	4.06	4.06	4.361e+40	0.0238
738	diHPCARP_I.pptmptmd	4.216e+43	4.10	4.10	4.322e+40	0.0235
739	diHPCARP_I.ttpmtmtd	1.453e+43	3.47	3.47	4.298e+40	0.0234
740	diHPCARP_I.tttmptpmd	5.235e+43	4.24	4.24	4.272e+40	0.0233
741	diHPCARP_I.pmtmtmmd	1.124e+44	4.70	4.70	4.229e+40	0.023
742	diHPCARP_I.ppppmtpmd	4.155e+43	4.11	4.11	4.214e+40	0.023
743	diHPCARP_I.mtmmmttd	1.756e+44	4.97	4.97	4.190e+40	0.0228
744	diHPCARP_I.tptpmtpmd	4.976e+43	4.22	4.22	4.185e+40	0.0228
745	diHPCARP_I.mmmptmtd	3.427e+43	4.01	4.01	4.110e+40	0.0224
746	diHPCARP_I.ptmptpmd	5.012e+43	4.24	4.24	4.053e+40	0.0221
747	diHPCARP_I.tptmptpmd	3.392e+43	4.01	4.01	4.047e+40	0.022
748	diHPCARP_I.tmtmptpmd	1.780e+44	5.01	5.01	3.997e+40	0.0218
749	diHPCARP_I.tttmptmtd	5.678e+43	4.33	4.33	3.987e+40	0.0217
750	diHPCARP_I.ppmptmtd	1.507e+44	4.91	4.91	3.976e+40	0.0217
751	diHPCARP_I.mptmptmmd	3.031e+43	3.96	3.96	3.959e+40	0.0216
752	diHPCARP_I.mtpmptpmd	1.970e+43	3.71	3.71	3.931e+40	0.0214
753	diHPCARP_I.tmpmptmmd	1.026e+44	4.70	4.70	3.864e+40	0.0211
754	diHPCARP_I.pppmptpmd	2.253e+43	3.80	3.80	3.849e+40	0.021
755	diHPCARP_I.mtpmptpmd	5.638e+43	4.35	4.35	3.849e+40	0.021
756	diHPCARP_I.mmmmtmtd	2.537e+44	5.26	5.26	3.756e+40	0.0205
757	diHPCARP_I.pmmmtmtd	3.146e+43	4.02	4.02	3.700e+40	0.0202
758	diHPCARP_I.mtpmptpmd	3.135e+43	4.03	4.03	3.641e+40	0.0198
759	diHPCARP_I.tmmptmtd	6.388e+43	4.46	4.46	3.627e+40	0.0198
760	diHPCARP_I.tptmptpmd	7.287e+43	4.55	4.55	3.510e+40	0.0191
761	diHPCARP_I.tmpmptpmd	3.593e+43	4.14	4.14	3.469e+40	0.0189
762	diHPCARP_I.tmtmptmmd	3.944e+43	4.21	4.21	3.358e+40	0.0183
763	diHPCARP_I.pttpmtmtd	6.917e+43	4.56	4.56	3.321e+40	0.0181
764	diHPCARP_I.pppmtmtd	1.261e+44	4.92	4.92	3.311e+40	0.018
765	diHPCARP_I.ttpmptpmd	2.820e+43	4.02	4.02	3.298e+40	0.018
766	diHPCARP_I.tmpmptpmd	2.553e+43	3.98	3.98	3.235e+40	0.0176
767	diHPCARP_I.tmtmptmtd	1.407e+44	5.00	5.00	3.232e+40	0.0176
768	diHPCARP_I.mtpmptmmd	1.798e+44	5.15	5.15	3.174e+40	0.0173
769	diHPCARP_I.mmtpmttd	9.576e+43	4.79	4.79	3.109e+40	0.0169

770	diHPCARP_I.tmmmtmtmd	5.345e+43	4.44	4.44	3.108e+40	0.0169
771	diHPCARP_I.mmmppmpd	2.664e+43	4.03	4.03	3.104e+40	0.0169
772	diHPCARP_I.mtpmpmtmd	1.754e+43	3.78	3.78	3.081e+40	0.0168
773	diHPCARP_I.pptpmmmmmd	9.708e+43	4.81	4.81	3.063e+40	0.0167
774	diHPCARP_I.tptmmtmmd	9.229e+43	4.79	4.79	2.986e+40	0.0163
775	diHPCARP_I.tptmpttmd	3.808e+43	4.27	4.27	2.943e+40	0.016
776	diHPCARP_I.mttptmtmd	8.638e+43	4.77	4.77	2.909e+40	0.0158
777	diHPCARP_I.ttmmmtppd	1.881e+44	5.24	5.24	2.860e+40	0.0156
778	diHPCARP_I.mmtmtttpd	9.959e+43	4.87	4.87	2.838e+40	0.0155
779	diHPCARP_I.tttpttpmd	2.984e+44	5.52	5.52	2.823e+40	0.0154
780	diHPCARP_I.mtmmmtppd	1.341e+44	5.05	5.05	2.815e+40	0.0153
781	diHPCARP_I.tmtmtttd	1.577e+44	5.15	5.15	2.810e+40	0.0153
782	diHPCARP_I.pppmpttmd	1.122e+44	4.96	4.96	2.741e+40	0.0149
783	diHPCARP_I.pppmptppd	2.715e+43	4.12	4.12	2.728e+40	0.0149
784	diHPCARP_I.mmtmptmpd	9.076e+43	4.86	4.86	2.626e+40	0.0143
785	diHPCARP_I.ptmmmmmpd	1.744e+43	3.87	3.87	2.624e+40	0.0143
786	diHPCARP_I.tmtmtmmd	2.278e+44	5.43	5.43	2.526e+40	0.0138
787	diHPCARP_I.ppttttmd	1.833e+44	5.32	5.32	2.458e+40	0.0134
788	diHPCARP_I.tmtmtmpd	1.671e+44	5.26	5.26	2.451e+40	0.0134
789	diHPCARP_I.pttptmpd	4.926e+43	4.54	4.54	2.444e+40	0.0133
790	diHPCARP_I.pptpmtmmd	4.169e+43	4.44	4.44	2.435e+40	0.0133
791	diHPCARP_I.pptpmpmmd	4.038e+43	4.42	4.42	2.425e+40	0.0132
792	diHPCARP_I.tmppttmd	3.642e+43	4.36	4.36	2.416e+40	0.0132
793	diHPCARP_I.mttptttd	6.917e+43	4.79	4.79	2.244e+40	0.0122
794	diHPCARP_I.ppppmttmd	1.408e+44	5.22	5.22	2.216e+40	0.0121
795	diHPCARP_I.tttmtmmd	5.500e+43	4.66	4.66	2.216e+40	0.0121
796	diHPCARP_I.pmtppmpd	1.894e+44	5.41	5.41	2.185e+40	0.0119
797	diHPCARP_I.tptptttd	1.827e+44	5.40	5.40	2.126e+40	0.0116
798	diHPCARP_I.ptpmpmpd	6.601e+42	3.42	3.42	2.113e+40	0.0115
799	diHPCARP_I.mtptppmpd	3.370e+43	4.40	4.40	2.113e+40	0.0115
800	diHPCARP_I.mmmmmtttd	2.094e+44	5.49	5.49	2.094e+40	0.0114
801	diHPCARP_I.ptmpttmd	3.699e+43	4.46	4.46	2.081e+40	0.0113
802	diHPCARP_I.tttmptttd	6.997e+43	4.84	4.84	2.071e+40	0.0113
803	diHPCARP_I.ttppttmd	3.468e+43	4.44	4.44	2.012e+40	0.011
804	diHPCARP_I.tmpmtttd	4.963e+43	4.66	4.66	1.996e+40	0.0109
805	diHPCARP_I.pppptttd	7.112e+43	4.88	4.88	1.980e+40	0.0108
806	diHPCARP_I.tmtppmpd	3.090e+44	5.76	5.76	1.972e+40	0.0107
807	diHPCARP_I.mtppppmpd	2.010e+43	4.14	4.14	1.930e+40	0.0105
808	diHPCARP_I.ttpppmpd	3.361e+43	4.46	4.46	1.909e+40	0.0104
809	diHPCARP_I.tttptmpd	6.527e+43	4.85	4.85	1.902e+40	0.0104
810	diHPCARP_I.mpppmpmd	5.045e+43	4.71	4.71	1.882e+40	0.0103
811	diHPCARP_I.tptppmpd	1.907e+44	5.50	5.50	1.873e+40	0.0102
812	diHPCARP_I.mttptmtd	5.566e+43	4.77	4.77	1.871e+40	0.0102
813	diHPCARP_I.pppptmpd	1.669e+44	5.42	5.42	1.867e+40	0.0102
814	diHPCARP_I.ptppmtmpd	1.499e+43	3.99	3.99	1.864e+40	0.0102
815	diHPCARP_I.pppptmmd	5.205e+43	4.73	4.73	1.862e+40	0.0101
816	diHPCARP_I.mmmmmtpd	1.517e+44	5.37	5.37	1.850e+40	0.0101
817	diHPCARP_I.tmtptmpd	9.798e+43	5.11	5.11	1.845e+40	0.0101
818	diHPCARP_I.mtppmttmd	2.986e+43	4.41	4.41	1.825e+40	0.00994
819	diHPCARP_I.pttptmpd	6.054e+43	4.84	4.84	1.791e+40	0.00976
820	diHPCARP_I.ptmmmtmd	1.216e+44	5.26	5.26	1.787e+40	0.00973
821	diHPCARP_I.tmmppmpd	4.691e+43	4.72	4.72	1.719e+40	0.00937
822	diHPCARP_I.pmtptmpd	7.254e+43	4.98	4.98	1.707e+40	0.0093
823	diHPCARP_I.pppmmtpmd	4.461e+43	4.70	4.70	1.685e+40	0.00918
824	diHPCARP_I.mmmmttppd	1.583e+44	5.46	5.46	1.680e+40	0.00915
825	diHPCARP_I.pptpmpd	1.295e+44	5.34	5.34	1.679e+40	0.00914
826	diHPCARP_I.ttpmpmpd	4.029e+43	4.65	4.65	1.656e+40	0.00902
827	diHPCARP_I.tmmpttmd	4.416e+43	4.71	4.71	1.631e+40	0.00888
828	diHPCARP_I.tmpmpmpd	1.628e+43	4.12	4.12	1.619e+40	0.00882
829	diHPCARP_I.pppmttmd	4.348e+43	4.71	4.71	1.612e+40	0.00878
830	diHPCARP_I.mttmtttd	6.426e+43	4.95	4.95	1.602e+40	0.00873
831	diHPCARP_I.pptptppd	7.200e+44	6.39	6.39	1.586e+40	0.00864
832	diHPCARP_I.pppmmppd	8.980e+43	5.15	5.15	1.586e+40	0.00864
833	diHPCARP_I.tpmmptppd	4.591e+43	4.75	4.75	1.584e+40	0.00863
834	diHPCARP_I.ttmtptmd	2.123e+44	5.68	5.68	1.534e+40	0.00836
835	diHPCARP_I.ttpmtptd	1.833e+43	4.23	4.23	1.530e+40	0.00834
836	diHPCARP_I.pmttpttd	9.477e+43	5.22	5.22	1.498e+40	0.00816
837	diHPCARP_I.pppptttd	2.601e+43	4.45	4.45	1.490e+40	0.00812
838	diHPCARP_I.pttmtmmd	1.247e+43	4.01	4.01	1.487e+40	0.0081
839	diHPCARP_I.mptmpmpd	1.167e+44	5.35	5.35	1.470e+40	0.00801
840	diHPCARP_I.ptpmppttd	2.908e+43	4.53	4.53	1.469e+40	0.008
841	diHPCARP_I.pppmptmpd	7.702e+43	5.11	5.11	1.460e+40	0.00796

842	diHPCARP_I.mmmmttmd	1.537e+44	5.53	5.53	1.431e+40	0.00779
843	diHPCARP_I.tptmptmd	5.998e+43	4.97	4.97	1.429e+40	0.00779
844	diHPCARP_I.tppptmppd	1.448e+44	5.51	5.51	1.399e+40	0.00762
845	diHPCARP_I.tpmpttttd	1.337e+44	5.47	5.47	1.376e+40	0.0075
846	diHPCARP_I.mmmmtmmpd	9.028e+43	5.24	5.24	1.373e+40	0.00748
847	diHPCARP_I.tptmptppd	8.003e+44	6.54	6.54	1.369e+40	0.00746
848	diHPCARP_I.tmpmttmd	1.644e+43	4.24	4.24	1.349e+40	0.00735
849	diHPCARP_I.mptpptmpd	7.182e+43	5.13	5.13	1.305e+40	0.00711
850	diHPCARP_I.tpmmtttmd	1.251e+44	5.47	5.47	1.301e+40	0.00709
851	diHPCARP_I.mttmtmmd	6.957e+43	5.12	5.12	1.298e+40	0.00707
852	diHPCARP_I.tmmmtppd	3.216e+44	6.04	6.04	1.273e+40	0.00693
853	diHPCARP_I.mppppmtpd	7.404e+43	5.17	5.17	1.272e+40	0.00693
854	diHPCARP_I.tmpptmmd	5.858e+43	5.04	5.04	1.242e+40	0.00677
855	diHPCARP_I.tmmpttttd	8.238e+43	5.25	5.25	1.229e+40	0.0067
856	diHPCARP_I.mptmptmd	8.225e+43	5.27	5.27	1.200e+40	0.00654
857	diHPCARP_I.tpmptmtpd	3.558e+43	4.77	4.77	1.199e+40	0.00653
858	diHPCARP_I.pptpptppd	2.301e+44	5.89	5.89	1.171e+40	0.00638
859	diHPCARP_I.mtmmtttd	2.436e+44	5.94	5.94	1.148e+40	0.00626
860	diHPCARP_I.tmtptmtd	9.022e+43	5.35	5.35	1.146e+40	0.00624
861	diHPCARP_I.tpppmtpd	3.976e+43	4.86	4.86	1.138e+40	0.0062
862	diHPCARP_I.tpttptmpd	7.074e+43	5.22	5.22	1.110e+40	0.00604
863	diHPCARP_I.pptmptpd	4.679e+43	4.98	4.98	1.105e+40	0.00602
864	diHPCARP_I.tppmtpmd	7.162e+43	5.24	5.24	1.094e+40	0.00596
865	diHPCARP_I.tmtmpttttd	1.478e+44	5.67	5.67	1.091e+40	0.00595
866	diHPCARP_I.ttmptmmd	2.272e+44	5.93	5.93	1.089e+40	0.00593
867	diHPCARP_I.ttmmtmtd	1.658e+44	5.77	5.77	1.039e+40	0.00566
868	diHPCARP_I.mtmtptmmd	3.567e+44	6.23	6.23	1.035e+40	0.00564
869	diHPCARP_I.pppmmmpmd	5.497e+43	5.11	5.11	1.034e+40	0.00563
870	diHPCARP_I.tppppptpd	1.264e+44	5.61	5.61	1.028e+40	0.0056
871	diHPCARP_I.pptmmtmd	3.057e+44	6.14	6.14	1.022e+40	0.00557
872	diHPCARP_I.pptmpttd	1.435e+44	5.69	5.69	1.020e+40	0.00555
873	diHPCARP_I.tptmmtmd	4.161e+43	4.96	4.96	1.019e+40	0.00555
874	diHPCARP_I.ptpmptmd	2.208e+43	4.59	4.59	1.009e+40	0.0055
875	diHPCARP_I.pppmptmd	3.773e+43	4.91	4.91	1.005e+40	0.00547
876	diHPCARP_I.mttmpttd	1.202e+44	5.60	5.60	1.001e+40	0.00545
877	diHPCARP_I.mmpmtpmd	2.095e+43	4.56	4.56	9.992e+39	0.00544
878	diHPCARP_I.ptppmtmd	2.867e+43	4.75	4.75	9.968e+39	0.00543
879	diHPCARP_I.mttmpttd	1.196e+44	5.60	5.60	9.943e+39	0.00542
880	diHPCARP_I.mppmtpmd	3.266e+43	4.83	4.83	9.932e+39	0.00541
881	diHPCARP_I.pmmmtmtpd	2.021e+43	4.54	4.54	9.927e+39	0.00541
882	diHPCARP_I.mtmtptmd	2.551e+44	6.06	6.06	9.868e+39	0.00538
883	diHPCARP_I.tmtmmpmmd	5.977e+43	5.20	5.20	9.806e+39	0.00534
884	diHPCARP_I.tptmppmmd	3.994e+43	4.97	4.97	9.644e+39	0.00525
885	diHPCARP_I.ptmmmtmd	2.279e+44	6.01	6.01	9.541e+39	0.0052
886	diHPCARP_I.ttmmtmmd	2.565e+43	4.73	4.73	9.236e+39	0.00503
887	diHPCARP_I.tppmmtmd	1.367e+44	5.73	5.73	9.217e+39	0.00502
888	diHPCARP_I.mptmmtmd	4.895e+43	5.12	5.12	9.193e+39	0.00501
889	diHPCARP_I.pptmmtmd	1.369e+44	5.73	5.73	9.178e+39	0.005
890	diHPCARP_I.tttptppd	4.330e+44	6.42	6.42	9.097e+39	0.00496
891	diHPCARP_I.mttmptmd	6.923e+43	5.33	5.33	9.019e+39	0.00491
892	diHPCARP_I.pptmptmd	3.855e+43	4.99	4.99	8.960e+39	0.00488
893	diHPCARP_I.pmmmtttmd	1.297e+44	5.72	5.72	8.787e+39	0.00479
894	diHPCARP_I.tmmptttmd	6.194e+43	5.29	5.29	8.722e+39	0.00475
895	diHPCARP_I.pptmptppd	2.434e+44	6.11	6.11	8.622e+39	0.0047
896	diHPCARP_I.tppppppmd	1.038e+44	5.61	5.61	8.562e+39	0.00466
897	diHPCARP_I.tppppppmd	1.738e+43	4.54	4.54	8.505e+39	0.00463
898	diHPCARP_I.mtppmtpmd	2.534e+43	4.79	4.79	8.183e+39	0.00446
899	diHPCARP_I.tmmpttttd	2.955e+44	6.26	6.26	8.164e+39	0.00445
900	diHPCARP_I.tmttpttd	1.657e+44	5.91	5.91	8.137e+39	0.00443
901	diHPCARP_I.pmtmptpd	1.013e+44	5.64	5.64	7.940e+39	0.00433
902	diHPCARP_I.mtmmtttd	2.996e+44	6.30	6.30	7.729e+39	0.00421
903	diHPCARP_I.pttpmtpd	3.339e+43	4.99	4.99	7.692e+39	0.00419
904	diHPCARP_I.pptpmtmd	6.783e+43	5.42	5.42	7.611e+39	0.00415
905	diHPCARP_I.mmmmtmtpd	3.494e+43	5.03	5.03	7.562e+39	0.00412
906	diHPCARP_I.mmtptppd	2.956e+44	6.30	6.30	7.561e+39	0.00412
907	diHPCARP_I.mptmtpmd	1.248e+44	5.80	5.80	7.478e+39	0.00407
908	diHPCARP_I.tmppttpd	8.387e+43	5.56	5.56	7.416e+39	0.00404
909	diHPCARP_I.tpmptmtpd	3.650e+43	5.07	5.07	7.336e+39	0.004
910	diHPCARP_I.pmtmpttd	7.746e+43	5.52	5.52	7.325e+39	0.00399
911	diHPCARP_I.mtmmtpmd	1.646e+44	5.98	5.98	7.300e+39	0.00398
912	diHPCARP_I.tptmmpmmd	2.144e+44	6.13	6.13	7.297e+39	0.00398
913	diHPCARP_I.mtmmtpmd	2.369e+44	6.19	6.19	7.290e+39	0.00397

914	diHPCARP_I.tppppptpmd	5.235e+43	5.30	5.30	7.199e+39	0.00392
915	diHPCARP_I.ttttptmmd	6.840e+43	5.47	5.47	7.143e+39	0.00389
916	diHPCARP_I.tpmppttmd	4.677e+43	5.25	5.25	7.054e+39	0.00384
917	diHPCARP_I.tmmtpptmd	2.590e+44	6.27	6.27	6.957e+39	0.00379
918	diHPCARP_I.mppmmttptd	3.174e+43	5.02	5.02	6.934e+39	0.00378
919	diHPCARP_I.pmtptmtd	5.136e+43	5.31	5.31	6.928e+39	0.00377
920	diHPCARP_I.tpppmtppd	1.406e+44	5.91	5.91	6.909e+39	0.00376
921	diHPCARP_I.pmttmtpd	3.204e+44	6.41	6.41	6.908e+39	0.00376
922	diHPCARP_I.mptpmtmd	2.608e+43	4.91	4.91	6.896e+39	0.00376
923	diHPCARP_I.mptpmtmmd	4.498e+43	5.24	5.24	6.831e+39	0.00372
924	diHPCARP_I.mmtppmtmd	1.178e+44	5.82	5.82	6.757e+39	0.00368
925	diHPCARP_I.mtmmtmmd	2.365e+43	4.87	4.87	6.747e+39	0.00368
926	diHPCARP_I.ttttptmpd	1.088e+44	5.79	5.79	6.638e+39	0.00362
927	diHPCARP_I.pptpmpmd	3.008e+44	6.39	6.39	6.631e+39	0.00361
928	diHPCARP_I.ptttmtpd	6.120e+43	5.45	5.45	6.602e+39	0.0036
929	diHPCARP_I.tmmpptttd	7.331e+43	5.56	5.56	6.566e+39	0.00358
930	diHPCARP_I.mtmmmmmmd	3.677e+43	5.15	5.15	6.552e+39	0.00357
931	diHPCARP_I.mptmpttmd	3.946e+43	5.19	5.19	6.510e+39	0.00355
932	diHPCARP_I.mptppmtpd	1.399e+44	5.95	5.95	6.499e+39	0.00354
933	diHPCARP_I.ttmtpptmd	1.925e+44	6.14	6.14	6.471e+39	0.00353
934	diHPCARP_I.ttpmtmtd	1.321e+44	5.92	5.92	6.470e+39	0.00352
935	diHPCARP_I.tptmptttd	1.516e+44	6.00	6.00	6.461e+39	0.00352
936	diHPCARP_I.tpppppppd	5.949e+43	5.45	5.45	6.387e+39	0.00348
937	diHPCARP_I.pptmmtmmd	6.382e+43	5.50	5.50	6.263e+39	0.00341
938	diHPCARP_I.mtmmtmmd	2.351e+44	6.28	6.28	6.218e+39	0.00339
939	diHPCARP_I.mptpmttd	5.361e+43	5.41	5.41	6.160e+39	0.00336
940	diHPCARP_I.ttttmttd	7.337e+43	5.60	5.60	6.131e+39	0.00334
941	diHPCARP_I.tptmtpd	1.064e+44	5.83	5.83	6.070e+39	0.00331
942	diHPCARP_I.tptpmpmd	2.146e+44	6.25	6.25	5.999e+39	0.00327
943	diHPCARP_I.tppptmmd	5.750e+43	5.47	5.47	5.908e+39	0.00322
944	diHPCARP_I.pptmtppd	6.019e+44	6.88	6.88	5.900e+39	0.00321
945	diHPCARP_I.tmmtpptd	2.645e+44	6.39	6.39	5.872e+39	0.0032
946	diHPCARP_I.mtppmmtmd	1.277e+44	5.96	5.96	5.843e+39	0.00318
947	diHPCARP_I.tmtmtpd	1.283e+44	5.96	5.96	5.798e+39	0.00316
948	diHPCARP_I.tmmppptmd	4.909e+43	5.39	5.39	5.766e+39	0.00314
949	diHPCARP_I.pptppmmd	7.608e+43	5.66	5.66	5.756e+39	0.00314
950	diHPCARP_I.pttpmtd	2.556e+43	5.01	5.01	5.726e+39	0.00312
951	diHPCARP_I.pttmptmd	1.591e+44	6.11	6.11	5.672e+39	0.00309
952	diHPCARP_I.pmptmtd	3.587e+43	5.22	5.22	5.663e+39	0.00309
953	diHPCARP_I.pmtptppd	2.659e+44	6.42	6.42	5.612e+39	0.00306
954	diHPCARP_I.tmptmtd	5.247e+43	5.46	5.46	5.518e+39	0.00301
955	diHPCARP_I.pptpmpmd	1.827e+44	6.21	6.21	5.499e+39	0.003
956	diHPCARP_I.tptmtmtd	9.913e+43	5.84	5.84	5.491e+39	0.00299
957	diHPCARP_I.tptpmpmmd	4.260e+43	5.34	5.34	5.490e+39	0.00299
958	diHPCARP_I.mptpmpmd	2.756e+44	6.46	6.46	5.405e+39	0.00294
959	diHPCARP_I.mtppmtd	3.463e+43	5.23	5.23	5.386e+39	0.00293
960	diHPCARP_I.mtttptmpd	1.207e+44	5.98	5.98	5.346e+39	0.00291
961	diHPCARP_I.tmmmtmtd	2.698e+44	6.46	6.46	5.315e+39	0.0029
962	diHPCARP_I.tptmttd	3.419e+44	6.60	6.60	5.298e+39	0.00289
963	diHPCARP_I.mptmmpmmd	2.573e+43	5.07	5.07	5.203e+39	0.00283
964	diHPCARP_I.tptpmpmmd	9.167e+43	5.83	5.83	5.199e+39	0.00283
965	diHPCARP_I.pmtmtpd	5.307e+43	5.52	5.52	5.080e+39	0.00277
966	diHPCARP_I.mttptmpd	9.977e+43	5.89	5.89	5.079e+39	0.00277
967	diHPCARP_I.ttmmtmtd	3.068e+43	5.19	5.19	5.065e+39	0.00276
968	diHPCARP_I.tttmmtmd	9.787e+43	5.89	5.89	5.042e+39	0.00275
969	diHPCARP_I.tptpmpd	2.355e+44	6.41	6.41	5.018e+39	0.00273
970	diHPCARP_I.tptttmtd	9.254e+43	5.86	5.86	4.972e+39	0.00271
971	diHPCARP_I.pmtpttd	2.323e+43	5.07	5.07	4.725e+39	0.00257
972	diHPCARP_I.tpmmpmtd	3.513e+43	5.32	5.32	4.672e+39	0.00255
973	diHPCARP_I.ttmtpmpd	1.812e+44	6.33	6.33	4.465e+39	0.00243
974	diHPCARP_I.tmpmtmtd	4.841e+43	5.54	5.54	4.460e+39	0.00243
975	diHPCARP_I.mmtmttd	1.394e+44	6.18	6.18	4.422e+39	0.00241
976	diHPCARP_I.tmmmtmtd	2.157e+44	6.44	6.44	4.415e+39	0.00241
977	diHPCARP_I.pmmtptmpd	9.675e+43	5.96	5.96	4.413e+39	0.0024
978	diHPCARP_I.pttpmtd	3.783e+44	6.78	6.78	4.333e+39	0.00236
979	diHPCARP_I.pptmmtmd	5.422e+43	5.62	5.62	4.332e+39	0.00236
980	diHPCARP_I.tmtmtpd	1.504e+44	6.24	6.24	4.301e+39	0.00234
981	diHPCARP_I.pttttptmd	2.843e+44	6.62	6.62	4.275e+39	0.00233
982	diHPCARP_I.tmpmmtmd	1.412e+43	4.84	4.84	4.237e+39	0.00231
983	diHPCARP_I.pptmtpd	3.174e+43	5.32	5.32	4.217e+39	0.0023
984	diHPCARP_I.tmtmtpd	1.242e+44	6.14	6.14	4.198e+39	0.00229
985	diHPCARP_I.pttppmmd	1.463e+43	4.87	4.87	4.149e+39	0.00226

986	diHPCARP_I.mttptppd	4.658e+44	6.94	6.94	4.106e+39	0.00224
987	diHPCARP_I.ppptmtmpd	4.749e+43	5.58	5.58	4.096e+39	0.00223
988	diHPCARP_I.tttmpttttd	3.051e+44	6.69	6.69	4.065e+39	0.00221
989	diHPCARP_I.tttmtttmd	1.550e+44	6.29	6.29	4.043e+39	0.0022
990	diHPCARP_I.mmtptppd	4.074e+44	6.87	6.87	4.009e+39	0.00218
991	diHPCARP_I.tptpmttmd	9.436e+43	6.01	6.01	3.977e+39	0.00217
992	diHPCARP_I.tmttmtppd	3.549e+44	6.80	6.80	3.959e+39	0.00216
993	diHPCARP_I.tmttptppd	3.062e+44	6.71	6.71	3.946e+39	0.00215
994	diHPCARP_I.ttmppmpmd	2.738e+44	6.65	6.65	3.945e+39	0.00215
995	diHPCARP_I.pptppmtpd	1.031e+44	6.07	6.07	3.925e+39	0.00214
996	diHPCARP_I.ppttpttpd	5.106e+44	7.03	7.03	3.879e+39	0.00211
997	diHPCARP_I.tmtppptpd	1.279e+44	6.20	6.20	3.867e+39	0.00211
998	diHPCARP_I.tttmptppd	5.473e+43	5.72	5.72	3.754e+39	0.00205
999	diHPCARP_I.pmttptmtd	1.502e+44	6.33	6.33	3.691e+39	0.00201
1000	diHPCARP_I.tptpmpmpd	4.556e+43	5.62	5.62	3.671e+39	0.002
1001	diHPCARP_I.ptpmpmtd	4.601e+43	5.63	5.63	3.659e+39	0.00199
1002	diHPCARP_I.ptppptmpd	7.584e+42	4.56	4.56	3.612e+39	0.00197
1003	diHPCARP_I.tmtpmpmtd	5.868e+43	5.78	5.78	3.600e+39	0.00196
1004	diHPCARP_I.mmmppmmmpd	1.683e+43	5.04	5.04	3.586e+39	0.00195
1005	diHPCARP_I.mtppmmmpmd	9.038e+43	6.04	6.04	3.582e+39	0.00195
1006	diHPCARP_I.tmtppmmpd	2.392e+44	6.62	6.62	3.577e+39	0.00195
1007	diHPCARP_I.tmtppmmpd	5.728e+43	5.78	5.78	3.549e+39	0.00193
1008	diHPCARP_I.ptmptmpd	1.623e+43	5.03	5.03	3.542e+39	0.00193
1009	diHPCARP_I.tmmmtmmpd	4.858e+43	5.68	5.68	3.541e+39	0.00193
1010	diHPCARP_I.mmmpttttd	7.896e+43	5.97	5.97	3.515e+39	0.00192
1011	diHPCARP_I.pmmmpmmpd	3.639e+43	5.52	5.52	3.491e+39	0.0019
1012	diHPCARP_I.tpttppmpd	2.286e+44	6.62	6.62	3.466e+39	0.00189
1013	diHPCARP_I.mmtpmtptd	4.553e+44	7.03	7.03	3.449e+39	0.00188
1014	diHPCARP_I.mttpttpmd	3.557e+44	6.88	6.88	3.447e+39	0.00188
1015	diHPCARP_I.pppptpmpd	2.902e+43	5.39	5.39	3.443e+39	0.00188
1016	diHPCARP_I.tttmptptd	1.136e+44	6.21	6.21	3.417e+39	0.00186
1017	diHPCARP_I.mppptmmpd	5.487e+43	5.78	5.78	3.403e+39	0.00185
1018	diHPCARP_I.mmpmttppd	1.316e+43	4.93	4.93	3.398e+39	0.00185
1019	diHPCARP_I.tmtmptppd	8.764e+43	6.06	6.06	3.353e+39	0.00183
1020	diHPCARP_I.tpptmtmpd	1.406e+44	6.35	6.35	3.351e+39	0.00183
1021	diHPCARP_I.ttttpttpd	6.532e+43	5.89	5.89	3.323e+39	0.00181
1022	diHPCARP_I.ppttmtmpd	2.571e+44	6.72	6.72	3.282e+39	0.00179
1023	diHPCARP_I.mtmtpttmd	2.844e+44	6.78	6.78	3.259e+39	0.00178
1024	diHPCARP_I.tmmpttptd	1.189e+44	6.26	6.26	3.249e+39	0.00177
1025	diHPCARP_I.mmmtptttd	3.352e+44	6.89	6.89	3.199e+39	0.00174
1026	diHPCARP_I.tttmpttpd	4.946e+43	5.76	5.76	3.175e+39	0.00173
1027	diHPCARP_I.tmmppmtpd	2.317e+43	5.31	5.31	3.120e+39	0.0017
1028	diHPCARP_I.tppmmmpmd	6.710e+43	5.95	5.95	3.097e+39	0.00169
1029	diHPCARP_I.tptmmtmpd	6.822e+43	5.96	5.96	3.087e+39	0.00168
1030	diHPCARP_I.ppptptmmd	9.473e+43	6.16	6.16	3.061e+39	0.00167
1031	diHPCARP_I.tmmtpptpd	1.320e+44	6.37	6.37	3.044e+39	0.00166
1032	diHPCARP_I.mmpptmmpd	2.048e+43	5.26	5.26	3.024e+39	0.00165
1033	diHPCARP_I.ppttptmpd	1.344e+44	6.39	6.39	2.957e+39	0.00161
1034	diHPCARP_I.ppppttpd	1.839e+44	6.58	6.58	2.952e+39	0.00161
1035	diHPCARP_I.pmttptmpd	2.715e+44	6.82	6.82	2.938e+39	0.0016
1036	diHPCARP_I.pppptmmpd	2.251e+44	6.71	6.71	2.927e+39	0.00159
1037	diHPCARP_I.tppmmpmtpd	1.148e+44	6.31	6.31	2.927e+39	0.00159
1038	diHPCARP_I.ptmppmmpd	1.466e+43	5.08	5.08	2.912e+39	0.00159
1039	diHPCARP_I.ttptppmpd	7.839e+43	6.10	6.10	2.832e+39	0.00154
1040	diHPCARP_I.mttmmtmpd	8.920e+43	6.18	6.18	2.817e+39	0.00153
1041	diHPCARP_I.tpptpttpd	2.532e+44	6.81	6.81	2.783e+39	0.00152
1042	diHPCARP_I.mptpmtmmd	1.104e+44	6.32	6.32	2.761e+39	0.0015
1043	diHPCARP_I.pmmptmtd	4.788e+43	5.82	5.82	2.748e+39	0.0015
1044	diHPCARP_I.ttttmtmd	1.395e+44	6.46	6.46	2.724e+39	0.00148
1045	diHPCARP_I.pmtmmpmmpd	1.853e+43	5.26	5.26	2.708e+39	0.00148
1046	diHPCARP_I.mptpmpmmd	4.817e+43	5.84	5.84	2.677e+39	0.00146
1047	diHPCARP_I.mppppptpd	1.169e+44	6.38	6.38	2.628e+39	0.00143
1048	diHPCARP_I.pttptmmpd	5.358e+43	5.92	5.92	2.617e+39	0.00143
1049	diHPCARP_I.ttmmpmmpd	2.827e+43	5.54	5.54	2.597e+39	0.00141
1050	diHPCARP_I.tppmptttd	1.142e+44	6.38	6.38	2.588e+39	0.00141
1051	diHPCARP_I.tmmmtmtpd	4.611e+43	5.84	5.84	2.574e+39	0.0014
1052	diHPCARP_I.ttttptmpd	2.386e+44	6.82	6.82	2.566e+39	0.0014
1053	diHPCARP_I.ttppmptpd	1.700e+43	5.25	5.25	2.538e+39	0.00138
1054	diHPCARP_I.tpttmtmpd	2.679e+44	6.92	6.92	2.442e+39	0.00133
1055	diHPCARP_I.tptmtmtpd	1.444e+44	6.55	6.55	2.433e+39	0.00133
1056	diHPCARP_I.tmtttttmpd	8.351e+44	7.60	7.60	2.420e+39	0.00132
1057	diHPCARP_I.pppmmpmtd	9.190e+43	6.32	6.32	2.297e+39	0.00125

1058	diHPCARP_I.mmpmptptd	5.713e+43	6.04	6.04	2.283e+39	0.00124
1059	diHPCARP_I.mpppmptpd	3.388e+43	5.74	5.74	2.244e+39	0.00122
1060	diHPCARP_I.tmmpttppd	6.190e+43	6.10	6.10	2.237e+39	0.00122
1061	diHPCARP_I.tpptptpmd	2.363e+44	6.90	6.90	2.232e+39	0.00122
1062	diHPCARP_I.pppmpttmd	8.745e+43	6.31	6.31	2.208e+39	0.0012
1063	diHPCARP_I.ttpptpmpd	4.578e+43	5.93	5.93	2.191e+39	0.00119
1064	diHPCARP_I.tppmmtpmd	1.868e+44	6.77	6.77	2.181e+39	0.00119
1065	diHPCARP_I.mptpptptd	1.910e+44	6.79	6.79	2.174e+39	0.00118
1066	diHPCARP_I.ttmtmtttd	2.082e+44	6.84	6.84	2.162e+39	0.00118
1067	diHPCARP_I.pmmmtttd	5.487e+43	6.05	6.05	2.150e+39	0.00117
1068	diHPCARP_I.mpppppmpd	8.241e+43	6.29	6.29	2.146e+39	0.00117
1069	diHPCARP_I.mmmptttd	5.877e+43	6.10	6.10	2.114e+39	0.00115
1070	diHPCARP_I.tmpmtmmd	6.754e+43	6.19	6.19	2.107e+39	0.00115
1071	diHPCARP_I.tmttptmpd	3.318e+44	7.13	7.13	2.105e+39	0.00115
1072	diHPCARP_I.tmmppmmmpd	3.418e+43	5.78	5.78	2.093e+39	0.00114
1073	diHPCARP_I.mmtptmtd	7.009e+43	6.21	6.21	2.089e+39	0.00114
1074	diHPCARP_I.mttmptppd	7.636e+43	6.27	6.27	2.083e+39	0.00113
1075	diHPCARP_I.ptmptpmpd	1.548e+44	6.71	6.71	2.018e+39	0.0011
1076	diHPCARP_I.pptmttppd	1.327e+44	6.62	6.62	2.001e+39	0.00109
1077	diHPCARP_I.pmmmtmtpd	2.581e+43	5.64	5.64	1.999e+39	0.00109
1078	diHPCARP_I.pmpmptmtd	5.828e+43	6.13	6.13	1.991e+39	0.00108
1079	diHPCARP_I.mttmttppd	9.411e+43	6.44	6.44	1.911e+39	0.00104
1080	diHPCARP_I.ppppptppd	4.223e+43	5.96	5.96	1.908e+39	0.00104
1081	diHPCARP_I.pptmtpmpd	1.213e+44	6.60	6.60	1.893e+39	0.00103
1082	diHPCARP_I.tpptpmpmd	2.118e+44	6.94	6.94	1.874e+39	0.00102
1083	diHPCARP_I.mmmmtmtpd	1.425e+44	6.71	6.71	1.855e+39	0.00101
1084	diHPCARP_I.pmmmtmmpd	4.085e+43	5.96	5.96	1.854e+39	0.00101
1085	diHPCARP_I.tptmmpmpd	2.011e+44	6.91	6.91	1.852e+39	0.00101
1086	diHPCARP_I.ttmtptppd	2.373e+44	7.01	7.01	1.851e+39	0.00101
1087	diHPCARP_I.mtpmptpmd	1.357e+43	5.31	5.31	1.847e+39	0.00101
1088	diHPCARP_I.tppptpmpd	3.561e+43	5.88	5.88	1.846e+39	0.00101
1089	diHPCARP_I.tmmtmpmpd	1.616e+43	5.42	5.42	1.823e+39	0.000993
1090	diHPCARP_I.ttpmtmmpd	2.198e+44	6.99	6.99	1.768e+39	0.000963
1091	diHPCARP_I.mtpppmpmd	5.816e+43	6.21	6.21	1.742e+39	0.000949
1092	diHPCARP_I.ptppmmpmd	1.197e+44	6.64	6.64	1.735e+39	0.000945
1093	diHPCARP_I.pppmppppd	2.309e+43	5.67	5.67	1.720e+39	0.000937
1094	diHPCARP_I.mmtmptttd	9.496e+43	6.51	6.51	1.720e+39	0.000937
1095	diHPCARP_I.mmpmptttd	4.773e+43	6.11	6.11	1.690e+39	0.000921
1096	diHPCARP_I.mtmtmtd	2.287e+44	7.05	7.05	1.669e+39	0.000909
1097	diHPCARP_I.mtpmptmtd	9.796e+43	6.55	6.55	1.664e+39	0.000907
1098	diHPCARP_I.pppmptmtd	6.903e+43	6.34	6.34	1.655e+39	0.000902
1099	diHPCARP_I.mpttptmpd	9.513e+43	6.53	6.53	1.652e+39	0.0009
1100	diHPCARP_I.tmpmttptd	5.993e+43	6.27	6.27	1.629e+39	0.000887
1101	diHPCARP_I.mmtmptptd	1.261e+44	6.71	6.71	1.622e+39	0.000884
1102	diHPCARP_I.ptmtpmmpd	6.161e+43	6.29	6.29	1.620e+39	0.000882
1103	diHPCARP_I.tptmmpmpd	6.184e+43	6.29	6.29	1.612e+39	0.000878
1104	diHPCARP_I.mmmptttd	6.371e+43	6.31	6.31	1.612e+39	0.000878
1105	diHPCARP_I.mttmtmtpd	1.248e+44	6.71	6.71	1.608e+39	0.000876
1106	diHPCARP_I.mtmtmtpmd	4.851e+44	7.52	7.52	1.606e+39	0.000875
1107	diHPCARP_I.mptpmptpd	4.818e+43	6.15	6.15	1.602e+39	0.000873
1108	diHPCARP_I.mtptppppd	3.701e+43	5.99	5.99	1.590e+39	0.000866
1109	diHPCARP_I.mmmtpmtd	2.394e+44	7.11	7.11	1.585e+39	0.000863
1110	diHPCARP_I.mtpttppd	8.270e+44	7.85	7.85	1.584e+39	0.000863
1111	diHPCARP_I.mtmpttmd	2.970e+44	7.24	7.24	1.568e+39	0.000854
1112	diHPCARP_I.tppmmtpmd	6.448e+43	6.34	6.34	1.544e+39	0.000841
1113	diHPCARP_I.tpttptpmd	2.453e+44	7.14	7.14	1.534e+39	0.000836
1114	diHPCARP_I.mmttptmpd	2.214e+44	7.08	7.08	1.528e+39	0.000832
1115	diHPCARP_I.tmmptptd	7.657e+43	6.45	6.45	1.522e+39	0.000829
1116	diHPCARP_I.ttmmmtmpd	5.933e+43	6.30	6.30	1.518e+39	0.000827
1117	diHPCARP_I.pptmtmmd	1.036e+44	6.64	6.64	1.508e+39	0.000821
1118	diHPCARP_I.mmttpttpd	1.330e+44	6.80	6.80	1.486e+39	0.00081
1119	diHPCARP_I.mppmptpmd	1.903e+43	5.64	5.64	1.469e+39	0.000801
1120	diHPCARP_I.mttmpttpd	7.102e+43	6.43	6.43	1.469e+39	0.0008
1121	diHPCARP_I.pmmpttmd	4.407e+43	6.15	6.15	1.465e+39	0.000798
1122	diHPCARP_I.mmmpttmd	2.595e+44	7.21	7.21	1.453e+39	0.000792
1123	diHPCARP_I.mttmmpmpd	1.407e+44	6.85	6.85	1.444e+39	0.000787
1124	diHPCARP_I.tppmtmtpd	6.507e+43	6.40	6.40	1.428e+39	0.000778
1125	diHPCARP_I.pttpttpd	7.796e+43	6.51	6.51	1.415e+39	0.000771
1126	diHPCARP_I.pmmmtmtd	4.685e+43	6.21	6.21	1.391e+39	0.000758
1127	diHPCARP_I.mptpptpmd	3.001e+44	7.33	7.33	1.376e+39	0.000749
1128	diHPCARP_I.ttptttd	2.563e+44	7.24	7.24	1.363e+39	0.000743
1129	diHPCARP_I.mtptmmpmd	1.299e+44	6.84	6.84	1.352e+39	0.000737

1130	diHPCARP_I.tmtpttmd	5.437e+44	7.70	7.70	1.330e+39	0.000725
1131	diHPCARP_I.mmmmtmtmd	4.077e+43	6.16	6.16	1.323e+39	0.000721
1132	diHPCARP_I.ppppppttmd	2.133e+44	7.15	7.15	1.317e+39	0.000718
1133	diHPCARP_I.mmmmtmttd	2.007e+44	7.11	7.11	1.317e+39	0.000718
1134	diHPCARP_I.tmpptmpd	2.231e+43	5.81	5.81	1.314e+39	0.000716
1135	diHPCARP_I.mppptpmd	4.449e+43	6.22	6.22	1.299e+39	0.000708
1136	diHPCARP_I.ppttptpd	2.963e+44	7.36	7.36	1.295e+39	0.000705
1137	diHPCARP_I.mmpmtmpd	2.442e+43	5.87	5.87	1.287e+39	0.000701
1138	diHPCARP_I.pptmtppd	3.018e+44	7.38	7.38	1.262e+39	0.000688
1139	diHPCARP_I.tpmppppd	3.291e+43	6.06	6.06	1.261e+39	0.000687
1140	diHPCARP_I.ttptmpmd	1.552e+44	6.99	6.99	1.253e+39	0.000682
1141	diHPCARP_I.ptppmpmd	4.974e+43	6.31	6.31	1.251e+39	0.000681
1142	diHPCARP_I.mpppttpd	5.624e+43	6.39	6.39	1.250e+39	0.000681
1143	diHPCARP_I.mmmtptpd	2.174e+44	7.20	7.20	1.241e+39	0.000676
1144	diHPCARP_I.mtptmpmd	3.539e+44	7.49	7.49	1.230e+39	0.00067
1145	diHPCARP_I.ppptmtmd	9.711e+43	6.73	6.73	1.223e+39	0.000666
1146	diHPCARP_I.tttptpmd	6.618e+43	6.50	6.50	1.222e+39	0.000666
1147	diHPCARP_I.tptpmpd	1.282e+44	6.90	6.90	1.206e+39	0.000657
1148	diHPCARP_I.mppppppd	6.114e+43	6.46	6.46	1.201e+39	0.000654
1149	diHPCARP_I.mmmppptmd	4.078e+43	6.22	6.22	1.196e+39	0.000652
1150	diHPCARP_I.tpttptpd	3.326e+44	7.48	7.48	1.187e+39	0.000646
1151	diHPCARP_I.ptmtmpmd	1.634e+44	7.06	7.06	1.184e+39	0.000645
1152	diHPCARP_I.mtpmppmd	9.051e+42	5.34	5.34	1.166e+39	0.000635
1153	diHPCARP_I.tmmppptpd	4.483e+43	6.30	6.30	1.161e+39	0.000632
1154	diHPCARP_I.pppmpttd	1.759e+44	7.11	7.11	1.160e+39	0.000632
1155	diHPCARP_I.tptmpppd	6.846e+43	6.55	6.55	1.152e+39	0.000628
1156	diHPCARP_I.tttmtmpd	1.480e+44	7.02	7.02	1.147e+39	0.000625
1157	diHPCARP_I.ttptmpd	1.984e+43	5.82	5.82	1.138e+39	0.00062
1158	diHPCARP_I.ttpmtpd	8.945e+43	6.72	6.72	1.134e+39	0.000618
1159	diHPCARP_I.mptmtmpd	1.444e+44	7.01	7.01	1.128e+39	0.000615
1160	diHPCARP_I.mtmtptpd	2.212e+44	7.27	7.27	1.125e+39	0.000613
1161	diHPCARP_I.pmtmtmpd	1.744e+44	7.13	7.13	1.114e+39	0.000607
1162	diHPCARP_I.pptmpmmd	8.820e+43	6.73	6.73	1.106e+39	0.000602
1163	diHPCARP_I.mppptpmd	2.021e+43	5.86	5.86	1.089e+39	0.000593
1164	diHPCARP_I.ppppmtmd	2.562e+44	7.38	7.38	1.076e+39	0.000586
1165	diHPCARP_I.tttptppd	6.707e+43	6.59	6.59	1.066e+39	0.000581
1166	diHPCARP_I.ppptmtpd	2.426e+44	7.36	7.36	1.064e+39	0.00058
1167	diHPCARP_I.tmtpttpd	1.445e+44	7.05	7.05	1.063e+39	0.000579
1168	diHPCARP_I.tmtmpttd	3.808e+44	7.63	7.63	1.053e+39	0.000574
1169	diHPCARP_I.ttttttmd	3.314e+44	7.55	7.55	1.050e+39	0.000572
1170	diHPCARP_I.tmpmptpd	2.052e+43	5.89	5.89	1.045e+39	0.000569
1171	diHPCARP_I.pppmptmd	4.420e+43	6.35	6.35	1.045e+39	0.000569
1172	diHPCARP_I.tmpmmtpd	2.051e+43	5.89	5.89	1.045e+39	0.000569
1173	diHPCARP_I.mtttptpd	8.810e+43	6.77	6.77	1.039e+39	0.000566
1174	diHPCARP_I.tmpptmpd	5.119e+43	6.44	6.44	1.035e+39	0.000564
1175	diHPCARP_I.mpppmtmd	1.997e+44	7.26	7.26	1.022e+39	0.000557
1176	diHPCARP_I.mptptpmd	2.657e+44	7.43	7.43	1.021e+39	0.000556
1177	diHPCARP_I.mptmmpmd	7.912e+43	6.71	6.71	1.021e+39	0.000556
1178	diHPCARP_I.mmpmttttd	9.551e+43	6.83	6.83	1.018e+39	0.000555
1179	diHPCARP_I.mtmtpttd	3.212e+44	7.55	7.55	1.014e+39	0.000552
1180	diHPCARP_I.mptmtptpd	3.354e+44	7.58	7.58	1.006e+39	0.000548
1181	diHPCARP_I.pptmttpd	1.969e+44	7.27	7.27	9.965e+38	0.000543
1182	diHPCARP_I.pmtmtmpd	2.639e+44	7.45	7.45	9.905e+38	0.00054
1183	diHPCARP_I.tpttttmd	3.517e+44	7.62	7.62	9.844e+38	0.000536
1184	diHPCARP_I.mptmpttd	3.045e+44	7.54	7.54	9.738e+38	0.000531
1185	diHPCARP_I.tpptpmd	1.164e+44	6.97	6.97	9.735e+38	0.00053
1186	diHPCARP_I.ttmttppd	1.519e+44	7.14	7.14	9.625e+38	0.000524
1187	diHPCARP_I.pppmtpd	1.454e+44	7.11	7.11	9.593e+38	0.000523
1188	diHPCARP_I.mptpmtmd	2.103e+44	7.33	7.33	9.573e+38	0.000522
1189	diHPCARP_I.mmmmtmtpd	5.774e+43	6.56	6.56	9.542e+38	0.00052
1190	diHPCARP_I.tptppmmd	7.610e+43	6.73	6.73	9.529e+38	0.000519
1191	diHPCARP_I.ttmmppmd	5.786e+43	6.57	6.57	9.496e+38	0.000517
1192	diHPCARP_I.pppptppd	6.465e+43	6.63	6.63	9.493e+38	0.000517
1193	diHPCARP_I.tptppppd	2.029e+44	7.32	7.32	9.455e+38	0.000515
1194	diHPCARP_I.pmpmtmd	1.992e+43	5.94	5.94	9.417e+38	0.000513
1195	diHPCARP_I.mptmmpmd	3.746e+43	6.31	6.31	9.416e+38	0.000513
1196	diHPCARP_I.mmmmtmtmd	2.013e+44	7.32	7.32	9.344e+38	0.000509
1197	diHPCARP_I.tmmmtpmd	3.468e+43	6.28	6.28	9.277e+38	0.000505
1198	diHPCARP_I.mtptmmpmd	1.529e+44	7.17	7.17	9.202e+38	0.000501
1199	diHPCARP_I.mtptmmtmd	2.640e+44	7.49	7.49	9.200e+38	0.000501
1200	diHPCARP_I.tmmmtmttd	2.130e+44	7.37	7.37	9.165e+38	0.000499
1201	diHPCARP_I.mptmtpd	2.120e+44	7.37	7.37	9.071e+38	0.000494

1202	diHPCARP_I_ppptppttd	3.328e+44	7.64	7.64	9.064e+38	0.000494
1203	diHPCARP_I_mttptmtpd	1.241e+44	7.05	7.05	9.056e+38	0.000493
1204	diHPCARP_I_mmtmpmtpd	5.246e+43	6.55	6.55	8.950e+38	0.000488
1205	diHPCARP_I_mptmmtmpd	8.396e+43	6.83	6.83	8.934e+38	0.000487
1206	diHPCARP_I_pmtmmtpd	1.148e+44	7.02	7.02	8.889e+38	0.000484
1207	diHPCARP_I_mpmmttppd	6.603e+43	6.69	6.69	8.877e+38	0.000484
1208	diHPCARP_I_ppmmmttd	3.631e+44	7.71	7.71	8.847e+38	0.000482
1209	diHPCARP_I_ttppttmttd	3.392e+44	7.67	7.67	8.806e+38	0.00048
1210	diHPCARP_I_ptmppmtpd	8.989e+44	8.25	8.25	8.794e+38	0.000479
1211	diHPCARP_I_tptptpppd	2.695e+44	7.54	7.54	8.692e+38	0.000474
1212	diHPCARP_I_ptmmpmpd	5.508e+43	6.59	6.59	8.690e+38	0.000473
1213	diHPCARP_I_mtpptmtpd	2.311e+43	6.08	6.08	8.631e+38	0.00047
1214	diHPCARP_I_ttpmpppmd	7.664e+42	5.42	5.42	8.583e+38	0.000468
1215	diHPCARP_I_mmtmmtpd	8.080e+43	6.83	6.83	8.581e+38	0.000468
1216	diHPCARP_I_ppptmtpd	6.355e+43	6.69	6.69	8.533e+38	0.000465
1217	diHPCARP_I_pmpmtpd	2.598e+43	6.16	6.16	8.485e+38	0.000462
1218	diHPCARP_I_mmpmtpd	5.851e+43	6.65	6.65	8.432e+38	0.000459
1219	diHPCARP_I_mtmmpmpd	5.522e+43	6.61	6.61	8.415e+38	0.000458
1220	diHPCARP_I_ppptmttd	7.432e+44	8.16	8.16	8.412e+38	0.000458
1221	diHPCARP_I_pmmptttd	1.187e+44	7.07	7.07	8.376e+38	0.000456
1222	diHPCARP_I_pttmttd	7.748e+43	6.82	6.82	8.308e+38	0.000453
1223	diHPCARP_I_mtmpppmd	2.115e+43	6.05	6.05	8.286e+38	0.000451
1224	diHPCARP_I_tptmmpd	3.024e+43	6.27	6.27	8.143e+38	0.000444
1225	diHPCARP_I_mmpmtmtpd	3.439e+43	6.37	6.37	7.933e+38	0.000432
1226	diHPCARP_I_tpmmpmtpd	8.913e+43	6.94	6.94	7.799e+38	0.000425
1227	diHPCARP_I_pptmtpd	1.688e+44	7.33	7.33	7.778e+38	0.000424
1228	diHPCARP_I_ttppttd	3.602e+44	7.80	7.80	7.507e+38	0.000409
1229	diHPCARP_I_tptmtpd	4.360e+44	7.91	7.91	7.506e+38	0.000409
1230	diHPCARP_I_pmmmmmpd	9.568e+42	5.64	5.64	7.495e+38	0.000408
1231	diHPCARP_I_tmmmpmtpd	4.334e+43	6.54	6.54	7.486e+38	0.000408
1232	diHPCARP_I_ppmmpmtpd	8.177e+43	6.92	6.92	7.454e+38	0.000406
1233	diHPCARP_I_mmmtpmtpd	1.484e+44	7.28	7.28	7.385e+38	0.000402
1234	diHPCARP_I_ttmpppmd	1.906e+43	6.06	6.06	7.341e+38	0.0004
1235	diHPCARP_I_tmtmtpd	2.964e+44	7.70	7.70	7.255e+38	0.000395
1236	diHPCARP_I_tmtppppd	2.028e+44	7.48	7.48	7.195e+38	0.000392
1237	diHPCARP_I_ppmtpmtpd	3.845e+43	6.49	6.49	7.140e+38	0.000389
1238	diHPCARP_I_pmmtttd	2.372e+44	7.59	7.59	6.993e+38	0.000381
1239	diHPCARP_I_mmtmtpd	3.097e+43	6.38	6.38	6.954e+38	0.000379
1240	diHPCARP_I_mmtmtmtpd	1.463e+44	7.33	7.33	6.710e+38	0.000366
1241	diHPCARP_I_mmtppptd	9.202e+43	7.05	7.05	6.702e+38	0.000365
1242	diHPCARP_I_tptmmpd	4.820e+43	6.67	6.67	6.700e+38	0.000365
1243	diHPCARP_I_tmpmtpd	7.123e+43	6.90	6.90	6.691e+38	0.000365
1244	diHPCARP_I_mmmmpmtpd	7.968e+43	6.97	6.97	6.632e+38	0.000361
1245	diHPCARP_I_pmtppmtpd	7.527e+43	6.94	6.94	6.606e+38	0.00036
1246	diHPCARP_I_mmtmtpd	8.925e+43	7.05	7.05	6.528e+38	0.000356
1247	diHPCARP_I_mptpmtd	3.236e+43	6.45	6.45	6.525e+38	0.000356
1248	diHPCARP_I_pmmmtmtpd	1.652e+44	7.42	7.42	6.521e+38	0.000355
1249	diHPCARP_I_tptmtmtpd	1.257e+44	7.26	7.26	6.469e+38	0.000352
1250	diHPCARP_I_tptpmpd	3.524e+44	7.88	7.88	6.455e+38	0.000352
1251	diHPCARP_I_ttpmtpd	1.461e+43	5.99	5.99	6.354e+38	0.000346
1252	diHPCARP_I_tptmtpd	1.624e+44	7.42	7.42	6.342e+38	0.000346
1253	diHPCARP_I_pmtmmmpd	2.669e+43	6.35	6.35	6.339e+38	0.000345
1254	diHPCARP_I_tmmmpmtpd	2.796e+43	6.39	6.39	6.215e+38	0.000339
1255	diHPCARP_I_mtmmpmpd	6.595e+43	6.90	6.90	6.215e+38	0.000339
1256	diHPCARP_I_ppptpmpd	2.689e+44	7.74	7.74	6.208e+38	0.000338
1257	diHPCARP_I_mmpmtpd	9.099e+43	7.09	7.09	6.205e+38	0.000338
1258	diHPCARP_I_tpmtpmtpd	1.323e+44	7.32	7.32	6.176e+38	0.000336
1259	diHPCARP_I_mtmtpmtpd	2.240e+44	7.63	7.63	6.148e+38	0.000335
1260	diHPCARP_I_tptpmpd	6.111e+43	6.86	6.86	6.121e+38	0.000333
1261	diHPCARP_I_tmmmtmtpd	2.017e+44	7.58	7.58	6.036e+38	0.000329
1262	diHPCARP_I_mtpmtpmtpd	5.976e+43	6.86	6.86	6.018e+38	0.000328
1263	diHPCARP_I_ppptmtpd	3.973e+44	8.00	8.00	5.945e+38	0.000324
1264	diHPCARP_I_mpppmmpd	1.309e+44	7.34	7.34	5.913e+38	0.000322
1265	diHPCARP_I_pmtmmpd	3.530e+43	6.56	6.56	5.908e+38	0.000322
1266	diHPCARP_I_ptmmpmtpd	4.611e+43	6.72	6.72	5.899e+38	0.000321
1267	diHPCARP_I_pptppppd	3.394e+44	7.91	7.91	5.869e+38	0.00032
1268	diHPCARP_I_tmpmmttd	4.173e+43	6.66	6.66	5.830e+38	0.000318
1269	diHPCARP_I_mmtmtpd	2.898e+44	7.82	7.82	5.800e+38	0.000316
1270	diHPCARP_I_mmmptmtpd	9.787e+43	7.18	7.18	5.798e+38	0.000316
1271	diHPCARP_I_mmpmtpd	8.564e+43	7.10	7.10	5.747e+38	0.000313
1272	diHPCARP_I_ttppttd	2.212e+44	7.67	7.67	5.718e+38	0.000312
1273	diHPCARP_I_ppptpmpd	2.303e+44	7.70	7.70	5.698e+38	0.00031

1274	diHPCARP_I_ppptmmpd	3.057e+44	7.87	7.87	5.686e+38	0.00031
1275	diHPCARP_I_mmpmtmtpd	6.601e+43	6.96	6.96	5.648e+38	0.000308
1276	diHPCARP_I_ptptmmpmd	1.318e+44	7.37	7.37	5.635e+38	0.000307
1277	diHPCARP_I.mtptmtmtd	8.329e+43	7.10	7.10	5.603e+38	0.000305
1278	diHPCARP_I.ppppppstd	3.924e+44	8.03	8.03	5.590e+38	0.000305
1279	diHPCARP_I.pmmmtmmtmd	2.211e+43	6.31	6.31	5.575e+38	0.000304
1280	diHPCARP_I.mmmmtmtd	2.875e+44	7.85	7.85	5.464e+38	0.000298
1281	diHPCARP_I.ptmtptmmd	1.410e+44	7.43	7.43	5.457e+38	0.000297
1282	diHPCARP_I.tpmptmtpd	5.845e+43	6.91	6.91	5.430e+38	0.000296
1283	diHPCARP_I.ptttmtmmd	4.248e+43	6.72	6.72	5.384e+38	0.000293
1284	diHPCARP_I.pmmtpmtd	2.297e+44	7.74	7.74	5.261e+38	0.000287
1285	diHPCARP_I.tppppmtd	2.590e+44	7.81	7.81	5.253e+38	0.000286
1286	diHPCARP_I.ptmttppd	4.166e+44	8.11	8.11	5.149e+38	0.000281
1287	diHPCARP_I.pppmmtmtd	1.761e+44	7.61	7.61	5.061e+38	0.000276
1288	diHPCARP_I.pmpmtpd	4.442e+43	6.79	6.79	5.050e+38	0.000275
1289	diHPCARP_I.mtmtmtpd	2.195e+44	7.74	7.74	5.038e+38	0.000275
1290	diHPCARP_I.ttpmmpmtd	7.146e+43	7.07	7.07	5.018e+38	0.000273
1291	diHPCARP_I.mpmmpmtd	6.489e+43	7.02	7.02	4.994e+38	0.000272
1292	diHPCARP_I.ttttppd	1.921e+44	7.67	7.67	4.986e+38	0.000272
1293	diHPCARP_I.mmtmtmtpd	3.454e+44	8.02	8.02	4.949e+38	0.00027
1294	diHPCARP_I.pptppmtd	2.622e+44	7.86	7.86	4.889e+38	0.000266
1295	diHPCARP_I.tpttppd	3.003e+44	7.95	7.95	4.867e+38	0.000265
1296	diHPCARP_I.mmmptmtd	7.854e+43	7.15	7.15	4.849e+38	0.000264
1297	diHPCARP_I.pptpppmd	2.288e+44	7.79	7.79	4.835e+38	0.000263
1298	diHPCARP_I.mtmpppmd	5.635e+43	6.96	6.96	4.810e+38	0.000262
1299	diHPCARP_I.mttptmtpd	9.243e+43	7.26	7.26	4.716e+38	0.000257
1300	diHPCARP_I.tpmmtmtd	1.770e+44	7.65	7.65	4.714e+38	0.000257
1301	diHPCARP_I.tptmtpmd	1.345e+44	7.49	7.49	4.695e+38	0.000256
1302	diHPCARP_I.pttpmtpd	1.033e+45	8.71	8.71	4.683e+38	0.000255
1303	diHPCARP_I.tmpmtpmtd	2.719e+43	6.54	6.54	4.662e+38	0.000254
1304	diHPCARP_I.mpmmpmtd	1.322e+44	7.49	7.49	4.658e+38	0.000254
1305	diHPCARP_I.mmmmpmtd	4.049e+43	6.78	6.78	4.626e+38	0.000252
1306	diHPCARP_I.pppmmtmtd	1.548e+44	7.59	7.59	4.576e+38	0.000249
1307	diHPCARP_I.pptmtpd	2.841e+43	6.59	6.59	4.462e+38	0.000243
1308	diHPCARP_I.mptpppmd	1.603e+44	7.63	7.63	4.459e+38	0.000243
1309	diHPCARP_I.ptmtmtpmd	1.076e+44	7.39	7.39	4.413e+38	0.00024
1310	diHPCARP_I.pppmmtmtd	1.510e+44	7.60	7.60	4.409e+38	0.00024
1311	diHPCARP_I.tpmmpmtd	1.114e+44	7.42	7.42	4.372e+38	0.000238
1312	diHPCARP_I.mtptmtpd	1.653e+43	6.28	6.28	4.365e+38	0.000238
1313	diHPCARP_I.mtttptmtd	3.391e+44	8.09	8.09	4.357e+38	0.000237
1314	diHPCARP_I.pppmmpd	1.747e+44	7.69	7.69	4.353e+38	0.000237
1315	diHPCARP_I.tppptppd	7.217e+43	7.17	7.17	4.340e+38	0.000236
1316	diHPCARP_I.tttmtpd	3.155e+44	8.05	8.05	4.326e+38	0.000236
1317	diHPCARP_I.pttptmtd	3.800e+44	8.16	8.16	4.286e+38	0.000233
1318	diHPCARP_I.mttptmtpd	1.815e+44	7.72	7.72	4.285e+38	0.000233
1319	diHPCARP_I.ttpmtpd	4.080e+43	6.83	6.83	4.282e+38	0.000233
1320	diHPCARP_I.pmmptmtd	2.091e+43	6.44	6.44	4.279e+38	0.000233
1321	diHPCARP_I.tppmtpd	1.270e+44	7.51	7.51	4.271e+38	0.000233
1322	diHPCARP_I.tptppmtd	8.581e+43	7.28	7.28	4.254e+38	0.000232
1323	diHPCARP_I.mppmtmtd	1.150e+44	7.46	7.46	4.227e+38	0.00023
1324	diHPCARP_I.pppmtpd	5.992e+43	7.07	7.07	4.212e+38	0.000229
1325	diHPCARP_I.mppptmtd	1.829e+44	7.74	7.74	4.189e+38	0.000228
1326	diHPCARP_I.pttpmmpd	1.488e+43	6.25	6.25	4.154e+38	0.000226
1327	diHPCARP_I.tttptmtd	3.091e+44	8.06	8.06	4.139e+38	0.000226
1328	diHPCARP_I.mmmmtmtd	5.815e+43	7.07	7.07	4.131e+38	0.000225
1329	diHPCARP_I.mtmmtmtd	5.774e+43	7.07	7.07	4.085e+38	0.000223
1330	diHPCARP_I.tmpmmpmtd	3.447e+43	6.77	6.77	4.015e+38	0.000219
1331	diHPCARP_I.pmpmtpd	5.378e+43	7.04	7.04	3.991e+38	0.000217
1332	diHPCARP_I.mptmmpmtd	3.282e+44	8.12	8.12	3.981e+38	0.000217
1333	diHPCARP_I.tmpptmtd	4.554e+43	6.95	6.95	3.970e+38	0.000216
1334	diHPCARP_I.mtppmtpd	3.552e+43	6.80	6.80	3.930e+38	0.000214
1335	diHPCARP_I.mptmpppmd	8.374e+43	7.32	7.32	3.903e+38	0.000213
1336	diHPCARP_I.pmmptmtd	8.002e+43	7.30	7.30	3.864e+38	0.000211
1337	diHPCARP_I.mppptmtd	4.417e+43	6.94	6.94	3.863e+38	0.00021
1338	diHPCARP_I.mptmmpmtd	1.963e+44	7.83	7.83	3.855e+38	0.00021
1339	diHPCARP_I.mptmtmtd	1.954e+44	7.83	7.83	3.838e+38	0.000209
1340	diHPCARP_I.mtmptmtd	1.697e+43	6.38	6.38	3.834e+38	0.000209
1341	diHPCARP_I.ptmptmtd	2.742e+44	8.04	8.04	3.828e+38	0.000209
1342	diHPCARP_I.mmmmpmtd	4.397e+43	6.95	6.95	3.822e+38	0.000208
1343	diHPCARP_I.pptppmtd	1.502e+44	7.69	7.69	3.779e+38	0.000206
1344	diHPCARP_I.tmmmtmtd	2.879e+44	8.08	8.08	3.730e+38	0.000203
1345	diHPCARP_I.mmpmtpd	2.823e+43	6.70	6.70	3.701e+38	0.000202

1346	diHPCARP_I.mpttpmpmd	2.624e+44	8.04	8.04	3.643e+38	0.000198
1347	diHPCARP_I.mmmmtmptd	3.878e+44	8.29	8.29	3.567e+38	0.000194
1348	diHPCARP_I.ppttptmmd	1.653e+44	7.79	7.79	3.491e+38	0.00019
1349	diHPCARP_I.mtptttmtd	2.786e+44	8.11	8.11	3.469e+38	0.000189
1350	diHPCARP_I.tmmtmntmd	4.938e+43	7.08	7.08	3.460e+38	0.000189
1351	diHPCARP_I.mppmtmpmd	3.214e+44	8.19	8.19	3.459e+38	0.000188
1352	diHPCARP_I.mmmtttptd	9.277e+43	7.46	7.46	3.389e+38	0.000185
1353	diHPCARP_I.ttpmmtmd	4.882e+43	7.08	7.08	3.379e+38	0.000184
1354	diHPCARP_I.tttmpmmpd	5.935e+43	7.20	7.20	3.358e+38	0.000183
1355	diHPCARP_I.mpmmtmpmd	1.062e+44	7.55	7.55	3.337e+38	0.000182
1356	diHPCARP_I.mpttmtptd	3.229e+44	8.22	8.22	3.291e+38	0.000179
1357	diHPCARP_I.mpptpmmd	8.673e+43	7.44	7.44	3.288e+38	0.000179
1358	diHPCARP_I.pmmtptppd	1.513e+44	7.78	7.78	3.242e+38	0.000177
1359	diHPCARP_I.ppptptttd	2.716e+44	8.14	8.14	3.209e+38	0.000175
1360	diHPCARP_I.tmpptttd	2.717e+44	8.14	8.14	3.194e+38	0.000174
1361	diHPCARP_I.pttpttppd	9.720e+44	8.90	8.90	3.192e+38	0.000174
1362	diHPCARP_I.pppptmpd	6.889e+43	7.33	7.33	3.152e+38	0.000172
1363	diHPCARP_I.tpptmtmmd	1.058e+44	7.59	7.59	3.127e+38	0.00017
1364	diHPCARP_I.ttttttppd	3.644e+44	8.33	8.33	3.112e+38	0.00017
1365	diHPCARP_I.pptpttmd	2.864e+44	8.19	8.19	3.078e+38	0.000168
1366	diHPCARP_I.ppttptpd	2.373e+44	8.08	8.08	3.072e+38	0.000167
1367	diHPCARP_I.ppptmtpd	4.868e+44	8.52	8.52	3.044e+38	0.000166
1368	diHPCARP_I.mpttptppd	4.095e+44	8.41	8.41	3.038e+38	0.000166
1369	diHPCARP_I.ptpnmtpmd	2.045e+43	6.63	6.63	3.008e+38	0.000164
1370	diHPCARP_I.mpptpmpmd	1.474e+44	7.81	7.81	2.989e+38	0.000163
1371	diHPCARP_I.mptmtpppd	1.421e+44	7.80	7.80	2.976e+38	0.000162
1372	diHPCARP_I.pppmmtpd	7.760e+43	7.44	7.44	2.964e+38	0.000161
1373	diHPCARP_I.pmmmtmtd	1.779e+44	7.94	7.94	2.907e+38	0.000158
1374	diHPCARP_I.mmmmmntmd	2.983e+44	8.26	8.26	2.873e+38	0.000157
1375	diHPCARP_I.mtpnmtpmd	3.492e+43	6.99	6.99	2.841e+38	0.000155
1376	diHPCARP_I.tpmpttpmd	5.400e+43	7.25	7.25	2.819e+38	0.000154
1377	diHPCARP_I.pmmtptptd	2.025e+44	8.04	8.04	2.811e+38	0.000153
1378	diHPCARP_I.mppppmpmd	6.569e+43	7.37	7.37	2.795e+38	0.000152
1379	diHPCARP_I.tpmtmtpmd	3.052e+44	8.29	8.29	2.779e+38	0.000151
1380	diHPCARP_I.tpptmtttd	5.277e+44	8.63	8.63	2.748e+38	0.00015
1381	diHPCARP_I.mptmtmpmd	5.731e+43	7.31	7.31	2.731e+38	0.000149
1382	diHPCARP_I.tpttmtpd	2.500e+44	8.19	8.19	2.724e+38	0.000148
1383	diHPCARP_I.mmmmpptmd	4.818e+44	8.58	8.58	2.686e+38	0.000146
1384	diHPCARP_I.ttttmnttd	4.719e+44	8.58	8.58	2.646e+38	0.000144
1385	diHPCARP_I.mtptmtpmd	2.861e+44	8.29	8.29	2.634e+38	0.000144
1386	diHPCARP_I.ptptptmpd	2.854e+43	6.91	6.91	2.631e+38	0.000143
1387	diHPCARP_I.ttttpttmd	3.564e+44	8.42	8.42	2.608e+38	0.000142
1388	diHPCARP_I.ptpptmtpd	6.637e+43	7.43	7.43	2.565e+38	0.00014
1389	diHPCARP_I.tmttmtpd	1.642e+44	7.97	7.97	2.551e+38	0.000139
1390	diHPCARP_I.mttmtpmd	2.904e+44	8.32	8.32	2.545e+38	0.000139
1391	diHPCARP_I.tmttmmpmd	3.062e+44	8.36	8.36	2.501e+38	0.000136
1392	diHPCARP_I.tmpmtmpmd	4.900e+43	7.27	7.27	2.485e+38	0.000135
1393	diHPCARP_I.tpmmtttd	4.033e+44	8.53	8.53	2.476e+38	0.000135
1394	diHPCARP_I.tmpppmpmd	1.970e+43	6.73	6.73	2.456e+38	0.000134
1395	diHPCARP_I.tpttmmpmd	1.077e+44	7.76	7.76	2.391e+38	0.00013
1396	diHPCARP_I.ptmmttppd	4.068e+44	8.56	8.56	2.366e+38	0.000129
1397	diHPCARP_I.pmmtmmttd	3.291e+43	7.06	7.06	2.361e+38	0.000129
1398	diHPCARP_I.ptptttmpd	1.436e+44	7.94	7.94	2.356e+38	0.000128
1399	diHPCARP_I.ptttptmmd	6.245e+43	7.45	7.45	2.345e+38	0.000128
1400	diHPCARP_I.mmmppmpmd	3.689e+43	7.13	7.13	2.345e+38	0.000128
1401	diHPCARP_I.mpttptmpd	2.994e+44	8.38	8.38	2.340e+38	0.000128
1402	diHPCARP_I.tppmmtttd	2.324e+44	8.23	8.23	2.336e+38	0.000127
1403	diHPCARP_I.ptpmpmpd	8.745e+42	6.29	6.29	2.300e+38	0.000125
1404	diHPCARP_I.mmmptppd	4.375e+43	7.25	7.25	2.286e+38	0.000125
1405	diHPCARP_I.pmtpmmmmd	2.491e+43	6.92	6.92	2.282e+38	0.000124
1406	diHPCARP_I.mpptptmpd	5.483e+43	7.39	7.39	2.273e+38	0.000124
1407	diHPCARP_I.mtttptppd	2.545e+44	8.31	8.31	2.251e+38	0.000123
1408	diHPCARP_I.mmppttppd	1.323e+44	7.92	7.92	2.235e+38	0.000122
1409	diHPCARP_I.mtpnmtpd	4.273e+43	7.25	7.25	2.229e+38	0.000121
1410	diHPCARP_I.mpptmtpd	7.618e+43	7.60	7.60	2.215e+38	0.000121
1411	diHPCARP_I.ptmptmpd	7.617e+43	7.61	7.61	2.184e+38	0.000119
1412	diHPCARP_I.ttpmtmpd	1.580e+43	6.67	6.67	2.175e+38	0.000118
1413	diHPCARP_I.ptpmtmpmd	3.519e+43	7.16	7.16	2.157e+38	0.000118
1414	diHPCARP_I.tptpttmd	3.239e+44	8.48	8.48	2.153e+38	0.000117
1415	diHPCARP_I.pmmtmtpd	2.990e+43	7.06	7.06	2.143e+38	0.000117
1416	diHPCARP_I.mmtmpmpd	7.653e+43	7.64	7.64	2.093e+38	0.000114
1417	diHPCARP_I.mpttptmpd	2.175e+44	8.26	8.26	2.086e+38	0.000114

1418	diHPCARP_I.pmmpptttd	4.374e+43	7.31	7.31	2.083e+38	0.000113
1419	diHPCARP_I.tpptppmmd	6.385e+43	7.53	7.53	2.082e+38	0.000113
1420	diHPCARP_I.mptpppppd	1.790e+44	8.15	8.15	2.065e+38	0.000113
1421	diHPCARP_I.mttmpmmd	2.327e+43	6.94	6.94	2.061e+38	0.000112
1422	diHPCARP_I.ptmtmtmd	2.395e+44	8.33	8.33	2.050e+38	0.000112
1423	diHPCARP_I.pmmmmmpd	3.078e+44	8.48	8.48	2.037e+38	0.000111
1424	diHPCARP_I.pppppmmd	4.459e+43	7.34	7.34	2.021e+38	0.000111
1425	diHPCARP_I.tpttptmmd	1.985e+44	8.23	8.23	2.012e+38	0.000111
1426	diHPCARP_I.tpptppppd	1.488e+44	8.06	8.06	2.006e+38	0.000109
1427	diHPCARP_I.tppppmmd	8.170e+43	7.70	7.70	2.000e+38	0.000109
1428	diHPCARP_I.tmttptmmd	4.790e+44	8.76	8.76	1.997e+38	0.000109
1429	diHPCARP_I.mttmmtppd	3.845e+44	8.63	8.63	1.989e+38	0.000108
1430	diHPCARP_I.mttpttmd	3.506e+44	8.58	8.58	1.974e+38	0.000108
1431	diHPCARP_I.ttmppppmd	4.474e+43	7.35	7.35	1.974e+38	0.000108
1432	diHPCARP_I.pmptmtttd	1.133e+44	7.91	7.91	1.968e+38	0.000107
1433	diHPCARP_I.tpttptttd	2.227e+44	8.31	8.31	1.960e+38	0.000107
1434	diHPCARP_I.pppmtpmtd	1.192e+44	7.94	7.94	1.945e+38	0.000106
1435	diHPCARP_I.mmtptmtd	3.517e+43	7.22	7.22	1.944e+38	0.000106
1436	diHPCARP_I.tmpmmttd	4.923e+43	7.42	7.42	1.943e+38	0.000106
1437	diHPCARP_I.mmtpppppd	2.435e+44	8.37	8.37	1.942e+38	0.000106
1438	diHPCARP_I.tppmmtppd	2.147e+44	8.30	8.30	1.925e+38	0.000105
1439	diHPCARP_I.ppppmttd	3.281e+43	7.18	7.18	1.919e+38	0.000105
1440	diHPCARP_I.mmmtpmmd	1.855e+44	8.22	8.22	1.909e+38	0.000104
1441	diHPCARP_I.pmmppttmd	3.002e+43	7.14	7.14	1.900e+38	0.000104
1442	diHPCARP_I.tmmppppmd	3.844e+43	7.28	7.28	1.897e+38	0.000103
1443	diHPCARP_I.tpmmttmd	2.515e+44	8.41	8.41	1.867e+38	0.000102
1444	diHPCARP_I.tttptmtd	1.696e+44	8.19	8.19	1.837e+38	0.000101
1445	diHPCARP_I.pttppmmd	5.142e+43	7.48	7.48	1.834e+38	9.99e-05
1446	diHPCARP_I.ptppppmmd	1.470e+43	6.73	6.73	1.830e+38	9.97e-05
1447	diHPCARP_I.tpttppppd	1.497e+44	8.12	8.12	1.815e+38	9.89e-05
1448	diHPCARP_I.ptppmmtmd	1.201e+44	7.99	7.99	1.808e+38	9.85e-05
1449	diHPCARP_I.pttmtmtd	1.795e+44	8.24	8.24	1.786e+38	9.73e-05
1450	diHPCARP_I.tpppppmd	8.787e+43	7.83	7.83	1.727e+38	9.41e-05
1451	diHPCARP_I.tppmpmtd	5.642e+43	7.57	7.57	1.714e+38	9.34e-05
1452	diHPCARP_I.pmpptppmd	4.145e+43	7.39	7.39	1.711e+38	9.32e-05
1453	diHPCARP_I.tptmmtmd	3.339e+44	8.64	8.64	1.696e+38	9.24e-05
1454	diHPCARP_I.pmtppppd	1.997e+44	8.34	8.34	1.692e+38	9.22e-05
1455	diHPCARP_I.pppmmttd	1.161e+44	8.02	8.02	1.681e+38	9.16e-05
1456	diHPCARP_I.mmmptmmd	6.745e+43	7.70	7.70	1.670e+38	9.1e-05
1457	diHPCARP_I.pmpptppd	4.695e+43	7.49	7.49	1.643e+38	8.95e-05
1458	diHPCARP_I.tmttppppd	7.084e+43	7.74	7.74	1.634e+38	8.9e-05
1459	diHPCARP_I.ptpmtmtd	3.798e+44	8.76	8.76	1.587e+38	8.64e-05
1460	diHPCARP_I.tptmmpmd	1.608e+44	8.25	8.25	1.581e+38	8.61e-05
1461	diHPCARP_I.mtttttmd	4.061e+44	8.81	8.81	1.540e+38	8.39e-05
1462	diHPCARP_I.tmttptmtd	9.064e+43	7.92	7.92	1.532e+38	8.35e-05
1463	diHPCARP_I.pmpmtpmd	8.895e+43	7.92	7.92	1.513e+38	8.24e-05
1464	diHPCARP_I.tpmmtppd	1.782e+44	8.33	8.33	1.512e+38	8.24e-05
1465	diHPCARP_I.mmpptmtd	1.015e+44	8.00	8.00	1.512e+38	8.24e-05
1466	diHPCARP_I.pmttptmd	5.417e+44	9.00	9.00	1.505e+38	8.2e-05
1467	diHPCARP_I.tpttpttd	2.318e+44	8.50	8.50	1.497e+38	8.16e-05
1468	diHPCARP_I.tmtmmpmd	8.640e+43	7.91	7.91	1.487e+38	8.1e-05
1469	diHPCARP_I.mtmtmmpd	8.004e+43	7.87	7.87	1.472e+38	8.02e-05
1470	diHPCARP_I.tppttttd	3.495e+44	8.75	8.75	1.471e+38	8.01e-05
1471	diHPCARP_I.mttttttd	1.245e+45	9.51	9.51	1.469e+38	8e-05
1472	diHPCARP_I.tptmpppd	8.511e+43	7.91	7.91	1.468e+38	8e-05
1473	diHPCARP_I.tpttppppd	2.705e+44	8.60	8.60	1.467e+38	7.99e-05
1474	diHPCARP_I.tttppppmd	2.067e+43	7.07	7.07	1.459e+38	7.95e-05
1475	diHPCARP_I.ttpptmtd	2.385e+43	7.17	7.17	1.415e+38	7.71e-05
1476	diHPCARP_I.mtppppmmd	2.920e+43	7.30	7.30	1.410e+38	7.68e-05
1477	diHPCARP_I.pmtppmmd	1.052e+44	8.07	8.07	1.390e+38	7.57e-05
1478	diHPCARP_I.ppttppmd	2.449e+44	8.57	8.57	1.388e+38	7.56e-05
1479	diHPCARP_I.tpmttttd	1.017e+45	9.42	9.42	1.387e+38	7.56e-05
1480	diHPCARP_I.pmmmtmtd	5.468e+43	7.69	7.69	1.378e+38	7.51e-05
1481	diHPCARP_I.tmpmpptd	3.721e+43	7.46	7.46	1.364e+38	7.43e-05
1482	diHPCARP_I.mttppppmd	2.090e+43	7.12	7.12	1.363e+38	7.42e-05
1483	diHPCARP_I.mtmtppppd	5.638e+43	7.72	7.72	1.333e+38	7.26e-05
1484	diHPCARP_I.tmpmmttd	1.609e+44	8.35	8.35	1.330e+38	7.25e-05
1485	diHPCARP_I.mtttmtppd	4.113e+44	8.91	8.91	1.330e+38	7.24e-05
1486	diHPCARP_I.ppmmttmd	4.395e+44	8.96	8.96	1.307e+38	7.12e-05
1487	diHPCARP_I.tpmtptmtd	3.176e+44	8.77	8.77	1.307e+38	7.12e-05
1488	diHPCARP_I.pptmpptd	2.096e+44	8.52	8.52	1.302e+38	7.09e-05
1489	diHPCARP_I.ppttptmd	6.429e+44	9.19	9.19	1.291e+38	7.04e-05

1490	diHPCARP_I.mppttppmd	3.605e+44	8.85	8.85	1.284e+38	7e-05
1491	diHPCARP_I.pttttppmd	4.823e+44	9.03	9.03	1.283e+38	6.99e-05
1492	diHPCARP_I.mmpmmtppmd	1.246e+43	6.86	6.86	1.256e+38	6.84e-05
1493	diHPCARP_I.pmtppmmmd	7.486e+43	7.93	7.93	1.251e+38	6.81e-05
1494	diHPCARP_I.tptpppppd	9.496e+43	8.08	8.08	1.240e+38	6.76e-05
1495	diHPCARP_I.mpttmtpd	4.555e+44	9.01	9.01	1.240e+38	6.76e-05
1496	diHPCARP_I.ppmttttd	4.261e+44	8.98	8.98	1.232e+38	6.71e-05
1497	diHPCARP_I.mttppmmmd	2.399e+43	7.26	7.26	1.230e+38	6.7e-05
1498	diHPCARP_I.mmmmtppmd	1.136e+43	6.82	6.82	1.224e+38	6.67e-05
1499	diHPCARP_I.pmmmtmtmd	1.356e+44	8.30	8.30	1.222e+38	6.66e-05
1500	diHPCARP_I.ppmtpppd	2.203e+43	7.22	7.22	1.205e+38	6.57e-05
1501	diHPCARP_I.mtmtppmpd	1.822e+44	8.48	8.48	1.203e+38	6.55e-05
1502	diHPCARP_I.tpptppttd	1.790e+44	8.49	8.49	1.174e+38	6.4e-05
1503	diHPCARP_I.tmtmttmd	5.970e+44	9.21	9.21	1.171e+38	6.38e-05
1504	diHPCARP_I.tpttpppd	2.691e+44	8.73	8.73	1.169e+38	6.37e-05
1505	diHPCARP_I.pmmptppd	9.539e+43	8.12	8.12	1.168e+38	6.37e-05
1506	diHPCARP_I.pmtptmmpd	1.046e+44	8.17	8.17	1.167e+38	6.36e-05
1507	diHPCARP_I.tmptpttd	2.049e+44	8.57	8.57	1.166e+38	6.35e-05
1508	diHPCARP_I.ppmtppmd	6.560e+44	9.27	9.27	1.157e+38	6.31e-05
1509	diHPCARP_I.pppmttttd	2.266e+44	8.64	8.64	1.155e+38	6.29e-05
1510	diHPCARP_I.tppmmtmd	1.647e+44	8.45	8.45	1.148e+38	6.25e-05
1511	diHPCARP_I.tmttppmpd	1.067e+44	8.20	8.20	1.141e+38	6.22e-05
1512	diHPCARP_I.tmmmtppd	3.310e+43	7.50	7.50	1.135e+38	6.19e-05
1513	diHPCARP_I.tpptmtppd	2.702e+44	8.76	8.76	1.131e+38	6.16e-05
1514	diHPCARP_I.mmmmpmptd	6.346e+43	7.89	7.89	1.130e+38	6.16e-05
1515	diHPCARP_I.mpptppmmd	7.132e+43	7.96	7.96	1.125e+38	6.13e-05
1516	diHPCARP_I.tmttppmmd	3.139e+44	8.85	8.85	1.112e+38	6.06e-05
1517	diHPCARP_I.pttmmmpmd	5.542e+43	7.82	7.82	1.109e+38	6.04e-05
1518	diHPCARP_I.ppttppmd	1.310e+44	8.35	8.35	1.084e+38	5.9e-05
1519	diHPCARP_I.ptttmtpd	1.278e+44	8.33	8.33	1.083e+38	5.9e-05
1520	diHPCARP_I.pmmmmmpmd	1.897e+44	8.57	8.57	1.080e+38	5.88e-05
1521	diHPCARP_I.mppmmtppd	1.203e+44	8.30	8.30	1.080e+38	5.88e-05
1522	diHPCARP_I.mppmmtppd	1.306e+44	8.36	8.36	1.065e+38	5.8e-05
1523	diHPCARP_I.pptmmpmd	2.670e+44	8.79	8.79	1.063e+38	5.79e-05
1524	diHPCARP_I.pppmmpmd	2.760e+44	8.81	8.81	1.054e+38	5.74e-05
1525	diHPCARP_I.ppptppmpd	4.668e+43	7.75	7.75	1.050e+38	5.72e-05
1526	diHPCARP_I.pptmmpmd	4.308e+44	9.09	9.09	1.037e+38	5.65e-05
1527	diHPCARP_I.tpttmmmd	1.683e+44	8.53	8.53	1.028e+38	5.6e-05
1528	diHPCARP_I.mpptmtpd	2.899e+44	8.85	8.85	1.027e+38	5.6e-05
1529	diHPCARP_I.tpttpttd	6.370e+44	9.34	9.34	9.986e+37	5.44e-05
1530	diHPCARP_I.mmtmptpd	3.918e+43	7.68	7.68	9.935e+37	5.41e-05
1531	diHPCARP_I.mpptptpd	3.839e+44	9.05	9.05	9.862e+37	5.37e-05
1532	diHPCARP_I.mpttppd	3.536e+44	9.00	9.00	9.846e+37	5.36e-05
1533	diHPCARP_I.pppmtpd	2.425e+43	7.40	7.40	9.834e+37	5.36e-05
1534	diHPCARP_I.pptmmpmd	4.077e+43	7.71	7.71	9.826e+37	5.35e-05
1535	diHPCARP_I.mpptmmmd	9.748e+43	8.24	8.24	9.757e+37	5.32e-05
1536	diHPCARP_I.ptptmtpd	4.082e+43	7.72	7.72	9.745e+37	5.31e-05
1537	diHPCARP_I.tppmmtptd	2.518e+44	8.81	8.81	9.665e+37	5.27e-05
1538	diHPCARP_I.tmtppmpd	6.361e+43	7.99	7.99	9.649e+37	5.26e-05
1539	diHPCARP_I.mppmtpppd	1.194e+44	8.37	8.37	9.612e+37	5.24e-05
1540	diHPCARP_I.mpttppmd	3.492e+44	9.01	9.01	9.597e+37	5.23e-05
1541	diHPCARP_I.mpptpppd	5.150e+43	7.87	7.87	9.577e+37	5.22e-05
1542	diHPCARP_I.tpmmtmtd	8.375e+44	9.54	9.54	9.418e+37	5.13e-05
1543	diHPCARP_I.pmmmtmtd	1.277e+44	8.42	8.42	9.348e+37	5.09e-05
1544	diHPCARP_I.mpttppmd	1.034e+44	8.30	8.30	9.216e+37	5.02e-05
1545	diHPCARP_I.ppttppd	2.425e+44	8.82	8.82	9.037e+37	4.92e-05
1546	diHPCARP_I.mpttppmd	2.924e+44	8.94	8.94	9.022e+37	4.92e-05
1547	diHPCARP_I.mppmtpppd	7.320e+43	8.11	8.11	8.984e+37	4.89e-05
1548	diHPCARP_I.mtpmtppmd	2.064e+43	7.36	7.36	8.961e+37	4.88e-05
1549	diHPCARP_I.ptpmmtmtd	1.487e+43	7.17	7.17	8.888e+37	4.84e-05
1550	diHPCARP_I.ptmppmpd	9.030e+43	8.25	8.25	8.879e+37	4.84e-05
1551	diHPCARP_I.pppmmtmd	1.870e+44	8.68	8.68	8.874e+37	4.83e-05
1552	diHPCARP_I.tppmtpppd	7.344e+43	8.13	8.13	8.763e+37	4.77e-05
1553	diHPCARP_I.mppmmtmtd	3.537e+43	7.70	7.70	8.752e+37	4.77e-05
1554	diHPCARP_I.pppmtpmd	2.246e+44	8.80	8.80	8.743e+37	4.76e-05
1555	diHPCARP_I.mmmmpptd	7.594e+43	8.15	8.15	8.711e+37	4.75e-05
1556	diHPCARP_I.tmtppmtd	1.073e+44	8.36	8.36	8.692e+37	4.74e-05
1557	diHPCARP_I.tppmtpd	1.088e+44	8.38	8.38	8.602e+37	4.69e-05
1558	diHPCARP_I.mtttpttd	4.672e+44	9.25	9.25	8.462e+37	4.61e-05
1559	diHPCARP_I.ttpmmtmtd	1.177e+44	8.43	8.43	8.444e+37	4.6e-05
1560	diHPCARP_I.tmpttptd	6.183e+44	9.42	9.42	8.423e+37	4.59e-05
1561	diHPCARP_I.mpttmtppd	3.247e+44	9.04	9.04	8.414e+37	4.58e-05

1562	diHPCARP_I.ttmtppmpd	1.420e+44	8.55	8.55	8.405e+37	4.58e-05
1563	diHPCARP_I.tppmppppd	4.498e+43	7.86	7.86	8.386e+37	4.57e-05
1564	diHPCARP_I.mmtptpptd	6.351e+44	9.45	9.45	8.342e+37	4.55e-05
1565	diHPCARP_I.tmttppptd	1.746e+44	8.68	8.68	8.315e+37	4.53e-05
1566	diHPCARP_I.mmmmmmpd	4.614e+43	7.89	7.89	8.284e+37	4.51e-05
1567	diHPCARP_I.tpptmpmmd	6.781e+43	8.12	8.12	8.207e+37	4.47e-05
1568	diHPCARP_I.tmpmttttd	1.859e+44	8.73	8.73	8.180e+37	4.46e-05
1569	diHPCARP_I.ttttmttmd	4.855e+44	9.31	9.31	8.058e+37	4.39e-05
1570	diHPCARP_I.tmmppptd	9.467e+43	8.34	8.34	8.010e+37	4.36e-05
1571	diHPCARP_I.mtmtptmpd	9.085e+43	8.31	8.31	7.981e+37	4.35e-05
1572	diHPCARP_I.tpptmpptd	3.579e+44	9.13	9.13	7.969e+37	4.34e-05
1573	diHPCARP_I.pttptttd	1.173e+44	8.47	8.47	7.927e+37	4.32e-05
1574	diHPCARP_I.tmpptpmm	3.065e+43	7.67	7.67	7.894e+37	4.3e-05
1575	diHPCARP_I.mtppmmppd	4.036e+43	7.84	7.84	7.851e+37	4.28e-05
1576	diHPCARP_I.ttpmtmpmd	1.856e+43	7.39	7.39	7.688e+37	4.19e-05
1577	diHPCARP_I.pppmmtmmd	4.802e+43	7.96	7.96	7.679e+37	4.18e-05
1578	diHPCARP_I.tpttppptd	1.925e+44	8.78	8.78	7.678e+37	4.18e-05
1579	diHPCARP_I.mmtptpmpd	1.483e+43	7.26	7.26	7.624e+37	4.15e-05
1580	diHPCARP_I.tttppmpmd	3.570e+43	7.79	7.79	7.604e+37	4.14e-05
1581	diHPCARP_I.tppmppptd	8.117e+43	8.28	8.28	7.599e+37	4.14e-05
1582	diHPCARP_I.pppmtmtd	2.745e+44	9.01	9.01	7.542e+37	4.11e-05
1583	diHPCARP_I.mppmmtmmd	2.561e+44	8.97	8.97	7.541e+37	4.11e-05
1584	diHPCARP_I.pppmpmtd	7.426e+43	8.23	8.23	7.470e+37	4.07e-05
1585	diHPCARP_I.tpptmpptd	2.737e+44	9.01	9.01	7.425e+37	4.05e-05
1586	diHPCARP_I.ttmtmmtd	7.056e+43	8.21	8.21	7.368e+37	4.01e-05
1587	diHPCARP_I.tppmmptd	1.775e+44	8.76	8.76	7.348e+37	4e-05
1588	diHPCARP_I.mmtpttmd	4.911e+44	9.37	9.37	7.315e+37	3.99e-05
1589	diHPCARP_I.mtttmtmd	1.236e+45	9.94	9.94	7.045e+37	3.84e-05
1590	diHPCARP_I.mtppppmpd	9.746e+43	8.44	8.44	6.975e+37	3.8e-05
1591	diHPCARP_I.mtppppmpd	1.227e+43	7.20	7.20	6.975e+37	3.8e-05
1592	diHPCARP_I.mtppmpptd	4.033e+43	7.91	7.91	6.931e+37	3.78e-05
1593	diHPCARP_I.mppmmttmd	5.465e+44	9.48	9.48	6.840e+37	3.73e-05
1594	diHPCARP_I.tppppptd	4.115e+43	7.93	7.93	6.834e+37	3.72e-05
1595	diHPCARP_I.mmtpppmd	1.641e+44	8.76	8.76	6.798e+37	3.7e-05
1596	diHPCARP_I.tpptmptd	3.750e+44	9.25	9.25	6.794e+37	3.7e-05
1597	diHPCARP_I.mtppmpmpd	7.907e+42	6.96	6.96	6.753e+37	3.68e-05
1598	diHPCARP_I.ttmtptmpd	4.688e+43	8.03	8.03	6.650e+37	3.62e-05
1599	diHPCARP_I.mppmmmpd	2.605e+44	9.05	9.05	6.629e+37	3.61e-05
1600	diHPCARP_I.tttppmmd	1.683e+43	7.43	7.43	6.504e+37	3.54e-05
1601	diHPCARP_I.tppmmpppd	2.234e+44	8.98	8.98	6.455e+37	3.52e-05
1602	diHPCARP_I.pppmpptd	8.384e+43	8.39	8.39	6.454e+37	3.52e-05
1603	diHPCARP_I.mppmtmpd	2.038e+44	8.92	8.92	6.426e+37	3.5e-05
1604	diHPCARP_I.tttmmtmd	1.070e+45	9.92	9.92	6.373e+37	3.47e-05
1605	diHPCARP_I.ppttmtmd	6.266e+44	9.60	9.60	6.342e+37	3.46e-05
1606	diHPCARP_I.pmtppmpd	4.463e+43	8.03	8.03	6.341e+37	3.45e-05
1607	diHPCARP_I.tmtmpptd	1.543e+44	8.77	8.77	6.322e+37	3.44e-05
1608	diHPCARP_I.tppppmtd	3.764e+43	7.93	7.93	6.264e+37	3.41e-05
1609	diHPCARP_I.mptmmpmd	6.307e+43	8.24	8.24	6.250e+37	3.41e-05
1610	diHPCARP_I.mpppptttd	5.062e+44	9.48	9.48	6.236e+37	3.4e-05
1611	diHPCARP_I.tmppptttd	1.781e+44	8.88	8.88	6.027e+37	3.28e-05
1612	diHPCARP_I.mppppmpmd	1.807e+43	7.52	7.52	6.015e+37	3.28e-05
1613	diHPCARP_I.mtptttmpd	1.047e+44	8.57	8.57	6.013e+37	3.28e-05
1614	diHPCARP_I.mppppmpd	1.753e+44	8.88	8.88	5.956e+37	3.24e-05
1615	diHPCARP_I.mmtppmmd	5.126e+43	8.15	8.15	5.942e+37	3.24e-05
1616	diHPCARP_I.mtmmmtmd	2.953e+44	9.19	9.19	5.930e+37	3.23e-05
1617	diHPCARP_I.pppmpmtd	8.037e+43	8.42	8.42	5.917e+37	3.22e-05
1618	diHPCARP_I.pppmpppd	3.350e+43	7.90	7.90	5.914e+37	3.22e-05
1619	diHPCARP_I.mppmmtttd	7.492e+44	9.75	9.75	5.914e+37	3.22e-05
1620	diHPCARP_I.tpptppptd	1.832e+44	8.91	8.91	5.900e+37	3.21e-05
1621	diHPCARP_I.mptmmtmpd	1.183e+44	8.65	8.65	5.898e+37	3.21e-05
1622	diHPCARP_I.ptptmmtmd	2.384e+44	9.08	9.08	5.836e+37	3.18e-05
1623	diHPCARP_I.tmtppmtd	6.814e+43	8.33	8.33	5.812e+37	3.17e-05
1624	diHPCARP_I.pttmtmtd	3.386e+44	9.29	9.29	5.774e+37	3.15e-05
1625	diHPCARP_I.tpmtmtpd	3.593e+44	9.33	9.33	5.738e+37	3.13e-05
1626	diHPCARP_I.tmtmpptd	1.328e+44	8.74	8.74	5.694e+37	3.1e-05
1627	diHPCARP_I.pppppmtd	1.648e+43	7.51	7.51	5.548e+37	3.02e-05
1628	diHPCARP_I.mtppmtpd	4.525e+43	8.12	8.12	5.489e+37	2.99e-05
1629	diHPCARP_I.mmtmtpd	1.429e+44	8.81	8.81	5.472e+37	2.98e-05
1630	diHPCARP_I.tptmmtmd	1.220e+44	8.72	8.72	5.398e+37	2.94e-05
1631	diHPCARP_I.mppptmpd	2.895e+44	9.25	9.25	5.319e+37	2.9e-05
1632	diHPCARP_I.ttpmpmpd	2.653e+43	7.84	7.84	5.136e+37	2.8e-05
1633	diHPCARP_I.ttmtmpmpd	1.022e+44	8.65	8.65	5.111e+37	2.78e-05

1634	diHPCARP_I.tmmppptmd	8.134e+43	8.52	8.52	5.083e+37	2.77e-05
1635	diHPCARP_I.tttppmmmd	1.765e+43	7.62	7.62	4.946e+37	2.69e-05
1636	diHPCARP_I.mppmttttd	1.148e+45	10.11	10.11	4.940e+37	2.69e-05
1637	diHPCARP_I.tmpmpmttd	7.186e+43	8.46	8.46	4.916e+37	2.68e-05
1638	diHPCARP_I.mppmpptmd	7.042e+43	8.46	8.46	4.823e+37	2.63e-05
1639	diHPCARP_I.ttpppmtmd	8.464e+43	8.58	8.58	4.759e+37	2.59e-05
1640	diHPCARP_I.mptppttmd	4.306e+44	9.55	9.55	4.757e+37	2.59e-05
1641	diHPCARP_I.mmtppmttd	1.763e+44	9.02	9.02	4.753e+37	2.59e-05
1642	diHPCARP_I.ppmmtttmd	4.954e+44	9.63	9.63	4.750e+37	2.59e-05
1643	diHPCARP_I.ptpmtttmd	8.384e+43	8.58	8.58	4.747e+37	2.59e-05
1644	diHPCARP_I.tmppttttd	3.460e+44	9.42	9.42	4.737e+37	2.58e-05
1645	diHPCARP_I.ptmpptmpd	9.578e+43	8.66	8.66	4.714e+37	2.57e-05
1646	diHPCARP_I.mppppmmpd	1.662e+44	8.99	8.99	4.678e+37	2.55e-05
1647	diHPCARP_I.tttmppmpd	2.587e+43	7.88	7.88	4.667e+37	2.54e-05
1648	diHPCARP_I.mtptmmpd	1.726e+44	9.02	9.02	4.652e+37	2.53e-05
1649	diHPCARP_I.pmmmtppmd	3.716e+43	8.11	8.11	4.617e+37	2.52e-05
1650	diHPCARP_I.pmpptttmd	7.821e+43	8.55	8.55	4.612e+37	2.51e-05
1651	diHPCARP_I.mppmmttmd	3.072e+44	9.37	9.37	4.594e+37	2.5e-05
1652	diHPCARP_I.mppmtttmd	7.084e+43	8.49	8.49	4.593e+37	2.5e-05
1653	diHPCARP_I.mmtppptmd	1.017e+44	8.71	8.71	4.590e+37	2.5e-05
1654	diHPCARP_I.pppmmpmmd	1.989e+43	7.74	7.74	4.582e+37	2.5e-05
1655	diHPCARP_I.pmttmmtpd	1.077e+44	8.75	8.75	4.566e+37	2.49e-05
1656	diHPCARP_I.pttmtttmd	2.868e+44	9.33	9.33	4.551e+37	2.48e-05
1657	diHPCARP_I.tmpmmtpd	7.151e+43	8.51	8.51	4.547e+37	2.48e-05
1658	diHPCARP_I.mppmmtpd	8.857e+43	8.64	8.64	4.528e+37	2.47e-05
1659	diHPCARP_I.tppmmtpd	1.183e+44	8.82	8.82	4.438e+37	2.42e-05
1660	diHPCARP_I.mtptmmttd	9.529e+43	8.71	8.71	4.277e+37	2.33e-05
1661	diHPCARP_I.mtptmmtmd	1.723e+44	9.07	9.07	4.221e+37	2.3e-05
1662	diHPCARP_I.mpmmtppd	3.813e+43	8.18	8.18	4.193e+37	2.28e-05
1663	diHPCARP_I.mppptppd	1.180e+44	8.86	8.86	4.154e+37	2.26e-05
1664	diHPCARP_I.ptpmttttd	1.472e+44	8.99	8.99	4.149e+37	2.26e-05
1665	diHPCARP_I.tpttmttd	6.367e+44	9.87	9.87	4.121e+37	2.24e-05
1666	diHPCARP_I.mppptmpd	9.689e+43	8.75	8.75	4.078e+37	2.22e-05
1667	diHPCARP_I.tppmmmtmd	7.534e+43	8.61	8.61	3.998e+37	2.18e-05
1668	diHPCARP_I.mtptmtpd	1.183e+44	8.88	8.88	3.996e+37	2.18e-05
1669	diHPCARP_I.mptmmpd	1.518e+44	9.04	9.04	3.957e+37	2.16e-05
1670	diHPCARP_I.mppmtmmd	8.305e+43	8.68	8.68	3.944e+37	2.15e-05
1671	diHPCARP_I.mptmmpd	3.404e+44	9.53	9.53	3.882e+37	2.12e-05
1672	diHPCARP_I.ptpppttd	4.282e+43	8.30	8.30	3.878e+37	2.11e-05
1673	diHPCARP_I.ptptmttd	4.985e+44	9.77	9.77	3.801e+37	2.07e-05
1674	diHPCARP_I.pmtmmpd	7.757e+43	8.67	8.67	3.746e+37	2.04e-05
1675	diHPCARP_I.mtmmmtmd	4.051e+44	9.66	9.66	3.713e+37	2.02e-05
1676	diHPCARP_I.tttppmpd	9.532e+42	7.44	7.44	3.651e+37	1.99e-05
1677	diHPCARP_I.mppptppd	7.057e+43	8.63	8.63	3.634e+37	1.98e-05
1678	diHPCARP_I.tmpmtpmd	2.513e+43	8.02	8.02	3.591e+37	1.96e-05
1679	diHPCARP_I.mptmtpd	4.233e+43	8.34	8.34	3.562e+37	1.94e-05
1680	diHPCARP_I.tmptttmd	1.769e+44	9.19	9.19	3.560e+37	1.94e-05
1681	diHPCARP_I.tptmpptd	8.953e+43	8.79	8.79	3.550e+37	1.93e-05
1682	diHPCARP_I.tmpptttmd	2.144e+44	9.32	9.32	3.474e+37	1.89e-05
1683	diHPCARP_I.pptmtpd	7.522e+43	8.70	8.70	3.473e+37	1.89e-05
1684	diHPCARP_I.tmpppptmd	5.199e+43	8.48	8.48	3.459e+37	1.88e-05
1685	diHPCARP_I.ptpmmmtmd	2.091e+43	7.94	7.94	3.427e+37	1.87e-05
1686	diHPCARP_I.tpmtttmd	4.587e+44	9.78	9.78	3.423e+37	1.86e-05
1687	diHPCARP_I.tppppmmpd	8.699e+43	8.81	8.81	3.314e+37	1.81e-05
1688	diHPCARP_I.mmmmttttd	3.948e+44	9.71	9.71	3.313e+37	1.81e-05
1689	diHPCARP_I.mptppppd	2.405e+44	9.42	9.42	3.295e+37	1.8e-05
1690	diHPCARP_I.ttptppmpd	1.158e+44	8.99	8.99	3.269e+37	1.78e-05
1691	diHPCARP_I.mptmtpd	7.864e+43	8.76	8.76	3.262e+37	1.78e-05
1692	diHPCARP_I.mmpmmtttd	6.696e+43	8.67	8.67	3.252e+37	1.77e-05
1693	diHPCARP_I.tptppmpd	1.147e+44	9.00	9.00	3.213e+37	1.75e-05
1694	diHPCARP_I.pppmmttd	6.045e+43	8.62	8.62	3.194e+37	1.74e-05
1695	diHPCARP_I.ppmtpptd	9.637e+43	8.90	8.90	3.185e+37	1.74e-05
1696	diHPCARP_I.tttmtpmd	1.781e+44	9.27	9.27	3.167e+37	1.73e-05
1697	diHPCARP_I.mtptppmpd	9.908e+43	8.92	8.92	3.163e+37	1.72e-05
1698	diHPCARP_I.tmtppppd	2.778e+44	9.54	9.54	3.134e+37	1.71e-05
1699	diHPCARP_I.mpmmtttmd	1.104e+44	8.99	8.99	3.130e+37	1.71e-05
1700	diHPCARP_I.mmttpttd	7.038e+44	10.09	10.09	3.123e+37	1.7e-05
1701	diHPCARP_I.mptmtpd	1.574e+44	9.21	9.21	3.068e+37	1.67e-05
1702	diHPCARP_I.mppmmmtmd	4.984e+43	8.53	8.53	3.023e+37	1.65e-05
1703	diHPCARP_I.pmmppptd	5.617e+43	8.62	8.62	2.975e+37	1.62e-05
1704	diHPCARP_I.ptpmtttmd	1.060e+43	7.63	7.63	2.942e+37	1.6e-05
1705	diHPCARP_I.mpmmtttmd	1.203e+44	9.08	9.08	2.939e+37	1.6e-05

1706	diHPCARP_I.ptptttttd	1.642e+44	9.27	9.27	2.891e+37	1.57e-05
1707	diHPCARP_I.mtttppmmpd	1.418e+44	9.19	9.19	2.880e+37	1.57e-05
1708	diHPCARP_I.mttmpmtd	1.421e+44	9.20	9.20	2.817e+37	1.53e-05
1709	diHPCARP_I.tppmmmtmd	3.917e+44	9.82	9.82	2.770e+37	1.51e-05
1710	diHPCARP_I.mppppmtpd	5.990e+43	8.70	8.70	2.767e+37	1.51e-05
1711	diHPCARP_I.mmtttttmd	7.136e+44	10.18	10.18	2.725e+37	1.48e-05
1712	diHPCARP_I.tmpmpmmpd	2.102e+43	8.08	8.08	2.714e+37	1.48e-05
1713	diHPCARP_I.ttmmtmtd	1.683e+44	9.33	9.33	2.690e+37	1.47e-05
1714	diHPCARP_I.mtmtmpmmpd	1.243e+44	9.16	9.16	2.652e+37	1.44e-05
1715	diHPCARP_I.ptttptppd	8.792e+44	10.33	10.33	2.603e+37	1.42e-05
1716	diHPCARP_I.tptmptmtd	1.246e+44	9.17	9.17	2.595e+37	1.41e-05
1717	diHPCARP_I.pmmppptpd	2.376e+43	8.18	8.18	2.594e+37	1.41e-05
1718	diHPCARP_I.mtpttmmmd	8.282e+43	8.93	8.93	2.571e+37	1.4e-05
1719	diHPCARP_I.mpttpptpd	1.748e+44	9.38	9.38	2.567e+37	1.4e-05
1720	diHPCARP_I.mmmppmtd	7.937e+43	8.91	8.91	2.546e+37	1.39e-05
1721	diHPCARP_I.tppppmmmd	2.694e+43	8.28	8.28	2.490e+37	1.36e-05
1722	diHPCARP_I.mpmmtmtd	1.372e+44	9.26	9.26	2.482e+37	1.35e-05
1723	diHPCARP_I.pppmmmmmd	1.048e+44	9.10	9.10	2.465e+37	1.34e-05
1724	diHPCARP_I.mpptmtpd	4.320e+43	8.58	8.58	2.412e+37	1.31e-05
1725	diHPCARP_I.pppmmppd	1.056e+44	9.12	9.12	2.384e+37	1.3e-05
1726	diHPCARP_I.ptmtmpmmpd	1.081e+44	9.14	9.14	2.383e+37	1.3e-05
1727	diHPCARP_I.tppmppptd	6.574e+43	8.85	8.85	2.364e+37	1.29e-05
1728	diHPCARP_I.tppmmpptd	2.937e+43	8.38	8.38	2.319e+37	1.26e-05
1729	diHPCARP_I.tmmmmppmd	1.139e+44	9.19	9.19	2.309e+37	1.26e-05
1730	diHPCARP_I.tppmmppd	9.200e+43	9.07	9.07	2.282e+37	1.24e-05
1731	diHPCARP_I.ppptptmtd	1.516e+44	9.37	9.37	2.280e+37	1.24e-05
1732	diHPCARP_I.mppmmpmmpd	2.923e+43	8.40	8.40	2.240e+37	1.22e-05
1733	diHPCARP_I.pmptpmmmd	1.663e+43	8.06	8.06	2.233e+37	1.22e-05
1734	diHPCARP_I.mmmpttpmd	4.553e+43	8.66	8.66	2.229e+37	1.21e-05
1735	diHPCARP_I.mmpmmmtmd	5.218e+43	8.75	8.75	2.212e+37	1.21e-05
1736	diHPCARP_I.tmttppppd	2.240e+44	9.62	9.62	2.191e+37	1.19e-05
1737	diHPCARP_I.mtttppmmpd	2.867e+43	8.40	8.40	2.184e+37	1.19e-05
1738	diHPCARP_I.mmttppptd	1.449e+44	9.37	9.37	2.175e+37	1.18e-05
1739	diHPCARP_I.tttppmtpd	2.617e+43	8.35	8.35	2.159e+37	1.18e-05
1740	diHPCARP_I.mpptmpppd	1.361e+44	9.34	9.34	2.143e+37	1.17e-05
1741	diHPCARP_I.ttpmtmtd	1.262e+44	9.30	9.30	2.136e+37	1.16e-05
1742	diHPCARP_I.mpmmtmtd	2.200e+44	9.63	9.63	2.116e+37	1.15e-05
1743	diHPCARP_I.tpmttppd	2.956e+44	9.82	9.82	2.088e+37	1.14e-05
1744	diHPCARP_I.mpptmmpd	4.715e+44	10.10	10.10	2.073e+37	1.13e-05
1745	diHPCARP_I.mttmmmmmd	3.620e+43	8.58	8.58	2.042e+37	1.11e-05
1746	diHPCARP_I.mmtmpptd	1.223e+44	9.31	9.31	2.009e+37	1.09e-05
1747	diHPCARP_I.mmpmmpmtd	9.814e+43	9.18	9.18	2.005e+37	1.09e-05
1748	diHPCARP_I.tpmtmpppd	2.024e+44	9.62	9.62	1.981e+37	1.08e-05
1749	diHPCARP_I.pmppttpd	2.646e+44	9.79	9.79	1.952e+37	1.06e-05
1750	diHPCARP_I.mpttppmmd	1.503e+44	9.47	9.47	1.912e+37	1.04e-05
1751	diHPCARP_I.pmttptmtd	1.056e+44	9.26	9.26	1.893e+37	1.03e-05
1752	diHPCARP_I.tpttppmmd	3.501e+44	9.99	9.99	1.852e+37	1.01e-05
1753	diHPCARP_I.tptppptmd	1.921e+44	9.64	9.64	1.823e+37	9.93e-06
1754	diHPCARP_I.mppmtmmmd	4.542e+43	8.78	8.78	1.819e+37	9.91e-06
1755	diHPCARP_I.mmmppmtd	9.297e+43	9.21	9.21	1.805e+37	9.83e-06
1756	diHPCARP_I.mpptmtpd	4.854e+44	10.20	10.20	1.803e+37	9.82e-06
1757	diHPCARP_I.tmttppmmpd	3.470e+44	10.01	10.01	1.776e+37	9.68e-06
1758	diHPCARP_I.pppmmtmmpd	3.874e+43	8.71	8.71	1.762e+37	9.6e-06
1759	diHPCARP_I.pmpttppd	2.075e+44	9.71	9.71	1.752e+37	9.54e-06
1760	diHPCARP_I.mtppmmpd	6.344e+43	9.01	9.01	1.736e+37	9.46e-06
1761	diHPCARP_I.tpmttpmtd	3.350e+44	10.01	10.01	1.710e+37	9.32e-06
1762	diHPCARP_I.tmmtmtd	3.548e+44	10.05	10.05	1.680e+37	9.15e-06
1763	diHPCARP_I.ptmtmtpd	7.684e+43	9.15	9.15	1.657e+37	9.03e-06
1764	diHPCARP_I.tmmtmmtd	3.936e+44	10.13	10.13	1.656e+37	9.02e-06
1765	diHPCARP_I.mmtmppptd	1.181e+44	9.41	9.41	1.636e+37	8.91e-06
1766	diHPCARP_I.mpptpttd	1.800e+44	9.67	9.67	1.614e+37	8.79e-06
1767	diHPCARP_I.mpmmtmmd	5.742e+43	9.00	9.00	1.586e+37	8.64e-06
1768	diHPCARP_I.ptttmmpd	2.391e+43	8.48	8.48	1.584e+37	8.63e-06
1769	diHPCARP_I.tppppmtd	1.383e+44	9.53	9.53	1.583e+37	8.62e-06
1770	diHPCARP_I.mppppmmpd	5.382e+43	8.98	8.98	1.557e+37	8.48e-06
1771	diHPCARP_I.pmmppmmpd	1.227e+43	8.11	8.11	1.517e+37	8.27e-06
1772	diHPCARP_I.tmtmppppd	9.234e+43	9.31	9.31	1.514e+37	8.25e-06
1773	diHPCARP_I.pmmtppmmpd	1.218e+44	9.49	9.49	1.497e+37	8.16e-06
1774	diHPCARP_I.tptmtpmtd	1.163e+44	9.46	9.46	1.486e+37	8.09e-06
1775	diHPCARP_I.pmmppmtd	2.306e+43	8.50	8.50	1.477e+37	8.05e-06
1776	diHPCARP_I.tmmtmtd	5.560e+44	10.40	10.40	1.475e+37	8.04e-06
1777	diHPCARP_I.tppppmtpd	7.854e+43	9.23	9.23	1.475e+37	8.04e-06

1778	diHPCARP_I.mmttttttd	1.018e+45	10.76	10.76	1.472e+37	8.02e-06
1779	diHPCARP_I.mprnmmtmd	3.268e+44	10.09	10.09	1.462e+37	7.97e-06
1780	diHPCARP_I.mtmtppmtmd	4.594e+44	10.29	10.29	1.457e+37	7.94e-06
1781	diHPCARP_I.ttmppppmd	5.062e+43	8.99	8.99	1.425e+37	7.76e-06
1782	diHPCARP_I.mmmtpmttd	6.692e+44	10.54	10.54	1.415e+37	7.71e-06
1783	diHPCARP_I.mmtmpmpmd	4.259e+43	8.92	8.92	1.342e+37	7.31e-06
1784	diHPCARP_I.mmtmpppd	5.033e+44	10.40	10.40	1.327e+37	7.23e-06
1785	diHPCARP_I.tttppmtmd	3.953e+43	8.89	8.89	1.313e+37	7.15e-06
1786	diHPCARP_I.mttmmmpmd	1.444e+44	9.68	9.68	1.289e+37	7.02e-06
1787	diHPCARP_I.pttmtppd	9.524e+43	9.43	9.43	1.289e+37	7.02e-06
1788	diHPCARP_I.mptmpppd	9.177e+43	9.42	9.42	1.270e+37	6.92e-06
1789	diHPCARP_I.pmttppmmd	2.193e+44	9.94	9.94	1.264e+37	6.89e-06
1790	diHPCARP_I.ptppmttd	2.179e+43	8.57	8.57	1.248e+37	6.8e-06
1791	diHPCARP_I.pmtppmtmd	3.823e+44	10.28	10.28	1.231e+37	6.71e-06
1792	diHPCARP_I.mmmtpppmd	8.327e+43	9.38	9.38	1.218e+37	6.63e-06
1793	diHPCARP_I.pppmptppd	1.131e+44	9.57	9.57	1.199e+37	6.53e-06
1794	diHPCARP_I.tptpppttd	3.902e+44	10.31	10.31	1.198e+37	6.53e-06
1795	diHPCARP_I.mmpppptpd	6.065e+43	9.20	9.20	1.197e+37	6.52e-06
1796	diHPCARP_I.pmtppmttd	7.413e+43	9.32	9.32	1.196e+37	6.52e-06
1797	diHPCARP_I.mptmpppmd	1.797e+44	9.85	9.85	1.193e+37	6.5e-06
1798	diHPCARP_I.ttptpmtmd	1.623e+44	9.80	9.80	1.177e+37	6.41e-06
1799	diHPCARP_I.pmtmpmttd	1.169e+44	9.61	9.61	1.159e+37	6.31e-06
1800	diHPCARP_I.pptppmtmd	2.424e+44	10.05	10.05	1.155e+37	6.29e-06
1801	diHPCARP_I.mppptppd	1.251e+44	9.66	9.66	1.151e+37	6.27e-06
1802	diHPCARP_I.tttppmttd	6.801e+43	9.30	9.30	1.147e+37	6.25e-06
1803	diHPCARP_I.mmmptmttd	1.177e+44	9.63	9.63	1.143e+37	6.23e-06
1804	diHPCARP_I.pmpmtmd	2.565e+44	10.10	10.10	1.129e+37	6.15e-06
1805	diHPCARP_I.ptttmtppd	8.032e+44	10.80	10.80	1.092e+37	5.95e-06
1806	diHPCARP_I.ttttppmd	1.018e+44	9.57	9.57	1.091e+37	5.95e-06
1807	diHPCARP_I.mmtppppd	3.892e+44	10.37	10.37	1.090e+37	5.94e-06
1808	diHPCARP_I.mmttppmd	1.098e+44	9.62	9.62	1.075e+37	5.86e-06
1809	diHPCARP_I.mtppmmmd	4.343e+43	9.07	9.07	1.064e+37	5.8e-06
1810	diHPCARP_I.pttpttmd	8.653e+44	10.86	10.86	1.055e+37	5.75e-06
1811	diHPCARP_I.tttppmmd	1.199e+44	9.69	9.69	1.053e+37	5.73e-06
1812	diHPCARP_I.mpttptmd	6.646e+44	10.72	10.72	1.039e+37	5.66e-06
1813	diHPCARP_I.ptmpppmd	7.747e+42	8.06	8.06	1.035e+37	5.64e-06
1814	diHPCARP_I.tmmptmmpd	1.245e+44	9.73	9.73	1.010e+37	5.5e-06
1815	diHPCARP_I.pmpppmtmd	2.078e+43	8.70	8.70	9.507e+36	5.18e-06
1816	diHPCARP_I.mtttppmd	9.821e+43	9.63	9.63	9.477e+36	5.16e-06
1817	diHPCARP_I.mtpmtmmpd	4.098e+43	9.12	9.12	9.322e+36	5.08e-06
1818	diHPCARP_I.mmpmpmpmd	1.242e+43	8.41	8.41	9.281e+36	5.06e-06
1819	diHPCARP_I.ttptpppd	2.518e+44	10.21	10.21	9.258e+36	5.04e-06
1820	diHPCARP_I.mppmmpmd	3.059e+43	8.95	8.95	9.186e+36	5e-06
1821	diHPCARP_I.tpmtppppd	3.125e+44	10.35	10.35	9.007e+36	4.91e-06
1822	diHPCARP_I.ttppptmpd	8.445e+43	9.57	9.57	9.003e+36	4.91e-06
1823	diHPCARP_I.ptmpppmd	3.327e+43	9.02	9.02	8.931e+36	4.87e-06
1824	diHPCARP_I.pmppppttd	1.373e+44	9.87	9.87	8.827e+36	4.81e-06
1825	diHPCARP_I.tttmmmmmd	2.731e+43	8.92	8.92	8.713e+36	4.75e-06
1826	diHPCARP_I.mpmtpmmpd	4.646e+43	9.24	9.24	8.617e+36	4.69e-06
1827	diHPCARP_I.pmtmmmmmd	1.225e+44	9.82	9.82	8.575e+36	4.67e-06
1828	diHPCARP_I.mttmmtmd	5.946e+44	10.78	10.78	8.367e+36	4.56e-06
1829	diHPCARP_I.mmttppmmd	3.860e+44	10.53	10.53	8.304e+36	4.52e-06
1830	diHPCARP_I.mtmtmtmd	7.063e+44	10.89	10.89	8.179e+36	4.46e-06
1831	diHPCARP_I.mpptmptd	2.391e+44	10.25	10.25	8.162e+36	4.45e-06
1832	diHPCARP_I.pmttppmmd	1.478e+44	9.97	9.97	8.027e+36	4.37e-06
1833	diHPCARP_I.mpttmtmd	8.632e+44	11.03	11.03	7.992e+36	4.35e-06
1834	diHPCARP_I.mmtppppmd	4.268e+43	9.24	9.24	7.914e+36	4.31e-06
1835	diHPCARP_I.tmmtpmptd	1.106e+45	11.18	11.18	7.874e+36	4.29e-06
1836	diHPCARP_I.tmmtpppmd	1.439e+43	8.60	8.60	7.763e+36	4.23e-06
1837	diHPCARP_I.ttptpmttd	1.647e+44	10.06	10.06	7.744e+36	4.22e-06
1838	diHPCARP_I.tpptpmpd	1.839e+44	10.13	10.13	7.613e+36	4.15e-06
1839	diHPCARP_I.mttppmmd	5.202e+43	9.39	9.39	7.470e+36	4.07e-06
1840	diHPCARP_I.tppmmptmd	2.629e+44	10.37	10.37	7.329e+36	3.99e-06
1841	diHPCARP_I.ttpmtptd	9.750e+43	9.78	9.78	7.296e+36	3.98e-06
1842	diHPCARP_I.ptmtptpd	5.148e+44	10.78	10.78	7.244e+36	3.95e-06
1843	diHPCARP_I.tmttppmpd	4.167e+44	10.65	10.65	7.230e+36	3.94e-06
1844	diHPCARP_I.tmpptppd	9.056e+43	9.75	9.75	7.187e+36	3.92e-06
1845	diHPCARP_I.mmpmtmtd	1.020e+45	11.19	11.19	7.185e+36	3.91e-06
1846	diHPCARP_I.tpmttptmd	1.018e+45	11.21	11.21	6.951e+36	3.79e-06
1847	diHPCARP_I.mmttppmmd	8.604e+44	11.12	11.12	6.817e+36	3.71e-06
1848	diHPCARP_I.mmpmpptpd	4.794e+43	9.41	9.41	6.694e+36	3.65e-06
1849	diHPCARP_I.mmpppmptd	1.407e+44	10.06	10.06	6.607e+36	3.6e-06

1850	diHPCARP_I_ppmptpmt	2.065e+44	10.30	10.30	6.503e+36	3.54e-06
1851	diHPCARP_I_pttmppmmd	1.537e+43	8.76	8.76	6.408e+36	3.49e-06
1852	diHPCARP_I_pmttmpppd	3.056e+44	10.55	10.55	6.344e+36	3.46e-06
1853	diHPCARP_I_ptmtptppd	5.270e+44	10.90	10.90	6.053e+36	3.3e-06
1854	diHPCARP_I_mppmmntpd	1.327e+44	10.11	10.11	5.689e+36	3.1e-06
1855	diHPCARP_I_pmttmppmd	8.723e+42	8.50	8.50	5.648e+36	3.08e-06
1856	diHPCARP_I_mtpmpptpd	2.937e+43	9.23	9.23	5.546e+36	3.02e-06
1857	diHPCARP_I_pttmppmmd	2.211e+43	9.07	9.07	5.424e+36	2.95e-06
1858	diHPCARP_I_mmppttptd	5.760e+44	11.02	11.02	5.421e+36	2.95e-06
1859	diHPCARP_I_mmmppptpmd	2.714e+43	9.20	9.20	5.399e+36	2.94e-06
1860	diHPCARP_I_mmpmtpppd	7.647e+44	11.19	11.19	5.380e+36	2.93e-06
1861	diHPCARP_I_mppmmntpd	3.039e+43	9.27	9.27	5.362e+36	2.92e-06
1862	diHPCARP_I_mppptpmt	4.390e+43	9.49	9.49	5.347e+36	2.91e-06
1863	diHPCARP_I_mmtmppppd	1.202e+44	10.09	10.09	5.346e+36	2.91e-06
1864	diHPCARP_I_tmmptmtmd	2.240e+44	10.47	10.47	5.315e+36	2.9e-06
1865	diHPCARP_I_tpttpptmd	8.523e+44	11.27	11.27	5.240e+36	2.86e-06
1866	diHPCARP_I_tttmmmpmd	1.356e+44	10.18	10.18	5.222e+36	2.85e-06
1867	diHPCARP_I_mmpmmmpmd	3.159e+43	9.31	9.31	5.220e+36	2.84e-06
1868	diHPCARP_I_tmpmmppmd	2.187e+44	10.46	10.46	5.208e+36	2.84e-06
1869	diHPCARP_I_ttpmpptpd	2.668e+43	9.22	9.22	5.139e+36	2.8e-06
1870	diHPCARP_I_mpmptttd	1.077e+45	11.43	11.43	5.092e+36	2.77e-06
1871	diHPCARP_I_pmtmmmpmd	1.119e+44	10.09	10.09	4.963e+36	2.7e-06
1872	diHPCARP_I_tpmppptpd	1.515e+44	10.28	10.28	4.883e+36	2.66e-06
1873	diHPCARP_I_tppmmppd	1.707e+44	10.36	10.36	4.874e+36	2.66e-06
1874	diHPCARP_I_mtpptmmpd	4.907e+43	9.63	9.63	4.770e+36	2.6e-06
1875	diHPCARP_I_tmmttmptd	6.136e+44	11.13	11.13	4.763e+36	2.6e-06
1876	diHPCARP_I_pmtmpmptd	8.744e+43	9.97	9.97	4.748e+36	2.59e-06
1877	diHPCARP_I_ptptmptd	5.750e+44	11.10	11.10	4.718e+36	2.57e-06
1878	diHPCARP_I_tttppmmd	4.178e+43	9.54	9.54	4.685e+36	2.55e-06
1879	diHPCARP_I_tmpmpmptd	1.036e+44	10.08	10.08	4.678e+36	2.55e-06
1880	diHPCARP_I_pmttppmpd	1.841e+44	10.43	10.43	4.676e+36	2.55e-06
1881	diHPCARP_I_tmtptmtd	2.457e+44	10.60	10.60	4.671e+36	2.54e-06
1882	diHPCARP_I_mmmppppmd	2.339e+43	9.20	9.20	4.668e+36	2.54e-06
1883	diHPCARP_I_ttpmtmmd	5.680e+43	9.75	9.75	4.470e+36	2.44e-06
1884	diHPCARP_I_mmpmppttd	2.030e+44	10.53	10.53	4.328e+36	2.36e-06
1885	diHPCARP_I_ttpppppd	1.736e+44	10.44	10.44	4.328e+36	2.36e-06
1886	diHPCARP_I_pmttppmtd	2.597e+44	10.69	10.69	4.248e+36	2.31e-06
1887	diHPCARP_I_tmmmmptmd	1.372e+44	10.31	10.31	4.203e+36	2.29e-06
1888	diHPCARP_I_ppmmtpttd	2.749e+44	10.75	10.75	4.036e+36	2.2e-06
1889	diHPCARP_I_pmpppptmd	1.150e+44	10.24	10.24	3.975e+36	2.17e-06
1890	diHPCARP_I_ptppmmmd	1.946e+43	9.19	9.19	3.915e+36	2.13e-06
1891	diHPCARP_I_tmpptppmd	2.226e+43	9.27	9.27	3.911e+36	2.13e-06
1892	diHPCARP_I_pmmppptmd	1.335e+44	10.36	10.36	3.817e+36	2.08e-06
1893	diHPCARP_I_tpmptpmt	2.426e+44	10.73	10.73	3.699e+36	2.02e-06
1894	diHPCARP_I_ptmtmtpd	3.547e+44	10.96	10.96	3.682e+36	2.01e-06
1895	diHPCARP_I_tmmptmtd	1.278e+44	10.38	10.38	3.530e+36	1.92e-06
1896	diHPCARP_I_mmmppmptd	9.400e+43	10.19	10.19	3.524e+36	1.92e-06
1897	diHPCARP_I_mppmptmptd	2.553e+43	9.43	9.43	3.458e+36	1.88e-06
1898	diHPCARP_I_tmptmmpmd	7.875e+43	10.12	10.12	3.363e+36	1.83e-06
1899	diHPCARP_I_tmpmmppmd	2.052e+43	9.32	9.32	3.350e+36	1.82e-06
1900	diHPCARP_I_mpmpttmd	4.933e+44	11.22	11.22	3.328e+36	1.81e-06
1901	diHPCARP_I_mpmmtmtd	2.283e+44	10.77	10.77	3.262e+36	1.78e-06
1902	diHPCARP_I_mpttmtmd	8.930e+44	11.60	11.60	3.172e+36	1.73e-06
1903	diHPCARP_I_mpmtpmptd	3.151e+44	10.99	10.99	3.128e+36	1.7e-06
1904	diHPCARP_I_tmttmtmd	3.720e+44	11.09	11.09	3.084e+36	1.68e-06
1905	diHPCARP_I_mpmtpptpd	1.174e+44	10.41	10.41	3.081e+36	1.68e-06
1906	diHPCARP_I_ppmttptd	3.045e+44	10.98	10.98	3.031e+36	1.65e-06
1907	diHPCARP_I_ptptmtpd	5.544e+44	11.34	11.34	3.024e+36	1.65e-06
1908	diHPCARP_I_ppmttpppd	1.654e+44	10.64	10.64	2.959e+36	1.61e-06
1909	diHPCARP_I_mtmmmpppd	1.310e+44	10.54	10.54	2.733e+36	1.49e-06
1910	diHPCARP_I_mttmppppd	8.911e+43	10.34	10.34	2.615e+36	1.42e-06
1911	diHPCARP_I_tttppmtd	6.724e+43	10.18	10.18	2.592e+36	1.41e-06
1912	diHPCARP_I_pppmmppmd	8.061e+43	10.30	10.30	2.536e+36	1.38e-06
1913	diHPCARP_I_mtmppmtd	2.444e+44	10.98	10.98	2.457e+36	1.34e-06
1914	diHPCARP_I_mttttmmd	7.618e+43	10.29	10.29	2.430e+36	1.32e-06
1915	diHPCARP_I_mpmtpptpd	1.481e+45	12.06	12.06	2.429e+36	1.32e-06
1916	diHPCARP_I_mmmtpmptd	3.987e+44	11.29	11.29	2.375e+36	1.29e-06
1917	diHPCARP_I_mmmppmtd	3.790e+43	9.89	9.89	2.372e+36	1.29e-06
1918	diHPCARP_I_pppmtmmd	6.028e+43	10.18	10.18	2.307e+36	1.26e-06
1919	diHPCARP_I_mppmmppmd	3.009e+43	9.79	9.79	2.228e+36	1.21e-06
1920	diHPCARP_I_mmmppppd	8.199e+43	10.40	10.40	2.165e+36	1.18e-06
1921	diHPCARP_I_pmmtpmtd	2.607e+44	11.10	11.10	2.144e+36	1.17e-06

1922	diHPCARP_I.ttpmmmtpd	5.133e+43	10.13	10.13	2.139e+36	1.17e-06
1923	diHPCARP_I.mpmtpmttd	5.928e+44	11.61	11.61	2.082e+36	1.13e-06
1924	diHPCARP_I.mpmmtmmtd	5.642e+43	10.21	10.21	2.068e+36	1.13e-06
1925	diHPCARP_I.tprmmpttd	2.970e+44	11.21	11.21	2.024e+36	1.1e-06
1926	diHPCARP_I.pmtmpmppd	6.333e+43	10.29	10.29	2.019e+36	1.1e-06
1927	diHPCARP_I.mmmptmppd	2.857e+44	11.19	11.19	2.000e+36	1.09e-06
1928	diHPCARP_I.mtppmppd	7.684e+44	11.80	11.80	1.953e+36	1.06e-06
1929	diHPCARP_I.pmmppmppd	1.638e+43	9.51	9.51	1.934e+36	1.05e-06
1930	diHPCARP_I.tpmtppttd	7.434e+44	11.80	11.80	1.889e+36	1.03e-06
1931	diHPCARP_I.mppmttppd	2.105e+44	11.06	11.06	1.847e+36	1.01e-06
1932	diHPCARP_I.tpptppmpd	6.708e+43	10.38	10.38	1.844e+36	1e-06
1933	diHPCARP_I.mmpptpmpd	1.037e+44	10.65	10.65	1.798e+36	9.8e-07
1934	diHPCARP_I.ppmtppttd	5.228e+44	11.63	11.63	1.776e+36	9.67e-07
1935	diHPCARP_I.pmmtpppmd	7.696e+43	10.49	10.49	1.755e+36	9.56e-07
1936	diHPCARP_I.tttmmmpmd	2.436e+44	11.18	11.18	1.755e+36	9.56e-07
1937	diHPCARP_I.pmpmpmmpd	1.200e+43	9.39	9.39	1.738e+36	9.47e-07
1938	diHPCARP_I.tttttmmmd	7.013e+43	10.45	10.45	1.700e+36	9.26e-07
1939	diHPCARP_I.mppnmmtmd	4.825e+43	10.24	10.24	1.662e+36	9.06e-07
1940	diHPCARP_I.mmtmtptmd	8.234e+43	10.57	10.57	1.644e+36	8.96e-07
1941	diHPCARP_I.mtppmpmtd	7.783e+43	10.54	10.54	1.633e+36	8.9e-07
1942	diHPCARP_I.ttpmtmmpd	5.451e+43	10.34	10.34	1.604e+36	8.74e-07
1943	diHPCARP_I.tttmmmpmd	2.906e+44	11.34	11.34	1.603e+36	8.73e-07
1944	diHPCARP_I.tmpmmmpmd	4.600e+43	10.27	10.27	1.512e+36	8.24e-07
1945	diHPCARP_I.mtmtmtpmd	9.820e+43	10.73	10.73	1.502e+36	8.18e-07
1946	diHPCARP_I.pmtmmmpmd	1.362e+44	10.93	10.93	1.477e+36	8.05e-07
1947	diHPCARP_I.pmmptmtd	2.479e+44	11.30	11.30	1.458e+36	7.94e-07
1948	diHPCARP_I.mmmmtmptd	3.963e+44	11.58	11.58	1.448e+36	7.89e-07
1949	diHPCARP_I.pmmtpmtd	3.720e+44	11.55	11.55	1.439e+36	7.84e-07
1950	diHPCARP_I.tmpptmmpd	9.089e+42	9.39	9.39	1.321e+36	7.2e-07
1951	diHPCARP_I.tmttptmd	3.141e+44	11.52	11.52	1.267e+36	6.91e-07
1952	diHPCARP_I.tmmppmptd	1.488e+44	11.08	11.08	1.265e+36	6.89e-07
1953	diHPCARP_I.mmmptmptd	1.197e+44	10.97	10.97	1.223e+36	6.66e-07
1954	diHPCARP_I.mpmttmtd	3.450e+44	11.60	11.60	1.217e+36	6.63e-07
1955	diHPCARP_I.ttpmptmd	6.439e+43	10.62	10.62	1.188e+36	6.47e-07
1956	diHPCARP_I.tttmtpmd	7.768e+43	10.75	10.75	1.140e+36	6.21e-07
1957	diHPCARP_I.ptttmmpmd	2.016e+44	11.37	11.37	1.055e+36	5.75e-07
1958	diHPCARP_I.tpmtppttd	3.788e+44	11.76	11.76	1.033e+36	5.63e-07
1959	diHPCARP_I.ttpmmmmmd	1.707e+43	9.91	9.91	1.032e+36	5.62e-07
1960	diHPCARP_I.tmmptmptd	1.857e+44	11.34	11.34	1.019e+36	5.55e-07
1961	diHPCARP_I.ptptmmmd	6.999e+43	10.78	10.78	9.849e+35	5.37e-07
1962	diHPCARP_I.tttmmpmd	2.539e+43	10.19	10.19	9.595e+35	5.23e-07
1963	diHPCARP_I.tpptmtd	6.115e+43	10.73	10.73	9.351e+35	5.09e-07
1964	diHPCARP_I.tmtmptmd	4.272e+44	11.95	11.95	8.474e+35	4.62e-07
1965	diHPCARP_I.tmmptmppd	1.784e+44	11.43	11.43	8.412e+35	4.58e-07
1966	diHPCARP_I.pmttptmd	5.904e+44	12.15	12.15	8.290e+35	4.52e-07
1967	diHPCARP_I.tttptmppd	5.864e+44	12.16	12.16	8.159e+35	4.45e-07
1968	diHPCARP_I.tmpmpmtd	4.939e+43	10.72	10.72	7.625e+35	4.15e-07
1969	diHPCARP_I.mtppmmpmd	1.263e+43	9.93	9.93	7.412e+35	4.04e-07
1970	diHPCARP_I.mppmmmmmd	4.589e+43	10.75	10.75	6.771e+35	3.69e-07
1971	diHPCARP_I.mtmtmppd	3.126e+44	11.91	11.91	6.613e+35	3.6e-07
1972	diHPCARP_I.ptptmmmd	6.889e+43	11.03	11.03	6.373e+35	3.47e-07
1973	diHPCARP_I.pmtmpmmpd	3.201e+43	10.60	10.60	6.114e+35	3.33e-07
1974	diHPCARP_I.mmmptmmpd	2.251e+44	11.76	11.76	6.097e+35	3.32e-07
1975	diHPCARP_I.tmmtpppmd	7.816e+43	11.13	11.13	6.050e+35	3.3e-07
1976	diHPCARP_I.pttmmmmmd	2.488e+43	10.46	10.46	5.991e+35	3.26e-07
1977	diHPCARP_I.mppmmpppd	8.948e+43	11.24	11.24	5.776e+35	3.15e-07
1978	diHPCARP_I.mtmtmppd	1.562e+44	11.58	11.58	5.680e+35	3.09e-07
1979	diHPCARP_I.ptpmmmmmd	5.574e+43	10.98	10.98	5.625e+35	3.06e-07
1980	diHPCARP_I.tmptmmmpd	9.318e+43	11.29	11.29	5.559e+35	3.03e-07
1981	diHPCARP_I.pmmtpmptd	2.210e+44	11.84	11.84	5.197e+35	2.83e-07
1982	diHPCARP_I.tttmmtpd	9.497e+43	11.35	11.35	5.119e+35	2.79e-07
1983	diHPCARP_I.tppmmtpd	7.214e+43	11.19	11.19	5.066e+35	2.76e-07
1984	diHPCARP_I.ttpmppmmd	1.000e+43	10.03	10.03	4.924e+35	2.68e-07
1985	diHPCARP_I.mtmmmpmd	3.675e+43	10.81	10.81	4.879e+35	2.66e-07
1986	diHPCARP_I.tttmmpmd	5.228e+43	11.03	11.03	4.825e+35	2.63e-07
1987	diHPCARP_I.ttmppptmd	1.047e+44	11.49	11.49	4.464e+35	2.43e-07
1988	diHPCARP_I.mmttppmtd	1.930e+44	11.86	11.86	4.445e+35	2.42e-07
1989	diHPCARP_I.ptmppmtd	1.196e+44	11.59	11.59	4.326e+35	2.36e-07
1990	diHPCARP_I.mmpmtmmpd	6.400e+43	11.23	11.23	4.205e+35	2.29e-07
1991	diHPCARP_I.tpmtpppd	1.637e+44	11.80	11.80	4.167e+35	2.27e-07
1992	diHPCARP_I.mmpptppmd	2.131e+43	10.59	10.59	4.083e+35	2.22e-07
1993	diHPCARP_I.pttppmmmd	7.223e+43	11.32	11.32	4.073e+35	2.22e-07

1994	diHPCARP_I.mttppmmpd	7.103e+43	11.36	11.36	3.757e+35	2.05e-07
1995	diHPCARP_I.mmtppptmd	7.106e+44	12.77	12.77	3.563e+35	1.94e-07
1996	diHPCARP_I.mmpmmptpd	4.677e+43	11.16	11.16	3.439e+35	1.87e-07
1997	diHPCARP_I.mmpmmmpd	4.759e+43	11.21	11.21	3.267e+35	1.78e-07
1998	diHPCARP_I.tppppppd	7.690e+43	11.51	11.51	3.181e+35	1.73e-07
1999	diHPCARP_I.tttptmtmd	5.946e+44	12.74	12.74	3.092e+35	1.68e-07
2000	diHPCARP_I.tmpmpmpmd	3.715e+43	11.16	11.16	2.775e+35	1.51e-07
2001	diHPCARP_I.pmpptmpd	1.345e+44	11.94	11.94	2.696e+35	1.47e-07
2002	diHPCARP_I.tttmpmpd	2.923e+44	12.40	12.40	2.689e+35	1.46e-07
2003	diHPCARP_I.pttmtmpd	2.556e+43	10.96	10.96	2.659e+35	1.45e-07
2004	diHPCARP_I.mppppmpmd	3.525e+43	11.16	11.16	2.596e+35	1.41e-07
2005	diHPCARP_I.tmpptmpd	1.591e+44	12.12	12.12	2.364e+35	1.29e-07
2006	diHPCARP_I.mmpmpptd	2.923e+44	12.49	12.49	2.345e+35	1.28e-07
2007	diHPCARP_I.mttmtmpd	8.373e+44	13.19	13.19	2.051e+35	1.12e-07
2008	diHPCARP_I.mttptmtmd	4.847e+44	12.87	12.87	2.049e+35	1.12e-07
2009	diHPCARP_I.tttmtmpd	3.706e+44	12.71	12.71	2.046e+35	1.11e-07
2010	diHPCARP_I.tttptmpd	9.330e+43	11.89	11.89	2.031e+35	1.11e-07
2011	diHPCARP_I.mmtmtmd	9.935e+44	13.31	13.31	1.985e+35	1.08e-07
2012	diHPCARP_I.mttttmtmd	1.059e+45	13.37	13.37	1.936e+35	1.05e-07
2013	diHPCARP_I.pmpmmmpd	2.695e+43	11.22	11.22	1.808e+35	9.85e-08
2014	diHPCARP_I.pmpmtmpd	4.192e+44	12.91	12.91	1.655e+35	9.02e-08
2015	diHPCARP_I.tmpmmmpd	3.404e+43	11.44	11.44	1.581e+35	8.62e-08
2016	diHPCARP_I.mppmpptd	6.575e+43	11.85	11.85	1.543e+35	8.41e-08
2017	diHPCARP_I.mmpmtmpd	7.686e+43	11.97	11.97	1.457e+35	7.94e-08
2018	diHPCARP_I.mttppmpd	2.108e+44	12.62	12.62	1.355e+35	7.38e-08
2019	diHPCARP_I.mttttmpd	3.760e+44	13.01	13.01	1.256e+35	6.84e-08
2020	diHPCARP_I.mmtmmmpmd	2.075e+44	12.80	12.80	9.780e+34	5.33e-08
2021	diHPCARP_I.pttttmtmd	1.107e+44	12.43	12.43	9.736e+34	5.3e-08
2022	diHPCARP_I.tttttmtmd	5.891e+44	13.45	13.45	9.355e+34	5.1e-08
2023	diHPCARP_I.tttttmpd	6.757e+44	13.59	13.59	8.440e+34	4.6e-08
2024	diHPCARP_I.mtpmpppd	4.007e+43	11.96	11.96	7.774e+34	4.24e-08
2025	diHPCARP_I.tmpptmpd	2.040e+44	13.03	13.03	6.601e+34	3.6e-08
2026	diHPCARP_I.ptppppmd	1.131e+43	11.35	11.35	6.057e+34	3.3e-08
2027	diHPCARP_I.tttppmpd	2.047e+44	13.20	13.20	4.968e+34	2.71e-08
2028	diHPCARP_I.tmpptppmd	2.562e+43	11.97	11.97	4.899e+34	2.67e-08
2029	diHPCARP_I.mtmppmpd	2.058e+44	13.25	13.25	4.583e+34	2.5e-08
2030	diHPCARP_I.tttmtmpd	3.284e+44	13.75	13.75	3.152e+34	1.72e-08
2031	diHPCARP_I.ttmppppd	3.639e+43	12.46	12.46	3.040e+34	1.66e-08
2032	diHPCARP_I.tmpptpmd	1.087e+45	14.51	14.51	2.915e+34	1.59e-08
2033	diHPCARP_I.mmpmmmpmd	2.291e+43	12.23	12.23	2.800e+34	1.53e-08
2034	diHPCARP_I.tmpmmntd	1.474e+44	13.36	13.36	2.722e+34	1.48e-08
2035	diHPCARP_I.tmppppmd	9.075e+44	14.58	14.58	2.157e+34	1.18e-08
2036	diHPCARP_I.mmpmmntd	1.418e+44	13.97	13.97	9.462e+33	5.16e-09
2037	diHPCARP_I.mmpptpmd	8.572e+44	15.17	15.17	7.679e+33	4.18e-09
2038	diHPCARP_I.tmpmmpd	3.317e+43	13.81	13.81	2.880e+33	1.57e-09
2039	diHPCARP_I.tmpmmmpd	3.940e+44	15.33	15.33	2.699e+33	1.47e-09
2040	diHPCARP_I.tmpmmmpmd	9.937e+43	14.72	14.72	1.872e+33	1.02e-09
2041	diHPCARP_I.tmpmmppmd	3.145e+43	14.95	14.95	4.056e+32	2.21e-10
2042	diHPCARP_I.mmpmmmpd	7.054e+43	15.81	15.81	2.133e+32	1.16e-10
2043	diHPCARP_I.mmpmmmpmd	3.101e+43	15.83	15.83	9.044e+31	4.93e-11
2044	diHPCARP_I.pmpppmpd	9.036e+43	17.31	17.31	2.201e+31	1.2e-11
2045	Total				1.835e+44	100

2046
2047
2048
2049 (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)
2050 =====

2051
2052 Population analysis at 300K. Vibrational scaling: 0.971.
2053 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
2054 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
2055 %: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
2057	-----				
2058	diHPCARP_Ib.mmmmpmtmpd	1.894e+43	0.00	0.00	1.894e+43 18.7
2059	diHPCARP_Ib.pmpptmtmd	1.682e+43	0.63	0.63	5.894e+42 5.83
2060	diHPCARP_Ib.pmpptmtmd	2.764e+43	1.09	1.09	4.462e+42 4.41
2061	diHPCARP_Ib.pppmmpmpd	1.103e+43	0.56	0.56	4.323e+42 4.28
2062	diHPCARP_Ib.pmmmpmtmd	8.734e+42	0.45	0.45	4.124e+42 4.08
2063	diHPCARP_Ib.pmpptmpd	3.371e+43	1.26	1.26	4.055e+42 4.01
2064	diHPCARP_Ib.tmmmpptpd	3.941e+43	1.61	1.61	2.645e+42 2.62
2065	diHPCARP_Ib.pppmmpppd	1.322e+43	1.11	1.11	2.041e+42 2.02

2066	diHPCARP_Ib.tmmmpmtmpd	3.327e+43	1.67	1.67	2.026e+42	2
2067	diHPCARP_Ib.mmmmppttmd	5.201e+43	1.95	1.95	1.981e+42	1.96
2068	diHPCARP_Ib.mmmmpptpmd	3.825e+43	1.77	1.77	1.962e+42	1.94
2069	diHPCARP_Ib.ppmnmttmd	5.606e+43	2.00	2.00	1.954e+42	1.93
2070	diHPCARP_Ib.mmpmpmtppd	2.628e+43	1.57	1.57	1.885e+42	1.86
2071	diHPCARP_Ib.mmmmpmtppd	3.404e+43	1.78	1.78	1.731e+42	1.71
2072	diHPCARP_Ib.tmmmpptppd	2.983e+43	1.70	1.70	1.724e+42	1.71
2073	diHPCARP_Ib.mmpmpmtppd	3.281e+43	1.80	1.80	1.611e+42	1.59
2074	diHPCARP_Ib.ppmnmtmmd	2.897e+43	1.75	1.75	1.539e+42	1.52
2075	diHPCARP_Ib.pptpmtppd	3.271e+43	1.86	1.86	1.442e+42	1.43
2076	diHPCARP_Ib.tmmmppttmd	5.319e+43	2.17	2.17	1.406e+42	1.39
2077	diHPCARP_Ib.ppmmpptppd	2.566e+43	1.78	1.78	1.289e+42	1.27
2078	diHPCARP_Ib.tmmmpmtmmd	4.820e+43	2.25	2.25	1.114e+42	1.1
2079	diHPCARP_Ib.mmmmpmtppd	2.772e+43	1.94	1.94	1.074e+42	1.06
2080	diHPCARP_Ib.mmpmpmtmpd	2.139e+43	1.79	1.79	1.054e+42	1.04
2081	diHPCARP_Ib.mttpmtppd	1.682e+44	3.04	3.04	1.020e+42	1.01
2082	diHPCARP_Ib.tmmmpptpmd	3.815e+43	2.30	2.30	8.077e+41	0.799
2083	diHPCARP_Ib.mtpmtppd	1.265e+43	1.64	1.64	8.041e+41	0.795
2084	diHPCARP_Ib.pmpmttmd	7.082e+43	2.68	2.68	7.925e+41	0.784
2085	diHPCARP_Ib.pmmmpmtmpd	4.817e+43	2.46	2.46	7.785e+41	0.77
2086	diHPCARP_Ib.pmtpptmmd	7.326e+43	2.74	2.74	7.445e+41	0.736
2087	diHPCARP_Ib.mtmmpmtppd	2.971e+44	3.58	3.58	7.296e+41	0.722
2088	diHPCARP_Ib.ptppmtpmd	1.281e+43	1.72	1.72	7.156e+41	0.708
2089	diHPCARP_Ib.pppppmpppd	2.060e+44	3.45	3.45	6.268e+41	0.62
2090	diHPCARP_Ib.pppppppppd	1.632e+44	3.35	3.35	5.953e+41	0.589
2091	diHPCARP_Ib.mmpmpmtppd	2.788e+43	2.36	2.36	5.346e+41	0.529
2092	diHPCARP_Ib.mttpptppd	1.052e+44	3.18	3.18	5.061e+41	0.501
2093	diHPCARP_Ib.pmmmpmtppd	3.468e+43	2.52	2.52	5.025e+41	0.497
2094	diHPCARP_Ib.pmmmpmtppd	3.907e+43	2.60	2.60	4.987e+41	0.493
2095	diHPCARP_Ib.pmtpmttmd	1.681e+44	3.47	3.47	4.956e+41	0.49
2096	diHPCARP_Ib.mmpppmmtmd	5.271e+43	2.80	2.80	4.833e+41	0.478
2097	diHPCARP_Ib.pmpmpmtmd	2.658e+43	2.41	2.41	4.628e+41	0.458
2098	diHPCARP_Ib.pmtpmtmmd	9.512e+43	3.24	3.24	4.174e+41	0.413
2099	diHPCARP_Ib.pppppptpd	8.321e+43	3.19	3.19	3.954e+41	0.391
2100	diHPCARP_Ib.pmpppptmd	6.101e+43	3.03	3.03	3.760e+41	0.372
2101	diHPCARP_Ib.pmpmttmd	6.305e+43	3.06	3.06	3.691e+41	0.365
2102	diHPCARP_Ib.pmpmpmpmd	1.712e+43	2.29	2.29	3.657e+41	0.362
2103	diHPCARP_Ib.mmpppmtppd	9.026e+43	3.30	3.30	3.586e+41	0.355
2104	diHPCARP_Ib.ptppmttmd	2.212e+43	2.51	2.51	3.273e+41	0.324
2105	diHPCARP_Ib.mmpmpmtppd	2.405e+43	2.60	2.60	3.076e+41	0.304
2106	diHPCARP_Ib.mtmnmtppd	8.707e+43	3.38	3.38	3.027e+41	0.299
2107	diHPCARP_Ib.mmpppptppd	5.544e+43	3.11	3.11	3.013e+41	0.298
2108	diHPCARP_Ib.pptmpptppd	1.482e+44	3.76	3.76	2.699e+41	0.267
2109	diHPCARP_Ib.tmmmmmtmd	8.440e+43	3.43	3.43	2.664e+41	0.264
2110	diHPCARP_Ib.pmmmmmtppd	5.889e+43	3.22	3.22	2.664e+41	0.263
2111	diHPCARP_Ib.mmtpmtmpd	1.359e+44	3.72	3.72	2.636e+41	0.261
2112	diHPCARP_Ib.pptpmtppd	6.675e+43	3.35	3.35	2.417e+41	0.239
2113	diHPCARP_Ib.pmpmpmtppd	1.907e+43	2.61	2.61	2.394e+41	0.237
2114	diHPCARP_Ib.mmtpptmpd	1.215e+44	3.72	3.72	2.386e+41	0.236
2115	diHPCARP_Ib.pptpppppd	1.467e+44	3.87	3.87	2.239e+41	0.222
2116	diHPCARP_Ib.tpmmpmmd	1.145e+43	2.35	2.35	2.238e+41	0.221
2117	diHPCARP_Ib.mtmppmtppd	1.332e+44	3.82	3.82	2.192e+41	0.217
2118	diHPCARP_Ib.pptppppmd	2.142e+44	4.11	4.11	2.187e+41	0.216
2119	diHPCARP_Ib.pmtpmtppd	5.991e+43	3.35	3.35	2.172e+41	0.215
2120	diHPCARP_Ib.mtppmpppd	1.319e+43	2.47	2.47	2.099e+41	0.208
2121	diHPCARP_Ib.tmtpmtppd	1.064e+44	3.72	3.72	2.061e+41	0.204
2122	diHPCARP_Ib.pptpmpppd	1.584e+44	3.98	3.98	1.997e+41	0.198
2123	diHPCARP_Ib.pmtpmpppd	7.926e+43	3.58	3.58	1.944e+41	0.192
2124	diHPCARP_Ib.pmtmmtmmd	5.070e+43	3.32	3.32	1.936e+41	0.191
2125	diHPCARP_Ib.mmmmpmtmmd	3.655e+43	3.14	3.14	1.892e+41	0.187
2126	diHPCARP_Ib.mttpmtmpd	1.042e+44	3.78	3.78	1.831e+41	0.181
2127	diHPCARP_Ib.pmmmmmpppd	5.206e+43	3.38	3.38	1.794e+41	0.177
2128	diHPCARP_Ib.tmtpmttmd	3.315e+43	3.13	3.13	1.743e+41	0.172
2129	diHPCARP_Ib.pmpmpmmd	2.275e+43	2.93	2.93	1.664e+41	0.165
2130	diHPCARP_Ib.tmtpmttmd	2.607e+44	4.39	4.39	1.650e+41	0.163
2131	diHPCARP_Ib.pptppppmmd	4.690e+43	3.37	3.37	1.640e+41	0.162
2132	diHPCARP_Ib.pptpmtmmd	4.529e+43	3.37	3.37	1.586e+41	0.157
2133	diHPCARP_Ib.mtpmtppd	1.331e+44	4.02	4.02	1.576e+41	0.156
2134	diHPCARP_Ib.tmmmmmpmd	8.744e+43	3.78	3.78	1.544e+41	0.153
2135	diHPCARP_Ib.pppmpmtppd	8.309e+43	3.75	3.75	1.540e+41	0.152
2136	diHPCARP_Ib.mtmnmtmpd	1.687e+44	4.20	4.20	1.482e+41	0.147
2137	diHPCARP_Ib.mmpmpmtppd	1.387e+43	2.73	2.73	1.434e+41	0.142

2138	diHPCARP_Ib.mmptpttpd	2.134e+44	4.37	4.37	1.408e+41	0.139
2139	diHPCARP_Ib.pmppttpmd	7.998e+43	3.78	3.78	1.400e+41	0.138
2140	diHPCARP_Ib.ppmtpttmd	6.666e+43	3.69	3.69	1.371e+41	0.136
2141	diHPCARP_Ib.pttpmtmpd	5.393e+44	4.94	4.94	1.370e+41	0.136
2142	diHPCARP_Ib.mttpttpmd	7.432e+43	3.76	3.76	1.363e+41	0.135
2143	diHPCARP_Ib.tmmmtmpd	2.527e+44	4.50	4.50	1.330e+41	0.132
2144	diHPCARP_Ib.pppmppppd	1.400e+43	2.78	2.78	1.330e+41	0.132
2145	diHPCARP_Ib.tpmmpmpmd	1.452e+43	2.82	2.82	1.281e+41	0.127
2146	diHPCARP_Ib.mmptmttpd	1.110e+44	4.05	4.05	1.251e+41	0.124
2147	diHPCARP_Ib.mmtptmtmd	5.106e+43	3.59	3.59	1.234e+41	0.122
2148	diHPCARP_Ib.ppmtmmpd	6.522e+43	3.75	3.75	1.201e+41	0.119
2149	diHPCARP_Ib.tpmmpmtmd	2.754e+43	3.24	3.24	1.194e+41	0.118
2150	diHPCARP_Ib.pmtmptmmd	3.268e+43	3.36	3.36	1.165e+41	0.115
2151	diHPCARP_Ib.mttmmtppd	1.153e+44	4.15	4.15	1.090e+41	0.108
2152	diHPCARP_Ib.pptmmpppd	2.779e+44	4.68	4.68	1.075e+41	0.106
2153	diHPCARP_Ib.tmmmttppd	2.332e+44	4.58	4.58	1.070e+41	0.106
2154	diHPCARP_Ib.mmtptmtpd	4.901e+43	3.66	3.66	1.064e+41	0.105
2155	diHPCARP_Ib.pmppttpmd	8.126e+43	3.96	3.96	1.064e+41	0.105
2156	diHPCARP_Ib.ppmtptmmd	3.708e+43	3.49	3.49	1.058e+41	0.105
2157	diHPCARP_Ib.mmpppmpd	8.858e+43	4.04	4.04	1.005e+41	0.0994
2158	diHPCARP_Ib.tptpmmtmd	4.007e+43	3.58	3.58	9.962e+40	0.0985
2159	diHPCARP_Ib.pptpmmpd	1.253e+44	4.28	4.28	9.616e+40	0.0951
2160	diHPCARP_Ib.pptmppppd	4.624e+43	3.69	3.69	9.470e+40	0.0937
2161	diHPCARP_Ib.tmmmmmmmd	8.746e+43	4.08	4.08	9.396e+40	0.0929
2162	diHPCARP_Ib.pptppptmd	6.353e+43	3.90	3.90	9.157e+40	0.0906
2163	diHPCARP_Ib.pptmmpmpd	2.129e+44	4.63	4.63	9.002e+40	0.089
2164	diHPCARP_Ib.pmptmtmmd	4.334e+43	3.69	3.69	8.885e+40	0.0879
2165	diHPCARP_Ib.mttptmtpd	6.410e+43	3.94	3.94	8.683e+40	0.0859
2166	diHPCARP_Ib.pmmmmmpd	3.987e+43	3.66	3.66	8.588e+40	0.0849
2167	diHPCARP_Ib.mmpptppd	4.275e+43	3.71	3.71	8.452e+40	0.0836
2168	diHPCARP_Ib.ppptmpppd	2.904e+44	4.87	4.87	8.261e+40	0.0817
2169	diHPCARP_Ib.ptppmttpd	2.665e+43	3.45	3.45	8.225e+40	0.0814
2170	diHPCARP_Ib.pppmpttmd	6.811e+43	4.01	4.01	8.118e+40	0.0803
2171	diHPCARP_Ib.tmtpmmpmd	1.205e+44	4.36	4.36	8.089e+40	0.08
2172	diHPCARP_Ib.ttpmpttpd	2.868e+43	3.50	3.50	8.062e+40	0.0797
2173	diHPCARP_Ib.ppmmtmtpd	4.185e+43	3.73	3.73	8.034e+40	0.0795
2174	diHPCARP_Ib.mtppppppd	1.300e+43	3.06	3.06	7.644e+40	0.0756
2175	diHPCARP_Ib.tpmppmtmd	2.405e+43	3.43	3.43	7.619e+40	0.0754
2176	diHPCARP_Ib.tmtppmpmd	1.353e+44	4.47	4.47	7.522e+40	0.0744
2177	diHPCARP_Ib.ttptmtmd	3.478e+43	3.66	3.66	7.520e+40	0.0744
2178	diHPCARP_Ib.mmmmtmtpd	1.691e+43	3.24	3.24	7.424e+40	0.0734
2179	diHPCARP_Ib.pmtpmmtmd	2.636e+43	3.52	3.52	7.177e+40	0.071
2180	diHPCARP_Ib.tmppttpd	5.807e+43	3.99	3.99	7.177e+40	0.071
2181	diHPCARP_Ib.pmpmttmd	3.233e+43	3.68	3.68	6.704e+40	0.0663
2182	diHPCARP_Ib.tmmmtmpd	1.518e+44	4.61	4.61	6.693e+40	0.0662
2183	diHPCARP_Ib.mmtmptmpd	6.789e+43	4.15	4.15	6.419e+40	0.0635
2184	diHPCARP_Ib.tttpttpd	3.445e+43	3.75	3.75	6.356e+40	0.0629
2185	diHPCARP_Ib.tmpptppd	8.139e+43	4.28	4.28	6.211e+40	0.0614
2186	diHPCARP_Ib.pttpmtmd	4.031e+43	3.87	3.87	6.093e+40	0.0603
2187	diHPCARP_Ib.mmtmmtmpd	1.567e+44	4.68	4.68	6.064e+40	0.06
2188	diHPCARP_Ib.pppmmmpmd	8.279e+43	4.32	4.32	5.923e+40	0.0586
2189	diHPCARP_Ib.mtttptppd	1.344e+44	4.61	4.61	5.889e+40	0.0583
2190	diHPCARP_Ib.tpmppmmmd	2.147e+43	3.53	3.53	5.779e+40	0.0572
2191	diHPCARP_Ib.ppmmttmd	8.884e+43	4.38	4.38	5.736e+40	0.0567
2192	diHPCARP_Ib.pptpmpmpd	6.551e+43	4.21	4.21	5.601e+40	0.0554
2193	diHPCARP_Ib.pptmptpd	2.113e+44	4.91	4.91	5.571e+40	0.0551
2194	diHPCARP_Ib.ptmmmtmpd	1.701e+44	4.78	4.78	5.564e+40	0.055
2195	diHPCARP_Ib.mmmmtmpd	1.196e+44	4.58	4.58	5.477e+40	0.0542
2196	diHPCARP_Ib.ttpmttmd	5.406e+43	4.11	4.11	5.454e+40	0.0539
2197	diHPCARP_Ib.tmmmpmpmd	3.320e+43	3.83	3.83	5.342e+40	0.0528
2198	diHPCARP_Ib.tmmmttmd	3.263e+44	5.20	5.20	5.319e+40	0.0526
2199	diHPCARP_Ib.ptmmmttmd	1.649e+44	4.80	4.80	5.269e+40	0.0521
2200	diHPCARP_Ib.pppppmpmd	3.994e+43	3.96	3.96	5.237e+40	0.0518
2201	diHPCARP_Ib.mmmmttmd	1.103e+44	4.57	4.57	5.149e+40	0.0509
2202	diHPCARP_Ib.mttmptppd	5.005e+43	4.11	4.11	5.094e+40	0.0504
2203	diHPCARP_Ib.pmttptmmd	8.972e+43	4.47	4.47	5.009e+40	0.0495
2204	diHPCARP_Ib.pppmmppmd	3.874e+43	3.98	3.98	4.886e+40	0.0483
2205	diHPCARP_Ib.pmtppmpd	1.154e+44	4.63	4.63	4.875e+40	0.0482
2206	diHPCARP_Ib.pptppmpmd	9.933e+43	4.54	4.54	4.872e+40	0.0482
2207	diHPCARP_Ib.tmmmtmmd	1.357e+44	4.74	4.74	4.769e+40	0.0472
2208	diHPCARP_Ib.mtmmtmmd	1.571e+44	4.83	4.83	4.731e+40	0.0468
2209	diHPCARP_Ib.pmttmtmmd	6.617e+43	4.33	4.33	4.611e+40	0.0456

2210	diHPCARP_Ib.pppppttpd	1.558e+44	4.85	4.85	4.598e+40	0.0455
2211	diHPCARP_Ib.tmmppmtmd	2.727e+43	3.81	3.81	4.554e+40	0.045
2212	diHPCARP_Ib.pttpptpmd	2.795e+44	5.21	5.21	4.457e+40	0.0441
2213	diHPCARP_Ib.tmtptmtpd	4.632e+44	5.52	5.52	4.445e+40	0.044
2214	diHPCARP_Ib.mtpmptmpd	2.252e+43	3.72	3.72	4.374e+40	0.0433
2215	diHPCARP_Ib.pmmptmmd	3.136e+43	3.93	3.93	4.300e+40	0.0425
2216	diHPCARP_Ib.tmmppmmpd	2.036e+43	3.68	3.68	4.267e+40	0.0422
2217	diHPCARP_Ib.mmpmtmtpd	7.538e+43	4.46	4.46	4.238e+40	0.0419
2218	diHPCARP_Ib.pppmptpmd	2.413e+43	3.79	3.79	4.216e+40	0.0417
2219	diHPCARP_Ib.pptpmtmd	9.891e+43	4.64	4.64	4.131e+40	0.0409
2220	diHPCARP_Ib.ppmmtmmd	4.031e+43	4.11	4.11	4.091e+40	0.0405
2221	diHPCARP_Ib.pmtptmtpd	3.979e+44	5.48	5.48	4.079e+40	0.0404
2222	diHPCARP_Ib.ttpmpttpd	4.075e+43	4.13	4.13	4.006e+40	0.0396
2223	diHPCARP_Ib.pptpmmmpd	7.970e+43	4.53	4.53	3.985e+40	0.0394
2224	diHPCARP_Ib.mmpptpmpd	1.161e+44	4.76	4.76	3.936e+40	0.0389
2225	diHPCARP_Ib.pppptpppd	8.549e+43	4.60	4.60	3.824e+40	0.0378
2226	diHPCARP_Ib.pptppptpd	1.669e+44	5.00	5.00	3.824e+40	0.0378
2227	diHPCARP_Ib.tmtptmtpd	1.310e+45	6.25	6.25	3.669e+40	0.0363
2228	diHPCARP_Ib.ppptpmtpd	1.323e+44	4.89	4.89	3.638e+40	0.036
2229	diHPCARP_Ib.mtpmpttpd	2.913e+43	3.99	3.99	3.596e+40	0.0356
2230	diHPCARP_Ib.ptppmpmpd	1.606e+43	3.64	3.64	3.596e+40	0.0356
2231	diHPCARP_Ib.mttmmtpd	6.332e+43	4.46	4.46	3.595e+40	0.0356
2232	diHPCARP_Ib.ppttmpppd	2.095e+44	5.17	5.17	3.582e+40	0.0354
2233	diHPCARP_Ib.pmtppmpd	1.222e+44	4.85	4.85	3.555e+40	0.0352
2234	diHPCARP_Ib.ptmmmtmmd	1.006e+44	4.75	4.75	3.489e+40	0.0345
2235	diHPCARP_Ib.pppmpttpd	1.535e+44	5.00	5.00	3.479e+40	0.0344
2236	diHPCARP_Ib.pppmmmpmd	1.047e+44	4.78	4.78	3.459e+40	0.0342
2237	diHPCARP_Ib.ptpppptpd	3.462e+43	4.13	4.13	3.420e+40	0.0338
2238	diHPCARP_Ib.mmpmpptpd	1.293e+43	3.54	3.54	3.399e+40	0.0336
2239	diHPCARP_Ib.pppmpmpd	1.581e+43	3.66	3.66	3.385e+40	0.0335
2240	diHPCARP_Ib.ttpppmtmd	3.667e+43	4.17	4.17	3.351e+40	0.0331
2241	diHPCARP_Ib.mtttmtppd	1.677e+44	5.09	5.09	3.281e+40	0.0325
2242	diHPCARP_Ib.pppmmpppd	1.814e+44	5.14	5.14	3.266e+40	0.0323
2243	diHPCARP_Ib.tppmmpmpd	1.902e+43	3.80	3.80	3.241e+40	0.0321
2244	diHPCARP_Ib.mmpmppppd	1.475e+43	3.66	3.66	3.194e+40	0.0316
2245	diHPCARP_Ib.pppmptmmd	2.194e+43	3.90	3.90	3.155e+40	0.0312
2246	diHPCARP_Ib.mmtptmtpd	2.641e+44	5.39	5.39	3.139e+40	0.0311
2247	diHPCARP_Ib.ttpmmpmmd	1.615e+43	3.73	3.73	3.097e+40	0.0306
2248	diHPCARP_Ib.mmpmptmtpd	3.875e+43	4.26	4.26	3.060e+40	0.0303
2249	diHPCARP_Ib.mttptmtpd	2.231e+44	5.30	5.30	3.059e+40	0.0303
2250	diHPCARP_Ib.tptpmmmpd	2.946e+44	5.47	5.47	3.045e+40	0.0301
2251	diHPCARP_Ib.tmmmmmtmd	2.185e+44	5.30	5.30	3.007e+40	0.0297
2252	diHPCARP_Ib.mmttmtmtpd	1.545e+44	5.10	5.10	2.994e+40	0.0296
2253	diHPCARP_Ib.pppppmmpd	2.494e+43	4.01	4.01	2.994e+40	0.0296
2254	diHPCARP_Ib.pptmpmpd	6.175e+43	4.56	4.56	2.949e+40	0.0292
2255	diHPCARP_Ib.tmtptmtpd	3.511e+44	5.61	5.61	2.853e+40	0.0282
2256	diHPCARP_Ib.ppttpmpd	2.412e+44	5.40	5.40	2.794e+40	0.0276
2257	diHPCARP_Ib.mttptmtpd	4.058e+43	4.35	4.35	2.759e+40	0.0273
2258	diHPCARP_Ib.pmtptmtpd	1.814e+44	5.28	5.28	2.599e+40	0.0257
2259	diHPCARP_Ib.pppmmpppd	1.258e+44	5.06	5.06	2.579e+40	0.0255
2260	diHPCARP_Ib.mmtptmtpd	1.211e+44	5.04	5.04	2.573e+40	0.0255
2261	diHPCARP_Ib.tptpmpmpd	1.619e+44	5.23	5.23	2.488e+40	0.0246
2262	diHPCARP_Ib.pppmmmtmd	1.077e+44	5.00	5.00	2.444e+40	0.0242
2263	diHPCARP_Ib.tmtptmtpd	3.758e+44	5.75	5.75	2.428e+40	0.024
2264	diHPCARP_Ib.pptppppd	1.766e+44	5.30	5.30	2.425e+40	0.024
2265	diHPCARP_Ib.pmpptmtpd	8.055e+43	4.87	4.87	2.286e+40	0.0226
2266	diHPCARP_Ib.mttmptmpd	5.663e+43	4.67	4.67	2.248e+40	0.0222
2267	diHPCARP_Ib.tmpmpttpd	4.910e+43	4.58	4.58	2.245e+40	0.0222
2268	diHPCARP_Ib.tmmmmtpmd	2.590e+44	5.58	5.58	2.224e+40	0.022
2269	diHPCARP_Ib.pmtmpttpd	1.827e+44	5.38	5.38	2.188e+40	0.0216
2270	diHPCARP_Ib.tptppmmmd	1.787e+44	5.38	5.38	2.143e+40	0.0212
2271	diHPCARP_Ib.pppmmmtmd	1.109e+44	5.10	5.10	2.141e+40	0.0212
2272	diHPCARP_Ib.pptmpttpd	2.176e+44	5.51	5.51	2.091e+40	0.0207
2273	diHPCARP_Ib.pppmmpmmd	6.766e+43	4.83	4.83	2.065e+40	0.0204
2274	diHPCARP_Ib.tptmpttpd	8.685e+43	4.98	4.98	2.055e+40	0.0203
2275	diHPCARP_Ib.tptpmmmpd	2.644e+44	5.68	5.68	1.932e+40	0.0191
2276	diHPCARP_Ib.mmpmmmtmd	8.548e+43	5.01	5.01	1.920e+40	0.019
2277	diHPCARP_Ib.pmtptmtpd	2.295e+44	5.61	5.61	1.888e+40	0.0187
2278	diHPCARP_Ib.tttptmmd	1.255e+44	5.25	5.25	1.867e+40	0.0185
2279	diHPCARP_Ib.pptmtpmd	1.240e+44	5.25	5.25	1.857e+40	0.0184
2280	diHPCARP_Ib.pmtptpmpd	1.733e+44	5.45	5.45	1.848e+40	0.0183
2281	diHPCARP_Ib.tmtmpttpd	5.015e+44	6.09	6.09	1.845e+40	0.0182

2282	diHPCARP_Ib.ptptmtpd	6.012e+43	4.82	4.82	1.841e+40	0.0182
2283	diHPCARP_Ib.mtppmtmd	4.270e+43	4.62	4.62	1.839e+40	0.0182
2284	diHPCARP_Ib.pptppmpd	1.647e+44	5.43	5.43	1.809e+40	0.0179
2285	diHPCARP_Ib.tmtppppmd	5.595e+43	4.80	4.80	1.796e+40	0.0178
2286	diHPCARP_Ib.tmtppmtpd	3.888e+44	5.95	5.95	1.793e+40	0.0177
2287	diHPCARP_Ib.tpppmmtmd	2.320e+44	5.65	5.65	1.787e+40	0.0177
2288	diHPCARP_Ib.tmtppptpd	3.865e+44	5.95	5.95	1.786e+40	0.0177
2289	diHPCARP_Ib.tptmpmtmd	1.257e+44	5.29	5.29	1.768e+40	0.0175
2290	diHPCARP_Ib.tpmmpmtpd	3.549e+43	4.54	4.54	1.750e+40	0.0173
2291	diHPCARP_Ib.tmtppmmmd	9.703e+43	5.15	5.15	1.732e+40	0.0171
2292	diHPCARP_Ib.pppmpttpd	6.688e+43	4.93	4.93	1.715e+40	0.017
2293	diHPCARP_Ib.tppppmtmd	1.268e+44	5.31	5.31	1.710e+40	0.0169
2294	diHPCARP_Ib.tptppmpmd	1.289e+44	5.33	5.33	1.697e+40	0.0168
2295	diHPCARP_Ib.mtmtmtmpd	1.340e+43	3.98	3.98	1.696e+40	0.0168
2296	diHPCARP_Ib.mtttptmpd	9.504e+43	5.15	5.15	1.696e+40	0.0168
2297	diHPCARP_Ib.tmmmpmmd	2.404e+43	4.34	4.34	1.647e+40	0.0163
2298	diHPCARP_Ib.pppmptpd	7.846e+43	5.06	5.06	1.629e+40	0.0161
2299	diHPCARP_Ib.pptppmtpd	1.566e+45	6.84	6.84	1.626e+40	0.0161
2300	diHPCARP_Ib.mtmmmttd	2.216e+44	5.68	5.68	1.625e+40	0.0161
2301	diHPCARP_Ib.pptpmtmd	1.734e+44	5.53	5.53	1.616e+40	0.016
2302	diHPCARP_Ib.tptpmtmd	1.097e+44	5.26	5.26	1.613e+40	0.016
2303	diHPCARP_Ib.tmtpppmmd	7.765e+43	5.06	5.06	1.608e+40	0.0159
2304	diHPCARP_Ib.ppptmttd	4.511e+44	6.11	6.11	1.591e+40	0.0157
2305	diHPCARP_Ib.mtppmtmd	2.876e+43	4.47	4.47	1.589e+40	0.0157
2306	diHPCARP_Ib.tmmmttd	1.098e+44	5.28	5.28	1.575e+40	0.0156
2307	diHPCARP_Ib.mtppmtmd	1.475e+43	4.09	4.09	1.546e+40	0.0153
2308	diHPCARP_Ib.tmmmttd	1.347e+44	5.42	5.42	1.515e+40	0.015
2309	diHPCARP_Ib.pppmpttd	2.418e+44	5.77	5.77	1.514e+40	0.015
2310	diHPCARP_Ib.tttpmtmd	9.597e+43	5.22	5.22	1.513e+40	0.015
2311	diHPCARP_Ib.tmmppmmd	2.041e+43	4.31	4.31	1.491e+40	0.0147
2312	diHPCARP_Ib.mmtppmtpd	2.447e+44	5.79	5.79	1.489e+40	0.0147
2313	diHPCARP_Ib.tttppmtpd	1.544e+44	5.51	5.51	1.489e+40	0.0147
2314	diHPCARP_Ib.pmtppmmpd	1.038e+44	5.29	5.29	1.455e+40	0.0144
2315	diHPCARP_Ib.pttppmtpd	2.167e+44	5.75	5.75	1.397e+40	0.0138
2316	diHPCARP_Ib.pmtppmtpd	1.639e+44	5.59	5.59	1.384e+40	0.0137
2317	diHPCARP_Ib.tppmptpd	3.108e+43	4.62	4.62	1.330e+40	0.0132
2318	diHPCARP_Ib.pptppmtpd	9.083e+43	5.27	5.27	1.318e+40	0.013
2319	diHPCARP_Ib.tppmmtmd	4.510e+43	4.85	4.85	1.316e+40	0.013
2320	diHPCARP_Ib.pmtppmmpd	9.472e+43	5.30	5.30	1.303e+40	0.0129
2321	diHPCARP_Ib.mmtppmtpd	3.683e+43	4.74	4.74	1.302e+40	0.0129
2322	diHPCARP_Ib.tppmpttd	6.018e+43	5.03	5.03	1.295e+40	0.0128
2323	diHPCARP_Ib.mtppmtpd	1.367e+44	5.53	5.53	1.273e+40	0.0126
2324	diHPCARP_Ib.pptpmttd	7.411e+43	5.17	5.17	1.273e+40	0.0126
2325	diHPCARP_Ib.pptmtpmpd	1.444e+44	5.57	5.57	1.271e+40	0.0126
2326	diHPCARP_Ib.pmmmtmtpd	2.647e+43	4.56	4.56	1.259e+40	0.0125
2327	diHPCARP_Ib.tmtppmtpd	1.055e+44	5.39	5.39	1.241e+40	0.0123
2328	diHPCARP_Ib.pppmmttd	5.198e+43	4.98	4.98	1.230e+40	0.0122
2329	diHPCARP_Ib.mtppmtpd	1.444e+44	5.59	5.59	1.223e+40	0.0121
2330	diHPCARP_Ib.ttpmmtmd	6.861e+43	5.15	5.15	1.213e+40	0.012
2331	diHPCARP_Ib.mtmtmtpd	1.054e+44	5.43	5.43	1.164e+40	0.0115
2332	diHPCARP_Ib.pmtppmtpd	1.317e+44	5.57	5.57	1.156e+40	0.0114
2333	diHPCARP_Ib.pmpmtpmd	7.308e+43	5.24	5.24	1.122e+40	0.0111
2334	diHPCARP_Ib.ptppmtpd	6.697e+43	5.20	5.20	1.099e+40	0.0109
2335	diHPCARP_Ib.tppmmtmd	2.347e+43	4.58	4.58	1.079e+40	0.0107
2336	diHPCARP_Ib.ppppmttd	5.181e+43	5.06	5.06	1.072e+40	0.0106
2337	diHPCARP_Ib.mmtppmtpd	2.143e+44	5.90	5.90	1.071e+40	0.0106
2338	diHPCARP_Ib.ptppmtpd	3.438e+43	4.82	4.82	1.057e+40	0.0105
2339	diHPCARP_Ib.mtppmtpd	2.595e+43	4.66	4.66	1.045e+40	0.0103
2340	diHPCARP_Ib.mmtppmtpd	7.580e+43	5.32	5.32	1.013e+40	0.01
2341	diHPCARP_Ib.mmtppmtpd	2.563e+43	4.68	4.68	9.994e+39	0.00989
2342	diHPCARP_Ib.tppmtpmd	7.182e+43	5.31	5.31	9.803e+39	0.0097
2343	diHPCARP_Ib.mppmpttd	2.811e+43	4.76	4.76	9.647e+39	0.00954
2344	diHPCARP_Ib.ppppmmpd	3.913e+44	6.33	6.33	9.532e+39	0.00943
2345	diHPCARP_Ib.tppppppmd	2.061e+44	5.95	5.95	9.473e+39	0.00937
2346	diHPCARP_Ib.tppmtpmd	5.541e+43	5.18	5.18	9.380e+39	0.00928
2347	diHPCARP_Ib.mtppmtpd	1.136e+44	5.61	5.61	9.272e+39	0.00917
2348	diHPCARP_Ib.tttppmtpd	2.114e+43	4.62	4.62	9.132e+39	0.00903
2349	diHPCARP_Ib.mttmtpmd	1.111e+44	5.61	5.61	9.069e+39	0.00897
2350	diHPCARP_Ib.tmmmmmmmd	5.897e+43	5.24	5.24	9.050e+39	0.00895
2351	diHPCARP_Ib.tmmppmtpd	5.343e+43	5.18	5.18	8.984e+39	0.00889
2352	diHPCARP_Ib.tppmtpd	4.772e+43	5.12	5.12	8.866e+39	0.00877
2353	diHPCARP_Ib.mtmtppmtpd	9.707e+43	5.56	5.56	8.677e+39	0.00858

2354	diHPCARP_Ib.mmpptmpd	2.141e+43	4.66	4.66	8.649e+39	0.00855
2355	diHPCARP_Ib.ptmmmpmpd	7.055e+43	5.37	5.37	8.641e+39	0.00855
2356	diHPCARP_Ib.mmmppmpd	1.386e+43	4.40	4.40	8.582e+39	0.00849
2357	diHPCARP_Ib.tmtmmtmpd	1.110e+45	7.02	7.02	8.528e+39	0.00844
2358	diHPCARP_Ib.pmntmmpd	1.330e+43	4.43	4.43	7.888e+39	0.0078
2359	diHPCARP_Ib.ptptmpmpd	4.046e+43	5.09	5.09	7.881e+39	0.0078
2360	diHPCARP_Ib.ttpmmtmd	4.071e+43	5.11	5.11	7.707e+39	0.00762
2361	diHPCARP_Ib.mmtmpttmd	1.566e+44	5.92	5.92	7.682e+39	0.0076
2362	diHPCARP_Ib.tptpmtmd	2.759e+44	6.27	6.27	7.448e+39	0.00737
2363	diHPCARP_Ib.mtppmtppd	4.634e+43	5.22	5.22	7.354e+39	0.00727
2364	diHPCARP_Ib.mmtppptpd	1.840e+44	6.04	6.04	7.342e+39	0.00726
2365	diHPCARP_Ib.ttpmptppd	8.535e+43	5.58	5.58	7.318e+39	0.00724
2366	diHPCARP_Ib.pttpmtpd	1.781e+43	4.66	4.66	7.209e+39	0.00713
2367	diHPCARP_Ib.tpmptmmd	4.951e+43	5.27	5.27	7.179e+39	0.0071
2368	diHPCARP_Ib.tptpmtppd	3.458e+44	6.44	6.44	7.092e+39	0.00701
2369	diHPCARP_Ib.pmtmpmpd	1.056e+44	5.73	5.73	7.084e+39	0.00701
2370	diHPCARP_Ib.mtmmttmd	1.421e+44	5.92	5.92	6.972e+39	0.0069
2371	diHPCARP_Ib.tptmmmmmd	1.608e+44	5.99	5.99	6.941e+39	0.00687
2372	diHPCARP_Ib.ptppmpmpd	1.324e+43	4.51	4.51	6.895e+39	0.00682
2373	diHPCARP_Ib.tppmptpd	2.733e+43	4.95	4.95	6.756e+39	0.00668
2374	diHPCARP_Ib.tptpmtmd	4.146e+44	6.58	6.58	6.648e+39	0.00658
2375	diHPCARP_Ib.mmtmptppd	1.701e+44	6.06	6.06	6.600e+39	0.00653
2376	diHPCARP_Ib.tpmptpmd	4.249e+43	5.23	5.23	6.567e+39	0.0065
2377	diHPCARP_Ib.mmtmtmpmd	3.472e+43	5.12	5.12	6.520e+39	0.00645
2378	diHPCARP_Ib.tmmtmtmpd	3.058e+43	5.04	5.04	6.505e+39	0.00643
2379	diHPCARP_Ib.tppmpmpd	5.709e+43	5.41	5.41	6.495e+39	0.00642
2380	diHPCARP_Ib.mpmmpmpd	1.751e+43	4.72	4.72	6.430e+39	0.00636
2381	diHPCARP_Ib.mmmpttmd	8.567e+43	5.66	5.66	6.401e+39	0.00633
2382	diHPCARP_Ib.tmpmpmpd	2.444e+43	4.93	4.93	6.254e+39	0.00619
2383	diHPCARP_Ib.pptpmtmpd	1.170e+44	5.86	5.86	6.251e+39	0.00618
2384	diHPCARP_Ib.tmpmpmpd	2.275e+43	4.90	4.90	6.178e+39	0.00611
2385	diHPCARP_Ib.tmmppmmpd	4.799e+43	5.34	5.34	6.141e+39	0.00607
2386	diHPCARP_Ib.pmpppmmd	3.098e+43	5.09	5.09	6.024e+39	0.00596
2387	diHPCARP_Ib.tmtmptppd	2.879e+44	6.43	6.43	5.991e+39	0.00593
2388	diHPCARP_Ib.mmmmttmd	1.061e+44	5.84	5.84	5.885e+39	0.00582
2389	diHPCARP_Ib.ttpmtmpd	6.438e+43	5.55	5.55	5.783e+39	0.00572
2390	diHPCARP_Ib.tmtmpmpmd	7.900e+43	5.68	5.68	5.738e+39	0.00568
2391	diHPCARP_Ib.tptmppmpd	8.380e+43	5.72	5.72	5.669e+39	0.00561
2392	diHPCARP_Ib.pptpmpmpd	5.052e+43	5.43	5.43	5.635e+39	0.00557
2393	diHPCARP_Ib.tptmmpmpd	1.671e+44	6.15	6.15	5.562e+39	0.0055
2394	diHPCARP_Ib.pptppmpd	6.636e+44	6.97	6.97	5.516e+39	0.00546
2395	diHPCARP_Ib.ppmptppd	3.627e+43	5.24	5.24	5.512e+39	0.00545
2396	diHPCARP_Ib.tmtmmpmpd	8.067e+43	5.72	5.72	5.478e+39	0.00542
2397	diHPCARP_Ib.pmntmmpmpd	1.806e+43	4.84	4.84	5.336e+39	0.00528
2398	diHPCARP_Ib.ptpmtmmd	8.729e+42	4.42	4.42	5.276e+39	0.00522
2399	diHPCARP_Ib.tmmptmtpd	8.073e+43	5.75	5.75	5.242e+39	0.00519
2400	diHPCARP_Ib.mmtmttmd	5.650e+43	5.54	5.54	5.236e+39	0.00518
2401	diHPCARP_Ib.tptmpmmd	1.123e+44	5.95	5.95	5.215e+39	0.00516
2402	diHPCARP_Ib.pttppttmd	1.277e+44	6.03	6.03	5.139e+39	0.00508
2403	diHPCARP_Ib.ppmppmpd	2.698e+43	5.11	5.11	5.132e+39	0.00508
2404	diHPCARP_Ib.tttmptmmd	7.057e+43	5.70	5.70	4.937e+39	0.00488
2405	diHPCARP_Ib.ppmptpmd	3.876e+43	5.35	5.35	4.902e+39	0.00485
2406	diHPCARP_Ib.tttppmmd	1.669e+44	6.22	6.22	4.879e+39	0.00483
2407	diHPCARP_Ib.mtppmtmpd	6.216e+43	5.64	5.64	4.822e+39	0.00477
2408	diHPCARP_Ib.pptppppmd	7.479e+43	5.76	5.76	4.776e+39	0.00472
2409	diHPCARP_Ib.mtmtptmpd	3.596e+44	6.70	6.70	4.746e+39	0.00469
2410	diHPCARP_Ib.ttptmmmd	3.836e+43	5.39	5.39	4.576e+39	0.00453
2411	diHPCARP_Ib.ttmmtmpd	3.155e+44	6.65	6.65	4.548e+39	0.0045
2412	diHPCARP_Ib.pptpttpd	2.861e+44	6.59	6.59	4.545e+39	0.0045
2413	diHPCARP_Ib.pmtmpmpd	1.077e+44	6.01	6.01	4.521e+39	0.00447
2414	diHPCARP_Ib.tpmpttmd	7.576e+43	5.80	5.80	4.497e+39	0.00445
2415	diHPCARP_Ib.ptptptpd	8.535e+43	5.88	5.88	4.443e+39	0.00439
2416	diHPCARP_Ib.tptpmtmpd	4.896e+44	6.92	6.92	4.429e+39	0.00438
2417	diHPCARP_Ib.pmtptpmd	4.311e+43	5.48	5.48	4.423e+39	0.00437
2418	diHPCARP_Ib.mmpmptpmd	1.389e+44	6.18	6.18	4.359e+39	0.00431
2419	diHPCARP_Ib.tptpptpmd	3.507e+44	6.74	6.74	4.334e+39	0.00429
2420	diHPCARP_Ib.mmpmptpmd	1.110e+44	6.06	6.06	4.310e+39	0.00426
2421	diHPCARP_Ib.mtptpmpd	3.300e+43	5.33	5.33	4.299e+39	0.00425
2422	diHPCARP_Ib.ttpmptmmd	2.145e+43	5.08	5.08	4.266e+39	0.00422
2423	diHPCARP_Ib.tttptpmd	6.778e+44	7.14	7.14	4.233e+39	0.00419
2424	diHPCARP_Ib.tmtmtmmd	4.057e+43	5.47	5.47	4.194e+39	0.00415
2425	diHPCARP_Ib.tmpmptmmd	2.750e+43	5.24	5.24	4.179e+39	0.00413

2426	diHPCARP_Ib.tpmpttmd	6.352e+43	5.75	5.75	4.097e+39	0.00405
2427	diHPCARP_Ib.tpttpmmd	3.717e+44	6.81	6.81	4.072e+39	0.00403
2428	diHPCARP_Ib.tmtpttpd	3.606e+44	6.80	6.80	4.036e+39	0.00399
2429	diHPCARP_Ib.mmtmptpd	1.160e+44	6.13	6.13	3.989e+39	0.00395
2430	diHPCARP_Ib.mpmmpptpd	5.657e+43	5.70	5.70	3.970e+39	0.00393
2431	diHPCARP_Ib.pmttptpd	2.690e+44	6.64	6.64	3.935e+39	0.00389
2432	diHPCARP_Ib.mmpmpmpd	6.826e+42	4.45	4.45	3.918e+39	0.00388
2433	diHPCARP_Ib.pmpptmmd	3.213e+43	5.38	5.38	3.903e+39	0.00386
2434	diHPCARP_Ib.ptpmptpd	5.738e+43	5.72	5.72	3.897e+39	0.00385
2435	diHPCARP_Ib.tpptmmpd	6.906e+44	7.21	7.21	3.880e+39	0.00384
2436	diHPCARP_Ib.tmtmptmd	1.419e+44	6.27	6.27	3.827e+39	0.00379
2437	diHPCARP_Ib.mpmmpmpd	4.265e+43	5.56	5.56	3.812e+39	0.00377
2438	diHPCARP_Ib.ptmmntpd	3.141e+44	6.75	6.75	3.808e+39	0.00377
2439	diHPCARP_Ib.pmmptmtd	2.065e+44	6.51	6.51	3.747e+39	0.00371
2440	diHPCARP_Ib.ttpmmntmd	4.585e+43	5.61	5.61	3.732e+39	0.00369
2441	diHPCARP_Ib.pttmptmd	1.404e+44	6.28	6.28	3.717e+39	0.00368
2442	diHPCARP_Ib.pmtmntpd	3.344e+44	6.80	6.80	3.703e+39	0.00366
2443	diHPCARP_Ib.tptmptpd	3.052e+44	6.75	6.75	3.668e+39	0.00363
2444	diHPCARP_Ib.tttmntmd	1.144e+44	6.17	6.17	3.667e+39	0.00363
2445	diHPCARP_Ib.mmpmmntmd	5.652e+43	5.76	5.76	3.580e+39	0.00354
2446	diHPCARP_Ib.mtpmptmd	2.203e+43	5.20	5.20	3.571e+39	0.00353
2447	diHPCARP_Ib.tmmptmtd	1.988e+44	6.52	6.52	3.530e+39	0.00349
2448	diHPCARP_Ib.tmtmptmd	1.019e+44	6.12	6.12	3.528e+39	0.00349
2449	diHPCARP_Ib.tptmptmd	9.298e+43	6.07	6.07	3.497e+39	0.00346
2450	diHPCARP_Ib.tpptmmtmd	3.750e+44	6.91	6.91	3.466e+39	0.00343
2451	diHPCARP_Ib.tmtmmpmmd	1.061e+44	6.16	6.16	3.461e+39	0.00342
2452	diHPCARP_Ib.tptptppd	2.681e+44	6.72	6.72	3.423e+39	0.00339
2453	diHPCARP_Ib.pmpmpmpd	8.874e+42	4.69	4.69	3.413e+39	0.00338
2454	diHPCARP_Ib.pmmpmptpd	1.135e+43	4.85	4.85	3.321e+39	0.00328
2455	diHPCARP_Ib.ttpmptmd	1.912e+43	5.17	5.17	3.280e+39	0.00324
2456	diHPCARP_Ib.mtpmmtmd	2.099e+43	5.23	5.23	3.274e+39	0.00324
2457	diHPCARP_Ib.pmttptmd	2.769e+44	6.76	6.76	3.270e+39	0.00323
2458	diHPCARP_Ib.pmmmtmpd	1.648e+44	6.47	6.47	3.210e+39	0.00318
2459	diHPCARP_Ib.mtmptmmd	6.559e+43	5.92	5.92	3.189e+39	0.00315
2460	diHPCARP_Ib.tttmptmd	1.412e+44	6.38	6.38	3.160e+39	0.00313
2461	diHPCARP_Ib.tptmptmd	2.005e+44	6.60	6.60	3.132e+39	0.0031
2462	diHPCARP_Ib.tppmptpd	1.426e+44	6.40	6.40	3.118e+39	0.00308
2463	diHPCARP_Ib.tmtmptmd	3.469e+43	5.56	5.56	3.111e+39	0.00308
2464	diHPCARP_Ib.tptmptmd	3.975e+44	7.01	7.01	3.106e+39	0.00307
2465	diHPCARP_Ib.mpmmpptpd	1.020e+44	6.21	6.21	3.062e+39	0.00303
2466	diHPCARP_Ib.pmtmptmd	2.399e+44	6.72	6.72	3.045e+39	0.00301
2467	diHPCARP_Ib.tmpmptmd	3.061e+43	5.50	5.50	3.012e+39	0.00298
2468	diHPCARP_Ib.tpmptmtd	4.987e+43	5.79	5.79	3.005e+39	0.00297
2469	diHPCARP_Ib.tmmptmtd	9.702e+43	6.21	6.21	2.926e+39	0.00289
2470	diHPCARP_Ib.mtmmtmmd	2.726e+43	5.45	5.45	2.923e+39	0.00289
2471	diHPCARP_Ib.ptmmtmmd	1.154e+44	6.32	6.32	2.884e+39	0.00285
2472	diHPCARP_Ib.pptmmpd	2.216e+44	6.71	6.71	2.860e+39	0.00283
2473	diHPCARP_Ib.mmpmptmd	4.132e+43	5.71	5.71	2.838e+39	0.00281
2474	diHPCARP_Ib.ptmmtmtd	8.148e+43	6.12	6.12	2.837e+39	0.00281
2475	diHPCARP_Ib.tptmmtmd	3.345e+44	6.97	6.97	2.815e+39	0.00278
2476	diHPCARP_Ib.mptmmtmd	1.521e+44	6.52	6.52	2.722e+39	0.00269
2477	diHPCARP_Ib.tmtmptpd	6.547e+44	7.39	7.39	2.692e+39	0.00266
2478	diHPCARP_Ib.ttpmmpd	9.996e+43	6.29	6.29	2.637e+39	0.00261
2479	diHPCARP_Ib.tmmptmtd	1.098e+44	6.34	6.34	2.632e+39	0.0026
2480	diHPCARP_Ib.pmmmtppd	2.520e+43	5.47	5.47	2.622e+39	0.00259
2481	diHPCARP_Ib.tptmmpd	1.877e+44	6.67	6.67	2.602e+39	0.00257
2482	diHPCARP_Ib.pmtmmpd	6.305e+43	6.03	6.03	2.547e+39	0.00252
2483	diHPCARP_Ib.tpppttpd	2.035e+44	6.73	6.73	2.538e+39	0.00251
2484	diHPCARP_Ib.mmtmntppd	5.177e+44	7.29	7.29	2.537e+39	0.00251
2485	diHPCARP_Ib.mmtmptmd	1.925e+44	6.70	6.70	2.529e+39	0.0025
2486	diHPCARP_Ib.tmmptmtd	1.338e+44	6.49	6.49	2.521e+39	0.00249
2487	diHPCARP_Ib.mmtmptmd	2.396e+44	6.84	6.84	2.507e+39	0.00248
2488	diHPCARP_Ib.tpmptmtd	6.773e+43	6.09	6.09	2.479e+39	0.00245
2489	diHPCARP_Ib.pppmpmpd	1.948e+44	6.72	6.72	2.478e+39	0.00245
2490	diHPCARP_Ib.pmtmntppd	2.447e+44	6.86	6.86	2.465e+39	0.00244
2491	diHPCARP_Ib.pptmmpd	1.112e+44	6.39	6.39	2.465e+39	0.00244
2492	diHPCARP_Ib.mtmmtmtd	3.401e+44	7.06	7.06	2.435e+39	0.00241
2493	diHPCARP_Ib.pmtmmtmd	1.098e+43	5.02	5.02	2.427e+39	0.0024
2494	diHPCARP_Ib.pppmnttpd	1.639e+44	6.63	6.63	2.410e+39	0.00238
2495	diHPCARP_Ib.pmmmtmtd	1.554e+44	6.61	6.61	2.395e+39	0.00237
2496	diHPCARP_Ib.mmtpttpd	1.864e+44	6.72	6.72	2.390e+39	0.00236
2497	diHPCARP_Ib.tmtmntppd	5.331e+44	7.34	7.34	2.381e+39	0.00236

2498	diHPCARP_Ib.tptpmtmmd	4.859e+44	7.29	7.29	2.376e+39	0.00235
2499	diHPCARP_Ib.mmttmtppd	3.360e+44	7.07	7.07	2.360e+39	0.00233
2500	diHPCARP_Ib.tmmmtmtpd	3.060e+44	7.02	7.02	2.350e+39	0.00232
2501	diHPCARP_Ib.tttmptmpd	5.828e+43	6.04	6.04	2.323e+39	0.0023
2502	diHPCARP_Ib.pptmptmpd	1.337e+44	6.54	6.54	2.311e+39	0.00229
2503	diHPCARP_Ib.tptmptppd	1.897e+44	6.75	6.75	2.297e+39	0.00227
2504	diHPCARP_Ib.tmttptppd	3.979e+44	7.19	7.19	2.289e+39	0.00226
2505	diHPCARP_Ib.pmmptmtd	1.504e+43	5.24	5.24	2.288e+39	0.00226
2506	diHPCARP_Ib.tppmptmtd	2.339e+43	5.52	5.52	2.244e+39	0.00222
2507	diHPCARP_Ib.ptttptpmd	1.926e+44	6.77	6.77	2.236e+39	0.00221
2508	diHPCARP_Ib.tttppmmmd	3.824e+43	5.82	5.82	2.195e+39	0.00217
2509	diHPCARP_Ib.tmttmppmd	1.431e+44	6.61	6.61	2.195e+39	0.00217
2510	diHPCARP_Ib.ptmtmtd	2.645e+43	5.60	5.60	2.189e+39	0.00216
2511	diHPCARP_Ib.mmmppmmpmd	3.150e+43	5.71	5.71	2.189e+39	0.00216
2512	diHPCARP_Ib.mppmppppd	2.650e+43	5.61	5.61	2.175e+39	0.00215
2513	diHPCARP_Ib.tmmtpmtd	3.651e+44	7.18	7.18	2.165e+39	0.00214
2514	diHPCARP_Ib.tmpmptmpd	4.787e+43	5.97	5.97	2.160e+39	0.00214
2515	diHPCARP_Ib.pppmmpmpd	3.833e+43	5.84	5.84	2.151e+39	0.00213
2516	diHPCARP_Ib.tttptppd	5.295e+44	7.41	7.41	2.134e+39	0.00211
2517	diHPCARP_Ib.pmttppmpd	9.549e+43	6.39	6.39	2.126e+39	0.0021
2518	diHPCARP_Ib.mttmmtmmd	1.051e+44	6.45	6.45	2.108e+39	0.00208
2519	diHPCARP_Ib.pmmppmmpd	9.821e+42	5.04	5.04	2.100e+39	0.00208
2520	diHPCARP_Ib.tptpmpd	3.027e+44	7.09	7.09	2.084e+39	0.00206
2521	diHPCARP_Ib.tmttptmpd	3.455e+44	7.17	7.17	2.074e+39	0.00205
2522	diHPCARP_Ib.ptmtpmtd	1.780e+44	6.78	6.78	2.039e+39	0.00202
2523	diHPCARP_Ib.pptmmpmpd	5.075e+44	7.41	7.41	2.024e+39	0.002
2524	diHPCARP_Ib.pppmmpmd	1.096e+44	6.50	6.50	2.005e+39	0.00198
2525	diHPCARP_Ib.pttmptpmd	7.684e+43	6.30	6.30	1.992e+39	0.00197
2526	diHPCARP_Ib.tttmmtmpd	1.064e+44	6.49	6.49	1.991e+39	0.00197
2527	diHPCARP_Ib.mmmppmtpd	5.413e+43	6.09	6.09	1.989e+39	0.00197
2528	diHPCARP_Ib.mmpmptmtd	6.889e+43	6.24	6.24	1.976e+39	0.00195
2529	diHPCARP_Ib.mtptpmpd	1.207e+45	7.95	7.95	1.966e+39	0.00194
2530	diHPCARP_Ib.ptpmpmpd	5.998e+43	6.16	6.16	1.962e+39	0.00194
2531	diHPCARP_Ib.tttmpttpd	1.162e+44	6.55	6.55	1.961e+39	0.00194
2532	diHPCARP_Ib.tptmptpmd	2.549e+44	7.02	7.02	1.956e+39	0.00193
2533	diHPCARP_Ib.tppmptmpd	2.544e+43	5.65	5.65	1.956e+39	0.00193
2534	diHPCARP_Ib.pmmtmptpd	2.385e+43	5.61	5.61	1.946e+39	0.00192
2535	diHPCARP_Ib.ptppmtmmd	1.564e+43	5.37	5.37	1.925e+39	0.0019
2536	diHPCARP_Ib.tmtptmmd	2.363e+44	6.99	6.99	1.918e+39	0.0019
2537	diHPCARP_Ib.tmmtpmpmd	1.895e+44	6.86	6.86	1.916e+39	0.00189
2538	diHPCARP_Ib.mppmptmpd	5.141e+43	6.09	6.09	1.892e+39	0.00187
2539	diHPCARP_Ib.mmmtpmtd	3.216e+44	7.18	7.18	1.887e+39	0.00187
2540	diHPCARP_Ib.ptmmtmtd	8.153e+43	6.36	6.36	1.884e+39	0.00186
2541	diHPCARP_Ib.ptmmpmpd	9.248e+43	6.45	6.45	1.839e+39	0.00182
2542	diHPCARP_Ib.mmttptppd	3.117e+44	7.18	7.18	1.824e+39	0.0018
2543	diHPCARP_Ib.ttttptmmd	1.550e+44	6.77	6.77	1.815e+39	0.0018
2544	diHPCARP_Ib.tttppmtd	3.643e+44	7.28	7.28	1.807e+39	0.00179
2545	diHPCARP_Ib.mtttptmmd	1.595e+44	6.79	6.79	1.805e+39	0.00179
2546	diHPCARP_Ib.tmtptmpd	2.027e+44	6.94	6.94	1.777e+39	0.00176
2547	diHPCARP_Ib.tppmptmtd	2.306e+44	7.02	7.02	1.770e+39	0.00175
2548	diHPCARP_Ib.tptpmpd	3.978e+44	7.35	7.35	1.766e+39	0.00175
2549	diHPCARP_Ib.mmttptpmd	2.365e+44	7.05	7.05	1.742e+39	0.00172
2550	diHPCARP_Ib.tmtmppmmd	5.245e+43	6.15	6.15	1.741e+39	0.00172
2551	diHPCARP_Ib.pptpmpmpd	4.131e+43	6.01	6.01	1.723e+39	0.0017
2552	diHPCARP_Ib.pmmppmppd	1.135e+43	5.24	5.24	1.716e+39	0.0017
2553	diHPCARP_Ib.tmmmtmtd	1.108e+45	7.98	7.98	1.715e+39	0.0017
2554	diHPCARP_Ib.tmmtpmtd	1.913e+44	6.93	6.93	1.703e+39	0.00168
2555	diHPCARP_Ib.pmtmmpmpd	7.869e+43	6.41	6.41	1.697e+39	0.00168
2556	diHPCARP_Ib.tppmpttpd	1.276e+44	6.69	6.69	1.694e+39	0.00168
2557	diHPCARP_Ib.mppmmttpd	1.050e+44	6.58	6.58	1.678e+39	0.00166
2558	diHPCARP_Ib.mmmmtmtd	1.039e+44	6.59	6.59	1.658e+39	0.00164
2559	diHPCARP_Ib.tmmtpmtd	2.138e+44	7.02	7.02	1.654e+39	0.00164
2560	diHPCARP_Ib.tpppmmmd	3.560e+43	5.95	5.95	1.642e+39	0.00162
2561	diHPCARP_Ib.pppmpttpd	2.886e+44	7.20	7.20	1.634e+39	0.00162
2562	diHPCARP_Ib.mmtmmtmtd	3.054e+44	7.24	7.24	1.631e+39	0.00161
2563	diHPCARP_Ib.pmtmpttpd	2.044e+44	7.00	7.00	1.614e+39	0.0016
2564	diHPCARP_Ib.tmttptpmd	9.268e+44	7.92	7.92	1.585e+39	0.00157
2565	diHPCARP_Ib.pppmptppd	2.329e+43	5.72	5.72	1.584e+39	0.00157
2566	diHPCARP_Ib.mppmpttpd	8.660e+43	6.51	6.51	1.570e+39	0.00155
2567	diHPCARP_Ib.mptpmpmtd	4.746e+43	6.15	6.15	1.569e+39	0.00155
2568	diHPCARP_Ib.mmmtpmtd	1.195e+44	6.70	6.70	1.568e+39	0.00155
2569	diHPCARP_Ib.pptmmtmtd	8.666e+44	7.88	7.88	1.566e+39	0.00155

2570	diHPCARP_Ib.tptpptomd	1.514e+45	8.22	8.22	1.564e+39	0.00155
2571	diHPCARP_Ib.mmmmpmtmd	3.591e+43	5.99	5.99	1.553e+39	0.00154
2572	diHPCARP_Ib.ttmtmmmpd	1.748e+44	6.94	6.94	1.542e+39	0.00153
2573	diHPCARP_Ib.pmmmmtpdpd	1.226e+44	6.73	6.73	1.531e+39	0.00151
2574	diHPCARP_Ib.pppmptmpd	3.470e+43	5.98	5.98	1.529e+39	0.00151
2575	diHPCARP_Ib.mpmtpmpmd	7.709e+43	6.47	6.47	1.503e+39	0.00149
2576	diHPCARP_Ib.mmmmpmmmpd	1.775e+43	5.59	5.59	1.502e+39	0.00149
2577	diHPCARP_Ib.mpmmmmtmpd	6.811e+43	6.40	6.40	1.472e+39	0.00146
2578	diHPCARP_Ib.tpppmtmpd	1.923e+44	7.02	7.02	1.471e+39	0.00146
2579	diHPCARP_Ib.ppmmtmpmd	4.492e+43	6.16	6.16	1.467e+39	0.00145
2580	diHPCARP_Ib.pptppmmd	7.968e+44	7.88	7.88	1.459e+39	0.00144
2581	diHPCARP_Ib.mmmmpmtppd	1.129e+44	6.72	6.72	1.436e+39	0.00142
2582	diHPCARP_Ib.mpmmpptppd	3.081e+43	5.95	5.95	1.420e+39	0.0014
2583	diHPCARP_Ib.tppptmpmd	1.292e+44	6.81	6.81	1.419e+39	0.0014
2584	diHPCARP_Ib.ttmmmmtmd	7.867e+43	6.52	6.52	1.410e+39	0.0014
2585	diHPCARP_Ib.pmmtpmpdpd	9.272e+43	6.63	6.63	1.366e+39	0.00135
2586	diHPCARP_Ib.tmpmpmpmd	3.403e+43	6.04	6.04	1.355e+39	0.00134
2587	diHPCARP_Ib.pmtpmmmmd	8.361e+43	6.58	6.58	1.346e+39	0.00133
2588	diHPCARP_Ib.tpppptppd	1.584e+44	6.96	6.96	1.343e+39	0.00133
2589	diHPCARP_Ib.tptmmtmpd	3.425e+44	7.43	7.43	1.333e+39	0.00132
2590	diHPCARP_Ib.ttpmmmmmd	3.659e+43	6.10	6.10	1.317e+39	0.0013
2591	diHPCARP_Ib.mmpmpmtmd	5.984e+43	6.40	6.40	1.307e+39	0.00129
2592	diHPCARP_Ib.pptmmtmpd	9.195e+44	8.03	8.03	1.295e+39	0.00128
2593	diHPCARP_Ib.pptpptomd	3.901e+44	7.53	7.53	1.274e+39	0.00126
2594	diHPCARP_Ib.pttmptomd	4.221e+43	6.21	6.21	1.272e+39	0.00126
2595	diHPCARP_Ib.ptttptmmd	1.134e+44	6.80	6.80	1.264e+39	0.00125
2596	diHPCARP_Ib.pmpptmpmd	9.288e+42	5.32	5.32	1.236e+39	0.00122
2597	diHPCARP_Ib.mmmmpptomd	4.455e+43	6.26	6.26	1.232e+39	0.00122
2598	diHPCARP_Ib.pptptmpd	3.969e+44	7.56	7.56	1.228e+39	0.00121
2599	diHPCARP_Ib.pmtppmpmd	1.331e+44	6.91	6.91	1.223e+39	0.00121
2600	diHPCARP_Ib.mmtmtmpd	2.893e+44	7.38	7.38	1.212e+39	0.0012
2601	diHPCARP_Ib.pmtppmmmd	5.363e+43	6.38	6.38	1.203e+39	0.00119
2602	diHPCARP_Ib.pmpmmmtpd	1.748e+43	5.71	5.71	1.200e+39	0.00119
2603	diHPCARP_Ib.tmpmmttd	4.796e+43	6.32	6.32	1.200e+39	0.00119
2604	diHPCARP_Ib.ptpppmmpd	1.577e+43	5.66	5.66	1.183e+39	0.00117
2605	diHPCARP_Ib.mptmpmtpd	5.936e+43	6.45	6.45	1.183e+39	0.00117
2606	diHPCARP_Ib.tppmpmmmd	2.142e+43	5.85	5.85	1.175e+39	0.00116
2607	diHPCARP_Ib.ttttptmpd	1.492e+44	7.02	7.02	1.157e+39	0.00114
2608	diHPCARP_Ib.tmtmtmpd	3.532e+44	7.53	7.53	1.150e+39	0.00114
2609	diHPCARP_Ib.mtpppmmpd	3.746e+43	6.20	6.20	1.140e+39	0.00113
2610	diHPCARP_Ib.ptmpttmd	1.575e+44	7.06	7.06	1.134e+39	0.00112
2611	diHPCARP_Ib.pmtppmmpd	1.301e+44	6.95	6.95	1.118e+39	0.00111
2612	diHPCARP_Ib.pmtmmpmpd	7.520e+43	6.64	6.64	1.103e+39	0.00109
2613	diHPCARP_Ib.mmtppmtmd	2.113e+44	7.25	7.25	1.098e+39	0.00109
2614	diHPCARP_Ib.mpmmmmpdpd	1.025e+44	6.83	6.83	1.088e+39	0.00108
2615	diHPCARP_Ib.ppttmmpdpd	8.896e+44	8.13	8.13	1.065e+39	0.00105
2616	diHPCARP_Ib.mptpmtmpd	4.533e+44	7.73	7.73	1.064e+39	0.00105
2617	diHPCARP_Ib.mmpmmpmpd	1.486e+43	5.69	5.69	1.064e+39	0.00105
2618	diHPCARP_Ib.tpppptomd	6.966e+44	8.00	8.00	1.042e+39	0.00103
2619	diHPCARP_Ib.mmtmpmtmd	5.605e+43	6.50	6.50	1.024e+39	0.00101
2620	diHPCARP_Ib.mppmtttd	9.011e+43	6.79	6.79	1.023e+39	0.00101
2621	diHPCARP_Ib.tptmmtppd	2.812e+44	7.47	7.47	1.020e+39	0.00101
2622	diHPCARP_Ib.pptmppmd	1.150e+44	6.94	6.94	1.019e+39	0.00101
2623	diHPCARP_Ib.tptmmtmmd	5.063e+44	7.82	7.82	1.014e+39	0.001
2624	diHPCARP_Ib.tmtppmmd	9.117e+43	6.80	6.80	1.008e+39	0.000997
2625	diHPCARP_Ib.tptmmtmpd	3.709e+44	7.64	7.64	1.005e+39	0.000994
2626	diHPCARP_Ib.tppmmtmd	1.473e+44	7.09	7.09	1.003e+39	0.000992
2627	diHPCARP_Ib.tptmmtmd	3.870e+44	7.67	7.67	1.001e+39	0.00099
2628	diHPCARP_Ib.pppmmpmpd	7.224e+43	6.69	6.69	9.727e+38	0.000962
2629	diHPCARP_Ib.mpmmpmtmd	3.134e+43	6.19	6.19	9.707e+38	0.00096
2630	diHPCARP_Ib.tptmpmtpd	6.669e+43	6.64	6.64	9.657e+38	0.000955
2631	diHPCARP_Ib.ptpmmmmpd	3.196e+43	6.21	6.21	9.641e+38	0.000954
2632	diHPCARP_Ib.pppmmpdpd	4.681e+43	6.44	6.44	9.511e+38	0.000941
2633	diHPCARP_Ib.ptmppmtmd	1.844e+44	7.26	7.26	9.436e+38	0.000933
2634	diHPCARP_Ib.ptppptomd	2.967e+44	7.55	7.55	9.394e+38	0.000929
2635	diHPCARP_Ib.mtmptmmd	1.759e+44	7.24	7.24	9.369e+38	0.000927
2636	diHPCARP_Ib.pptptttd	1.134e+45	8.35	8.35	9.353e+38	0.000925
2637	diHPCARP_Ib.mmtppmpdpd	3.659e+44	7.68	7.68	9.297e+38	0.00092
2638	diHPCARP_Ib.tmmmpmtppd	9.974e+43	6.91	6.91	9.199e+38	0.00091
2639	diHPCARP_Ib.ptttmtmpd	2.252e+44	7.40	7.40	9.184e+38	0.000908
2640	diHPCARP_Ib.tmmppttd	6.421e+43	6.66	6.66	9.047e+38	0.000895
2641	diHPCARP_Ib.mmpmmmmpd	1.984e+43	5.96	5.96	9.046e+38	0.000895

2642	diHPCARP_Ib.mttmpttmd	1.683e+44	7.23	7.23	9.042e+38	0.000894
2643	diHPCARP_Ib.pnmtmpmpd	1.382e+43	5.74	5.74	9.031e+38	0.000893
2644	diHPCARP_Ib.tmmptmpd	1.462e+44	7.15	7.15	9.031e+38	0.000893
2645	diHPCARP_Ib.tnmtmttmd	5.981e+44	7.99	7.99	9.004e+38	0.000891
2646	diHPCARP_Ib.mtmtmttmd	4.642e+44	7.84	7.84	8.954e+38	0.000886
2647	diHPCARP_Ib.tpptmtppd	5.830e+44	7.98	7.98	8.894e+38	0.00088
2648	diHPCARP_Ib.pmttmppd	1.284e+44	7.08	7.08	8.877e+38	0.000878
2649	diHPCARP_Ib.ttpppmmpd	2.057e+43	5.99	5.99	8.869e+38	0.000877
2650	diHPCARP_Ib.pmtmpmmpd	5.987e+43	6.64	6.64	8.685e+38	0.000859
2651	diHPCARP_Ib.tnmtptpmd	2.026e+44	7.38	7.38	8.565e+38	0.000847
2652	diHPCARP_Ib.mptpmttmd	1.769e+44	7.30	7.30	8.440e+38	0.000835
2653	diHPCARP_Ib.tnmtpttmd	3.982e+44	7.79	7.79	8.361e+38	0.000827
2654	diHPCARP_Ib.tmmpttmd	4.151e+43	6.46	6.46	8.204e+38	0.000812
2655	diHPCARP_Ib.tpppmtmpd	9.510e+43	6.95	6.95	8.160e+38	0.000807
2656	diHPCARP_Ib.mtppmpmpd	3.588e+43	6.38	6.38	8.137e+38	0.000805
2657	diHPCARP_Ib.ttppttmd	3.569e+44	7.75	7.75	8.012e+38	0.000793
2658	diHPCARP_Ib.mmpmtmmd	1.414e+43	5.84	5.84	7.937e+38	0.000785
2659	diHPCARP_Ib.pnmmmtmpd	8.912e+43	6.93	6.93	7.907e+38	0.000782
2660	diHPCARP_Ib.mmmmtmmd	1.992e+44	7.42	7.42	7.894e+38	0.000781
2661	diHPCARP_Ib.tnmtptmmd	2.100e+44	7.45	7.45	7.883e+38	0.00078
2662	diHPCARP_Ib.mptpmtmpd	7.022e+44	8.17	8.17	7.806e+38	0.000772
2663	diHPCARP_Ib.mnmtmttmd	2.427e+44	7.55	7.55	7.682e+38	0.00076
2664	diHPCARP_Ib.tppmpmpd	4.785e+43	6.58	6.58	7.670e+38	0.000759
2665	diHPCARP_Ib.mmmmmmpmd	2.133e+44	7.48	7.48	7.629e+38	0.000755
2666	diHPCARP_Ib.mttmtmmd	2.129e+44	7.48	7.48	7.585e+38	0.00075
2667	diHPCARP_Ib.tpppmmmpd	1.780e+43	6.01	6.01	7.485e+38	0.00074
2668	diHPCARP_Ib.tpppmtmd	4.012e+44	7.88	7.88	7.318e+38	0.000724
2669	diHPCARP_Ib.tttmpmmd	2.709e+43	6.27	6.27	7.283e+38	0.00072
2670	diHPCARP_Ib.pmmpmtmpd	1.578e+43	5.96	5.96	7.205e+38	0.000713
2671	diHPCARP_Ib.tnmtpmmmd	1.330e+44	7.23	7.23	7.196e+38	0.000712
2672	diHPCARP_Ib.ttmtpttmd	2.319e+44	7.56	7.56	7.172e+38	0.000709
2673	diHPCARP_Ib.mnmtptppd	1.618e+44	7.35	7.35	7.159e+38	0.000708
2674	diHPCARP_Ib.tmtmpmpd	7.666e+43	6.91	6.91	7.149e+38	0.000707
2675	diHPCARP_Ib.ptmtmmpmd	1.715e+44	7.40	7.40	6.960e+38	0.000688
2676	diHPCARP_Ib.pttppmpd	3.871e+43	6.52	6.52	6.885e+38	0.000681
2677	diHPCARP_Ib.mtppptppd	4.298e+43	6.59	6.59	6.848e+38	0.000677
2678	diHPCARP_Ib.ptppmpmpd	5.267e+42	5.34	5.34	6.775e+38	0.00067
2679	diHPCARP_Ib.tttmtmmd	1.542e+44	7.36	7.36	6.723e+38	0.000665
2680	diHPCARP_Ib.mpmtpttmd	2.339e+44	7.61	7.61	6.711e+38	0.000664
2681	diHPCARP_Ib.mttpttmd	4.911e+44	8.05	8.05	6.708e+38	0.000663
2682	diHPCARP_Ib.ptmtmmd	2.328e+44	7.62	7.62	6.585e+38	0.000651
2683	diHPCARP_Ib.tpttptpmd	3.974e+44	7.94	7.94	6.559e+38	0.000649
2684	diHPCARP_Ib.tptpttmd	5.760e+44	8.17	8.17	6.489e+38	0.000642
2685	diHPCARP_Ib.ptmpmpmpd	1.250e+44	7.26	7.26	6.434e+38	0.000636
2686	diHPCARP_Ib.tmmppmmd	2.942e+43	6.40	6.40	6.375e+38	0.000631
2687	diHPCARP_Ib.mnmppttmd	5.692e+43	6.80	6.80	6.319e+38	0.000625
2688	diHPCARP_Ib.pnmtmtppd	6.758e+43	6.92	6.92	6.179e+38	0.000611
2689	diHPCARP_Ib.pnmtptmmd	1.012e+44	7.16	7.16	6.159e+38	0.000609
2690	diHPCARP_Ib.mnmtpppmd	2.705e+44	7.75	7.75	6.064e+38	0.0006
2691	diHPCARP_Ib.mnmtmtppd	1.811e+44	7.52	7.52	6.058e+38	0.000599
2692	diHPCARP_Ib.tttmttmd	2.132e+44	7.62	7.62	6.043e+38	0.000598
2693	diHPCARP_Ib.tttmtpmd	1.204e+44	7.28	7.28	6.005e+38	0.000594
2694	diHPCARP_Ib.tmmptmpd	3.306e+43	6.51	6.51	5.973e+38	0.000591
2695	diHPCARP_Ib.mnmpmtmmd	1.159e+44	7.26	7.26	5.919e+38	0.000586
2696	diHPCARP_Ib.pppppmpd	2.910e+43	6.44	6.44	5.893e+38	0.000583
2697	diHPCARP_Ib.mtptmmpd	4.206e+44	8.04	8.04	5.844e+38	0.000578
2698	diHPCARP_Ib.mnmmmmmpd	1.271e+44	7.33	7.33	5.833e+38	0.000577
2699	diHPCARP_Ib.tttmttmd	1.897e+44	7.57	7.57	5.794e+38	0.000573
2700	diHPCARP_Ib.ttpmpmpd	2.394e+43	6.35	6.35	5.678e+38	0.000562
2701	diHPCARP_Ib.tnmpmpppd	2.585e+43	6.40	6.40	5.658e+38	0.00056
2702	diHPCARP_Ib.ptmtmtmd	2.519e+43	6.38	6.38	5.625e+38	0.000556
2703	diHPCARP_Ib.tttmtpttd	1.675e+44	7.53	7.53	5.482e+38	0.000542
2704	diHPCARP_Ib.tttmpmmd	6.991e+43	7.01	7.01	5.482e+38	0.000542
2705	diHPCARP_Ib.ptmtmmpd	2.203e+43	6.32	6.32	5.480e+38	0.000542
2706	diHPCARP_Ib.tpptmttmd	4.724e+44	8.16	8.16	5.413e+38	0.000535
2707	diHPCARP_Ib.pnmtpttmd	5.119e+43	6.83	6.83	5.405e+38	0.000535
2708	diHPCARP_Ib.tptmpmpd	1.733e+44	7.56	7.56	5.403e+38	0.000534
2709	diHPCARP_Ib.tpppmttmd	1.684e+44	7.54	7.54	5.394e+38	0.000534
2710	diHPCARP_Ib.pnmtmttmd	8.234e+43	7.14	7.14	5.177e+38	0.000512
2711	diHPCARP_Ib.tppmpmpd	3.472e+43	6.64	6.64	5.047e+38	0.000499
2712	diHPCARP_Ib.tpttptppd	2.593e+44	7.85	7.85	4.978e+38	0.000492
2713	diHPCARP_Ib.tttpttmd	1.600e+44	7.56	7.56	4.954e+38	0.00049

2714	diHPCARP_Ib.ppptmtmpd	1.793e+44	7.65	7.65	4.828e+38	0.000478
2715	diHPCARP_Ib.mptpmmmmd	7.243e+44	8.48	8.48	4.826e+38	0.000477
2716	diHPCARP_Ib.ptmtptmmd	1.177e+44	7.40	7.40	4.782e+38	0.000473
2717	diHPCARP_Ib.tpttmtmpd	4.967e+44	8.26	8.26	4.767e+38	0.000472
2718	diHPCARP_Ib.tptmptmmd	2.919e+44	7.94	7.94	4.766e+38	0.000471
2719	diHPCARP_Ib.ppptmmpdp	2.993e+44	7.96	7.96	4.743e+38	0.000469
2720	diHPCARP_Ib.ttpmptmpd	1.010e+43	5.94	5.94	4.727e+38	0.000468
2721	diHPCARP_Ib.tmtttmpmmd	1.130e+44	7.40	7.40	4.633e+38	0.000458
2722	diHPCARP_Ib.tppmmmtmd	1.062e+44	7.36	7.36	4.623e+38	0.000457
2723	diHPCARP_Ib.tpttmtppd	3.574e+44	8.09	8.09	4.598e+38	0.000455
2724	diHPCARP_Ib.mptmpttmd	9.890e+44	8.71	8.71	4.475e+38	0.000443
2725	diHPCARP_Ib.tttmptppd	1.266e+44	7.49	7.49	4.433e+38	0.000439
2726	diHPCARP_Ib.tpptmtmpd	1.527e+45	8.98	8.98	4.389e+38	0.000434
2727	diHPCARP_Ib.ppttptmmd	1.118e+45	8.79	8.79	4.385e+38	0.000434
2728	diHPCARP_Ib.ppttptmmd	7.815e+44	8.58	8.58	4.376e+38	0.000433
2729	diHPCARP_Ib.ttpmttppd	2.491e+44	7.91	7.91	4.331e+38	0.000428
2730	diHPCARP_Ib.tppmmppmd	1.530e+44	7.62	7.62	4.309e+38	0.000426
2731	diHPCARP_Ib.mmtppppmd	1.645e+44	7.66	7.66	4.308e+38	0.000426
2732	diHPCARP_Ib.ppmtpmpmd	6.431e+43	7.11	7.11	4.284e+38	0.000424
2733	diHPCARP_Ib.mtmppmtpd	6.507e+43	7.12	7.12	4.204e+38	0.000416
2734	diHPCARP_Ib.pmttmmpmd	1.997e+44	7.80	7.80	4.185e+38	0.000414
2735	diHPCARP_Ib.ttpmtmpmd	9.829e+44	8.75	8.75	4.142e+38	0.00041
2736	diHPCARP_Ib.pptmttppd	8.571e+44	8.67	8.67	4.119e+38	0.000407
2737	diHPCARP_Ib.pmmppmmpmd	4.517e+42	5.55	5.55	4.116e+38	0.000407
2738	diHPCARP_Ib.pmmmtmtpd	3.688e+43	6.80	6.80	4.081e+38	0.000404
2739	diHPCARP_Ib.ttttmttmd	2.019e+45	9.19	9.19	4.079e+38	0.000403
2740	diHPCARP_Ib.tmmppmtmd	1.612e+44	7.69	7.69	4.061e+38	0.000402
2741	diHPCARP_Ib.ppttppmpmd	4.337e+44	8.28	8.28	4.051e+38	0.000401
2742	diHPCARP_Ib.tttttmpmmd	1.043e+44	7.43	7.43	4.024e+38	0.000398
2743	diHPCARP_Ib.ttttppmmd	1.044e+44	7.43	7.43	4.021e+38	0.000398
2744	diHPCARP_Ib.ptttmtmmd	1.076e+44	7.46	7.46	3.930e+38	0.000389
2745	diHPCARP_Ib.pmpmpttppd	4.677e+43	6.97	6.97	3.902e+38	0.000386
2746	diHPCARP_Ib.tppmmttppd	2.454e+44	7.96	7.96	3.900e+38	0.000386
2747	diHPCARP_Ib.tpttptmpd	4.636e+44	8.34	8.34	3.894e+38	0.000385
2748	diHPCARP_Ib.pptmptmpd	5.505e+43	7.08	7.08	3.812e+38	0.000377
2749	diHPCARP_Ib.ttmppttmd	4.466e+43	6.96	6.96	3.797e+38	0.000376
2750	diHPCARP_Ib.mtmpttmd	2.275e+44	7.94	7.94	3.734e+38	0.000369
2751	diHPCARP_Ib.tmmppmmpmd	1.855e+43	6.45	6.45	3.719e+38	0.000368
2752	diHPCARP_Ib.pmmtpmmpd	4.375e+43	6.96	6.96	3.695e+38	0.000365
2753	diHPCARP_Ib.tppmmptppd	6.037e+43	7.16	7.16	3.674e+38	0.000363
2754	diHPCARP_Ib.mtppmmtppd	1.382e+44	7.67	7.67	3.562e+38	0.000352
2755	diHPCARP_Ib.tmtppppppd	2.062e+44	7.92	7.92	3.534e+38	0.00035
2756	diHPCARP_Ib.ttptptppd	7.966e+44	8.72	8.72	3.526e+38	0.000349
2757	diHPCARP_Ib.tpttpttppd	1.818e+45	9.21	9.21	3.523e+38	0.000348
2758	diHPCARP_Ib.ttttmtmpd	1.512e+44	7.74	7.74	3.485e+38	0.000345
2759	diHPCARP_Ib.mpmpttppd	1.233e+44	7.62	7.62	3.469e+38	0.000343
2760	diHPCARP_Ib.pptmmttppd	6.819e+44	8.64	8.64	3.466e+38	0.000343
2761	diHPCARP_Ib.ptttpttmd	1.470e+44	7.73	7.73	3.410e+38	0.000337
2762	diHPCARP_Ib.pptmmpmmd	2.386e+44	8.02	8.02	3.407e+38	0.000337
2763	diHPCARP_Ib.mptppmpmd	4.273e+44	8.37	8.37	3.399e+38	0.000336
2764	diHPCARP_Ib.mmmmpmtmd	1.161e+44	7.60	7.60	3.384e+38	0.000335
2765	diHPCARP_Ib.mptmptppd	1.086e+44	7.57	7.57	3.334e+38	0.00033
2766	diHPCARP_Ib.mppmmppppd	7.585e+43	7.36	7.36	3.308e+38	0.000327
2767	diHPCARP_Ib.mppmpttmd	4.107e+43	7.00	7.00	3.253e+38	0.000322
2768	diHPCARP_Ib.pmmtpmtpd	4.037e+44	8.37	8.37	3.233e+38	0.00032
2769	diHPCARP_Ib.tttmptmmd	5.773e+43	7.21	7.21	3.219e+38	0.000318
2770	diHPCARP_Ib.ptmppmmd	1.118e+44	7.61	7.61	3.215e+38	0.000318
2771	diHPCARP_Ib.mmmtpmmd	1.808e+44	7.90	7.90	3.165e+38	0.000313
2772	diHPCARP_Ib.tppppptppd	1.435e+44	7.77	7.77	3.122e+38	0.000309
2773	diHPCARP_Ib.ptmpttppd	1.059e+45	8.97	8.97	3.103e+38	0.000307
2774	diHPCARP_Ib.mmtppmmpmd	2.125e+44	8.02	8.02	3.079e+38	0.000305
2775	diHPCARP_Ib.tppmmmmmd	6.394e+43	7.30	7.30	3.066e+38	0.000303
2776	diHPCARP_Ib.tmttmmmmd	8.516e+43	7.48	7.48	3.044e+38	0.000301
2777	diHPCARP_Ib.mmpmpttmd	1.230e+44	7.72	7.72	2.926e+38	0.000289
2778	diHPCARP_Ib.mpppmmpmd	1.359e+44	7.79	7.79	2.853e+38	0.000282
2779	diHPCARP_Ib.ttttpttmd	6.719e+44	8.75	8.75	2.850e+38	0.000282
2780	diHPCARP_Ib.tpttptmmd	6.038e+44	8.69	8.69	2.798e+38	0.000277
2781	diHPCARP_Ib.ttttptppd	4.505e+44	8.53	8.53	2.745e+38	0.000272
2782	diHPCARP_Ib.tttmmmmmd	6.727e+43	7.40	7.40	2.728e+38	0.00027
2783	diHPCARP_Ib.ptttppmpd	1.471e+44	7.88	7.88	2.652e+38	0.000262
2784	diHPCARP_Ib.pmmtptppd	3.369e+44	8.38	8.38	2.639e+38	0.000261
2785	diHPCARP_Ib.mtptmmtmd	2.522e+44	8.21	8.21	2.622e+38	0.000259

2786	diHPCARP_Ib.tmtppmppd	2.120e+44	8.12	8.12	2.591e+38	0.000256
2787	diHPCARP_Ib.tpnmpptpd	1.134e+44	7.74	7.74	2.590e+38	0.000256
2788	diHPCARP_Ib.ppmtpptpd	2.130e+44	8.12	8.12	2.590e+38	0.000256
2789	diHPCARP_Ib.mmmppmppd	1.397e+43	6.50	6.50	2.581e+38	0.000255
2790	diHPCARP_Ib.mpmtppmppd	1.419e+44	7.89	7.89	2.534e+38	0.000251
2791	diHPCARP_Ib.mmmppmtmd	2.697e+43	6.91	6.91	2.487e+38	0.000246
2792	diHPCARP_Ib.mtmtmtmd	2.590e+44	8.26	8.26	2.470e+38	0.000244
2793	diHPCARP_Ib.mptpptmmd	4.735e+44	8.63	8.63	2.431e+38	0.00024
2794	diHPCARP_Ib.tttmmtppd	4.567e+44	8.63	8.63	2.354e+38	0.000233
2795	diHPCARP_Ib.pnmtptppd	3.013e+44	8.38	8.38	2.351e+38	0.000233
2796	diHPCARP_Ib.tpttmtmpd	5.459e+44	8.74	8.74	2.333e+38	0.000231
2797	diHPCARP_Ib.mmtppmtppd	7.643e+43	7.57	7.57	2.333e+38	0.000231
2798	diHPCARP_Ib.pmtmmmmmd	5.334e+43	7.36	7.36	2.317e+38	0.000229
2799	diHPCARP_Ib.ttpmtmmd	3.608e+44	8.50	8.50	2.308e+38	0.000228
2800	diHPCARP_Ib.tmmppptpd	5.396e+43	7.38	7.38	2.272e+38	0.000225
2801	diHPCARP_Ib.mmmmpmpmd	5.424e+43	7.39	7.39	2.256e+38	0.000223
2802	diHPCARP_Ib.tttmmtmpd	3.509e+44	8.51	8.51	2.234e+38	0.000221
2803	diHPCARP_Ib.mptmpmpmd	1.779e+44	8.11	8.11	2.212e+38	0.000219
2804	diHPCARP_Ib.ptptptmd	5.200e+43	7.38	7.38	2.187e+38	0.000216
2805	diHPCARP_Ib.pmmmmmmmd	2.700e+43	7.00	7.00	2.163e+38	0.000214
2806	diHPCARP_Ib.pttmppptpd	4.893e+43	7.35	7.35	2.151e+38	0.000213
2807	diHPCARP_Ib.mpmtppppd	1.317e+44	7.95	7.95	2.127e+38	0.00021
2808	diHPCARP_Ib.ptmtpptpd	1.047e+44	7.82	7.82	2.119e+38	0.00021
2809	diHPCARP_Ib.mmtmpmtmd	7.477e+43	7.63	7.63	2.061e+38	0.000204
2810	diHPCARP_Ib.tpppmpptpd	1.533e+44	8.06	8.06	2.050e+38	0.000203
2811	diHPCARP_Ib.ptmtpttpd	4.696e+44	8.74	8.74	2.007e+38	0.000198
2812	diHPCARP_Ib.pmppmmmpd	6.452e+42	6.19	6.19	1.999e+38	0.000198
2813	diHPCARP_Ib.mtppptmmd	7.823e+43	7.68	7.68	1.992e+38	0.000197
2814	diHPCARP_Ib.ppmtppppd	9.057e+43	7.77	7.77	1.989e+38	0.000197
2815	diHPCARP_Ib.mtppmmtmd	2.168e+44	8.29	8.29	1.966e+38	0.000194
2816	diHPCARP_Ib.mmtptmmd	2.848e+44	8.46	8.46	1.963e+38	0.000194
2817	diHPCARP_Ib.tpnmpmpmd	3.450e+43	7.20	7.20	1.955e+38	0.000193
2818	diHPCARP_Ib.tpptptppd	3.728e+44	8.63	8.63	1.936e+38	0.000192
2819	diHPCARP_Ib.mppppptmd	1.258e+44	7.98	7.98	1.928e+38	0.000191
2820	diHPCARP_Ib.ttmppmmmd	2.494e+43	7.02	7.02	1.927e+38	0.000191
2821	diHPCARP_Ib.mmtmmtmmd	2.533e+44	8.41	8.41	1.900e+38	0.000188
2822	diHPCARP_Ib.mtppmmmpd	1.324e+43	6.66	6.66	1.874e+38	0.000185
2823	diHPCARP_Ib.mmmmmmmppd	2.387e+44	8.40	8.40	1.812e+38	0.000179
2824	diHPCARP_Ib.tpnmmmtmd	1.164e+44	7.97	7.97	1.810e+38	0.000179
2825	diHPCARP_Ib.tmtptppd	3.473e+44	8.63	8.63	1.809e+38	0.000179
2826	diHPCARP_Ib.ttpmppmmd	7.080e+42	6.31	6.31	1.807e+38	0.000179
2827	diHPCARP_Ib.tmtptmmd	1.210e+44	8.00	8.00	1.806e+38	0.000179
2828	diHPCARP_Ib.tmtmtmpd	3.417e+44	8.62	8.62	1.803e+38	0.000178
2829	diHPCARP_Ib.tmtptpmd	3.504e+44	8.63	8.63	1.799e+38	0.000178
2830	diHPCARP_Ib.pttmpttpd	1.695e+44	8.21	8.21	1.771e+38	0.000175
2831	diHPCARP_Ib.mtppmmtmd	1.407e+44	8.10	8.10	1.755e+38	0.000174
2832	diHPCARP_Ib.tttptppd	4.193e+44	8.76	8.76	1.750e+38	0.000173
2833	diHPCARP_Ib.tpptpttpd	4.026e+44	8.74	8.74	1.741e+38	0.000172
2834	diHPCARP_Ib.mmmppptpd	5.206e+43	7.52	7.52	1.738e+38	0.000172
2835	diHPCARP_Ib.pmpptpmd	8.043e+43	7.78	7.78	1.730e+38	0.000171
2836	diHPCARP_Ib.tttpttpd	5.564e+44	8.94	8.94	1.722e+38	0.00017
2837	diHPCARP_Ib.tmtppmmpd	2.287e+44	8.42	8.42	1.681e+38	0.000166
2838	diHPCARP_Ib.tpptmtmd	8.766e+44	9.23	9.23	1.667e+38	0.000165
2839	diHPCARP_Ib.tmtppmpd	1.270e+44	8.09	8.09	1.634e+38	0.000162
2840	diHPCARP_Ib.tpppmtmmd	1.459e+44	8.17	8.17	1.621e+38	0.00016
2841	diHPCARP_Ib.ttpptmmd	5.815e+43	7.65	7.65	1.563e+38	0.000155
2842	diHPCARP_Ib.ptmpptpmd	5.154e+43	7.58	7.58	1.548e+38	0.000153
2843	diHPCARP_Ib.mttmptpmd	1.062e+44	8.03	8.03	1.510e+38	0.000149
2844	diHPCARP_Ib.mtppppppd	3.550e+43	7.37	7.37	1.509e+38	0.000149
2845	diHPCARP_Ib.tppppmppd	1.040e+44	8.04	8.04	1.453e+38	0.000144
2846	diHPCARP_Ib.tppmmtppd	1.660e+44	8.32	8.32	1.438e+38	0.000142
2847	diHPCARP_Ib.ptmtmtpd	6.666e+44	9.15	9.15	1.433e+38	0.000142
2848	diHPCARP_Ib.mppmtmpd	3.113e+43	7.34	7.34	1.395e+38	0.000138
2849	diHPCARP_Ib.mmmmmmtppd	9.824e+43	8.05	8.05	1.348e+38	0.000133
2850	diHPCARP_Ib.mpnmpptpmd	3.058e+43	7.36	7.36	1.332e+38	0.000132
2851	diHPCARP_Ib.mmtmtmmd	4.019e+44	8.91	8.91	1.298e+38	0.000128
2852	diHPCARP_Ib.pmpptmpd	1.560e+43	6.98	6.98	1.294e+38	0.000128
2853	diHPCARP_Ib.tttmtmpd	5.542e+44	9.11	9.11	1.290e+38	0.000128
2854	diHPCARP_Ib.pppmmmpmd	1.783e+44	8.43	8.43	1.278e+38	0.000126
2855	diHPCARP_Ib.ttpmmpmd	2.746e+44	8.70	8.70	1.265e+38	0.000125
2856	diHPCARP_Ib.tpptpmpd	6.825e+44	9.25	9.25	1.256e+38	0.000124
2857	diHPCARP_Ib.tttmtppd	7.987e+44	9.34	9.34	1.250e+38	0.000124

2858	diHPCARP_Ib.mmptmptpd	2.563e+44	8.67	8.67	1.241e+38	0.000123
2859	diHPCARP_Ib.mmtmptmd	2.095e+44	8.55	8.55	1.236e+38	0.000122
2860	diHPCARP_Ib.mtptmtpmd	1.745e+44	8.45	8.45	1.227e+38	0.000121
2861	diHPCARP_Ib.tmtmpmpmd	8.800e+44	9.41	9.41	1.227e+38	0.000121
2862	diHPCARP_Ib.pppppmpmd	5.420e+43	7.76	7.76	1.199e+38	0.000119
2863	diHPCARP_Ib.tptmptpd	2.904e+44	8.79	8.79	1.157e+38	0.000114
2864	diHPCARP_Ib.mptmptmd	1.733e+44	8.48	8.48	1.149e+38	0.000114
2865	diHPCARP_Ib.tttmmtmd	4.332e+44	9.04	9.04	1.130e+38	0.000112
2866	diHPCARP_Ib.pttmptmpd	4.670e+43	7.71	7.71	1.124e+38	0.000111
2867	diHPCARP_Ib.mtppmmmpd	6.796e+43	7.94	7.94	1.116e+38	0.00011
2868	diHPCARP_Ib.tptmtmmd	5.547e+44	9.19	9.19	1.115e+38	0.00011
2869	diHPCARP_Ib.mmtmmpmpd	1.962e+44	8.57	8.57	1.114e+38	0.00011
2870	diHPCARP_Ib.mttmppppd	1.445e+44	8.40	8.40	1.101e+38	0.000109
2871	diHPCARP_Ib.tptmtpmd	2.391e+44	8.71	8.71	1.088e+38	0.000108
2872	diHPCARP_Ib.tmpmpmmmd	2.811e+43	7.44	7.44	1.073e+38	0.000106
2873	diHPCARP_Ib.tmtmtpdpd	2.771e+44	8.81	8.81	1.063e+38	0.000105
2874	diHPCARP_Ib.ttpptmpd	7.253e+43	8.01	8.01	1.060e+38	0.000105
2875	diHPCARP_Ib.mppppptmd	1.272e+44	8.35	8.35	1.048e+38	0.000104
2876	diHPCARP_Ib.tpmmmtpmd	9.697e+43	8.19	8.19	1.040e+38	0.000103
2877	diHPCARP_Ib.mptmpmpmd	2.817e+44	8.85	8.85	1.002e+38	9.91e-05
2878	diHPCARP_Ib.tpmmmtpmd	5.020e+44	9.22	9.22	9.688e+37	9.58e-05
2879	diHPCARP_Ib.mptmpmpmd	1.466e+44	8.48	8.48	9.667e+37	9.56e-05
2880	diHPCARP_Ib.tppmpmpmd	6.777e+43	8.03	8.03	9.624e+37	9.52e-05
2881	diHPCARP_Ib.pppmmtpmd	1.481e+44	8.50	8.50	9.465e+37	9.36e-05
2882	diHPCARP_Ib.tpnmpmmmd	1.969e+44	8.68	8.68	9.415e+37	9.31e-05
2883	diHPCARP_Ib.mtttptpmd	4.346e+44	9.15	9.15	9.326e+37	9.23e-05
2884	diHPCARP_Ib.mppppmpmd	6.822e+43	8.06	8.06	9.191e+37	9.09e-05
2885	diHPCARP_Ib.tmtmmtmd	1.547e+44	8.56	8.56	8.999e+37	8.9e-05
2886	diHPCARP_Ib.mtttptmd	6.867e+44	9.45	9.45	8.980e+37	8.88e-05
2887	diHPCARP_Ib.pppppptpd	8.763e+43	8.22	8.22	8.935e+37	8.84e-05
2888	diHPCARP_Ib.mppmpmpmd	4.528e+43	7.84	7.84	8.819e+37	8.72e-05
2889	diHPCARP_Ib.mpppmtmd	1.291e+44	8.46	8.46	8.804e+37	8.71e-05
2890	diHPCARP_Ib.mmmmpmmmd	2.865e+43	7.57	7.57	8.791e+37	8.7e-05
2891	diHPCARP_Ib.mmmmtmptpd	5.961e+43	8.01	8.01	8.772e+37	8.68e-05
2892	diHPCARP_Ib.mptpmtmd	2.010e+44	8.73	8.73	8.761e+37	8.67e-05
2893	diHPCARP_Ib.mmtmppmpd	1.841e+44	8.68	8.68	8.712e+37	8.62e-05
2894	diHPCARP_Ib.mtptmpppd	6.250e+43	8.04	8.04	8.687e+37	8.59e-05
2895	diHPCARP_Ib.pttmmpmpd	1.210e+44	8.44	8.44	8.670e+37	8.58e-05
2896	diHPCARP_Ib.mmtmppppd	2.123e+44	8.77	8.77	8.645e+37	8.55e-05
2897	diHPCARP_Ib.tttmpmpmd	9.835e+43	8.32	8.32	8.588e+37	8.49e-05
2898	diHPCARP_Ib.mtpppmtpd	1.908e+44	8.71	8.71	8.567e+37	8.47e-05
2899	diHPCARP_Ib.tpppppppd	7.211e+43	8.14	8.14	8.503e+37	8.41e-05
2900	diHPCARP_Ib.ptptmmpmd	1.927e+44	8.74	8.74	8.269e+37	8.18e-05
2901	diHPCARP_Ib.tpmmmtpmd	3.190e+44	9.05	9.05	8.212e+37	8.12e-05
2902	diHPCARP_Ib.mmtmppppd	4.340e+44	9.24	9.24	8.051e+37	7.96e-05
2903	diHPCARP_Ib.mttmmtpmd	3.939e+44	9.19	9.19	7.988e+37	7.9e-05
2904	diHPCARP_Ib.tpmmmtpmd	3.498e+44	9.12	9.12	7.940e+37	7.85e-05
2905	diHPCARP_Ib.tpmmmtpmd	1.658e+44	8.68	8.68	7.833e+37	7.75e-05
2906	diHPCARP_Ib.tpmmmtpmd	1.973e+43	7.43	7.43	7.583e+37	7.5e-05
2907	diHPCARP_Ib.tmpmpmpmd	1.998e+43	7.45	7.45	7.471e+37	7.39e-05
2908	diHPCARP_Ib.tttmmttpd	4.256e+44	9.28	9.28	7.421e+37	7.34e-05
2909	diHPCARP_Ib.tmptmtpd	2.973e+45	10.44	10.44	7.420e+37	7.34e-05
2910	diHPCARP_Ib.mppptpmd	7.858e+43	8.28	8.28	7.348e+37	7.27e-05
2911	diHPCARP_Ib.mmtppmpdpd	3.888e+44	9.23	9.23	7.305e+37	7.23e-05
2912	diHPCARP_Ib.mppppmpmd	8.138e+43	8.30	8.30	7.261e+37	7.18e-05
2913	diHPCARP_Ib.tpmmmtpmd	9.011e+43	8.37	8.37	7.214e+37	7.14e-05
2914	diHPCARP_Ib.mmtmmpmpd	2.509e+44	8.98	8.98	7.211e+37	7.13e-05
2915	diHPCARP_Ib.tppmmmmmd	1.494e+44	8.68	8.68	7.112e+37	7.03e-05
2916	diHPCARP_Ib.tpptmptpd	2.967e+44	9.10	9.10	7.019e+37	6.94e-05
2917	diHPCARP_Ib.mptmmtmmd	6.448e+44	9.58	9.58	6.771e+37	6.7e-05
2918	diHPCARP_Ib.ptptpmpd	2.164e+43	7.57	7.57	6.626e+37	6.55e-05
2919	diHPCARP_Ib.ptmtptpmd	1.378e+44	8.67	8.67	6.617e+37	6.55e-05
2920	diHPCARP_Ib.tmmmmtpd	2.122e+44	8.93	8.93	6.603e+37	6.53e-05
2921	diHPCARP_Ib.ptmtmtpmd	1.326e+44	8.66	8.66	6.552e+37	6.48e-05
2922	diHPCARP_Ib.mppppmpmd	9.322e+43	8.46	8.46	6.415e+37	6.35e-05
2923	diHPCARP_Ib.tmtmptpd	1.701e+44	8.83	8.83	6.297e+37	6.23e-05
2924	diHPCARP_Ib.pppppptpd	2.026e+44	8.94	8.94	6.223e+37	6.16e-05
2925	diHPCARP_Ib.mtmtptpmd	2.552e+44	9.08	9.08	6.221e+37	6.15e-05
2926	diHPCARP_Ib.tppmmtpmd	6.666e+44	9.66	9.66	6.158e+37	6.09e-05
2927	diHPCARP_Ib.mptppmpmd	2.940e+44	9.17	9.17	6.152e+37	6.08e-05
2928	diHPCARP_Ib.ttmptmtpd	5.259e+43	8.17	8.17	5.897e+37	5.83e-05
2929	diHPCARP_Ib.mmmmmmmmd	1.728e+44	8.88	8.88	5.859e+37	5.79e-05

2930	diHPCARP_Ib.mmptmpppd	1.370e+44	8.75	8.75	5.801e+37	5.74e-05
2931	diHPCARP_Ib.mpttptpmd	5.478e+44	9.58	9.58	5.762e+37	5.7e-05
2932	diHPCARP_Ib.pmmppptmpd	4.750e+43	8.12	8.12	5.734e+37	5.67e-05
2933	diHPCARP_Ib.mptmmmpmd	3.887e+44	9.38	9.38	5.722e+37	5.66e-05
2934	diHPCARP_Ib.mptmptmmd	1.241e+44	8.70	8.70	5.710e+37	5.65e-05
2935	diHPCARP_Ib.tmpmptmmd	3.181e+43	7.89	7.89	5.699e+37	5.64e-05
2936	diHPCARP_Ib.mtptmmpmd	2.491e+44	9.12	9.12	5.657e+37	5.6e-05
2937	diHPCARP_Ib.mpmtmptpd	9.575e+43	8.55	8.55	5.636e+37	5.57e-05
2938	diHPCARP_Ib.ptmppmmpd	1.811e+43	7.56	7.56	5.636e+37	5.57e-05
2939	diHPCARP_Ib.ttmpmttpd	4.678e+43	8.13	8.13	5.567e+37	5.51e-05
2940	diHPCARP_Ib.tptmpppd	2.055e+44	9.02	9.02	5.564e+37	5.5e-05
2941	diHPCARP_Ib.ttmpmmpmd	9.168e+43	8.55	8.55	5.438e+37	5.38e-05
2942	diHPCARP_Ib.ttmpmmpd	8.456e+43	8.50	8.50	5.427e+37	5.37e-05
2943	diHPCARP_Ib.tptmpmpd	2.086e+44	9.04	9.04	5.402e+37	5.34e-05
2944	diHPCARP_Ib.mmpmptmmd	3.241e+43	7.93	7.93	5.397e+37	5.34e-05
2945	diHPCARP_Ib.mtppmmmd	4.803e+43	8.17	8.17	5.352e+37	5.29e-05
2946	diHPCARP_Ib.ptppmmpd	1.931e+44	9.01	9.01	5.266e+37	5.21e-05
2947	diHPCARP_Ib.ptptpmtmd	2.073e+44	9.06	9.06	5.186e+37	5.13e-05
2948	diHPCARP_Ib.tmmppmmpd	6.689e+43	8.40	8.40	5.106e+37	5.05e-05
2949	diHPCARP_Ib.mtmtmtpmd	2.851e+44	9.26	9.26	5.099e+37	5.04e-05
2950	diHPCARP_Ib.ptmpptmmd	3.835e+43	8.09	8.09	4.910e+37	4.86e-05
2951	diHPCARP_Ib.tpptpttmd	4.402e+44	9.55	9.55	4.846e+37	4.79e-05
2952	diHPCARP_Ib.mtppptmpd	6.650e+43	8.43	8.43	4.829e+37	4.78e-05
2953	diHPCARP_Ib.tmptmtppd	9.766e+44	10.04	10.04	4.773e+37	4.72e-05
2954	diHPCARP_Ib.pmtmmpmmd	4.561e+43	8.22	8.22	4.671e+37	4.62e-05
2955	diHPCARP_Ib.tmpppttpd	2.188e+44	9.17	9.17	4.599e+37	4.55e-05
2956	diHPCARP_Ib.mmpmppmmd	2.800e+43	7.94	7.94	4.575e+37	4.52e-05
2957	diHPCARP_Ib.tmtmmpmpd	1.844e+44	9.07	9.07	4.532e+37	4.48e-05
2958	diHPCARP_Ib.pmmppptmmd	8.329e+42	7.23	7.23	4.487e+37	4.44e-05
2959	diHPCARP_Ib.mptppttmd	8.113e+44	9.97	9.97	4.444e+37	4.4e-05
2960	diHPCARP_Ib.ttmpmptmd	5.476e+43	8.37	8.37	4.340e+37	4.29e-05
2961	diHPCARP_Ib.tpmtmmmd	1.020e+44	8.76	8.76	4.204e+37	4.16e-05
2962	diHPCARP_Ib.pmmpttpd	3.725e+43	8.16	8.16	4.201e+37	4.16e-05
2963	diHPCARP_Ib.tmmmmmpd	2.657e+44	9.34	9.34	4.157e+37	4.11e-05
2964	diHPCARP_Ib.mptmppmd	3.215e+44	9.46	9.46	4.146e+37	4.1e-05
2965	diHPCARP_Ib.mpppmtmmd	7.097e+43	8.56	8.56	4.140e+37	4.09e-05
2966	diHPCARP_Ib.pttmntmpd	1.193e+44	8.87	8.87	4.124e+37	4.08e-05
2967	diHPCARP_Ib.pmpptppd	3.456e+43	8.13	8.13	4.118e+37	4.07e-05
2968	diHPCARP_Ib.pttptmpd	1.352e+44	8.95	8.95	4.070e+37	4.03e-05
2969	diHPCARP_Ib.pmmppptpd	4.889e+43	8.36	8.36	3.950e+37	3.91e-05
2970	diHPCARP_Ib.tmpmptpd	3.618e+43	8.18	8.18	3.946e+37	3.9e-05
2971	diHPCARP_Ib.mmttpppmd	2.848e+44	9.42	9.42	3.942e+37	3.9e-05
2972	diHPCARP_Ib.ptmpmtmpd	1.914e+43	7.81	7.81	3.939e+37	3.9e-05
2973	diHPCARP_Ib.tppppmmd	4.415e+43	8.30	8.30	3.937e+37	3.89e-05
2974	diHPCARP_Ib.ptptmtpmd	9.636e+43	8.77	8.77	3.937e+37	3.89e-05
2975	diHPCARP_Ib.mpmtmmpd	6.628e+43	8.55	8.55	3.896e+37	3.85e-05
2976	diHPCARP_Ib.mmmppmtpd	4.367e+43	8.31	8.31	3.844e+37	3.8e-05
2977	diHPCARP_Ib.mtppmmpmd	1.037e+44	8.83	8.83	3.842e+37	3.8e-05
2978	diHPCARP_Ib.ptptmtpmd	1.187e+44	8.91	8.91	3.817e+37	3.78e-05
2979	diHPCARP_Ib.pmttppmmd	7.143e+43	8.61	8.61	3.809e+37	3.77e-05
2980	diHPCARP_Ib.tpmmntppd	9.192e+43	8.77	8.77	3.773e+37	3.73e-05
2981	diHPCARP_Ib.pmppttpd	4.391e+43	8.37	8.37	3.513e+37	3.47e-05
2982	diHPCARP_Ib.mtppmpmpd	1.780e+43	7.84	7.84	3.483e+37	3.44e-05
2983	diHPCARP_Ib.mtttmtmpd	5.155e+44	9.85	9.85	3.452e+37	3.41e-05
2984	diHPCARP_Ib.mpmppmmpd	7.789e+43	8.73	8.73	3.406e+37	3.37e-05
2985	diHPCARP_Ib.tptppmpd	4.224e+44	9.74	9.74	3.397e+37	3.36e-05
2986	diHPCARP_Ib.ttttppmpd	4.204e+44	9.74	9.74	3.393e+37	3.36e-05
2987	diHPCARP_Ib.tmpmmttpd	5.728e+43	8.56	8.56	3.351e+37	3.31e-05
2988	diHPCARP_Ib.tppmmmpmd	1.933e+44	9.28	9.28	3.340e+37	3.3e-05
2989	diHPCARP_Ib.tmtmppppd	1.572e+44	9.16	9.16	3.328e+37	3.29e-05
2990	diHPCARP_Ib.mttmmtmpd	6.688e+43	8.66	8.66	3.287e+37	3.25e-05
2991	diHPCARP_Ib.mptmmtmpd	7.149e+44	10.08	10.08	3.242e+37	3.21e-05
2992	diHPCARP_Ib.tppmmpmmd	9.374e+43	8.87	8.87	3.235e+37	3.2e-05
2993	diHPCARP_Ib.mtptmppmd	2.544e+44	9.47	9.47	3.215e+37	3.18e-05
2994	diHPCARP_Ib.mpppmpmmd	3.123e+43	8.22	8.22	3.194e+37	3.16e-05
2995	diHPCARP_Ib.tmpmttppd	3.763e+44	9.71	9.71	3.178e+37	3.14e-05
2996	diHPCARP_Ib.mtmppptpd	1.030e+44	8.94	8.94	3.172e+37	3.14e-05
2997	diHPCARP_Ib.tmpmpmpd	1.048e+44	8.96	8.96	3.127e+37	3.09e-05
2998	diHPCARP_Ib.mmtppmtpd	8.570e+44	10.21	10.21	3.119e+37	3.08e-05
2999	diHPCARP_Ib.mpmtmtpd	2.328e+44	9.46	9.46	2.994e+37	2.96e-05
3000	diHPCARP_Ib.ttpmptmpd	4.482e+43	8.48	8.48	2.986e+37	2.95e-05
3001	diHPCARP_Ib.mtmptmpd	1.137e+44	9.04	9.04	2.975e+37	2.94e-05

3002	diHPCARP_Ib.tppmptmmd	5.898e+43	8.65	8.65	2.964e+37	2.93e-05
3003	diHPCARP_Ib.mpptmptmd	1.541e+44	9.23	9.23	2.935e+37	2.9e-05
3004	diHPCARP_Ib.pmtppmpmd	1.704e+44	9.29	9.29	2.924e+37	2.89e-05
3005	diHPCARP_Ib.tptpppppd	2.076e+44	9.41	9.41	2.908e+37	2.88e-05
3006	diHPCARP_Ib.mpptmtmd	4.288e+44	9.84	9.84	2.897e+37	2.87e-05
3007	diHPCARP_Ib.mttppmmtmd	7.294e+43	8.79	8.79	2.872e+37	2.84e-05
3008	diHPCARP_Ib.mtmppmmpmd	8.084e+43	8.86	8.86	2.863e+37	2.83e-05
3009	diHPCARP_Ib.tmtmmpppd	1.246e+44	9.12	9.12	2.822e+37	2.79e-05
3010	diHPCARP_Ib.mtptmptpd	2.354e+44	9.51	9.51	2.791e+37	2.76e-05
3011	diHPCARP_Ib.mptmpppmmd	1.450e+44	9.22	9.22	2.781e+37	2.75e-05
3012	diHPCARP_Ib.tpptmpppd	1.420e+44	9.21	9.21	2.779e+37	2.75e-05
3013	diHPCARP_Ib.tpmtmptmd	2.341e+44	9.51	9.51	2.750e+37	2.72e-05
3014	diHPCARP_Ib.tpptmtmpd	2.172e+44	9.47	9.47	2.747e+37	2.72e-05
3015	diHPCARP_Ib.tmppttppd	1.266e+45	10.53	10.53	2.682e+37	2.65e-05
3016	diHPCARP_Ib.ppppppppd	5.578e+43	8.68	8.68	2.672e+37	2.64e-05
3017	diHPCARP_Ib.mpttmtmpd	4.536e+44	9.93	9.93	2.649e+37	2.62e-05
3018	diHPCARP_Ib.tmpppttmd	1.187e+44	9.13	9.13	2.645e+37	2.62e-05
3019	diHPCARP_Ib.tmpmmtpmd	2.131e+43	8.11	8.11	2.613e+37	2.58e-05
3020	diHPCARP_Ib.tptmppppd	7.794e+43	8.89	8.89	2.612e+37	2.58e-05
3021	diHPCARP_Ib.tmpmttmd	2.856e+44	9.66	9.66	2.611e+37	2.58e-05
3022	diHPCARP_Ib.ptptmttmd	3.291e+44	9.75	9.75	2.600e+37	2.57e-05
3023	diHPCARP_Ib.mpptpppmmd	5.448e+43	8.68	8.68	2.583e+37	2.55e-05
3024	diHPCARP_Ib.mmtppmpmd	4.272e+44	9.91	9.91	2.566e+37	2.54e-05
3025	diHPCARP_Ib.pmmmmptmd	1.352e+44	9.23	9.23	2.552e+37	2.52e-05
3026	diHPCARP_Ib.ptppmmtmd	1.065e+44	9.11	9.11	2.460e+37	2.43e-05
3027	diHPCARP_Ib.ttttptmmd	2.580e+44	9.64	9.64	2.447e+37	2.42e-05
3028	diHPCARP_Ib.mttppmmmpd	1.790e+44	9.43	9.43	2.430e+37	2.4e-05
3029	diHPCARP_Ib.ptppmmmmmd	5.031e+43	8.68	8.68	2.409e+37	2.38e-05
3030	diHPCARP_Ib.pmttmmmmmd	7.377e+43	8.90	8.90	2.405e+37	2.38e-05
3031	diHPCARP_Ib.mpmtmtmpd	1.417e+44	9.30	9.30	2.388e+37	2.36e-05
3032	diHPCARP_Ib.tmpmppppd	3.380e+43	8.47	8.47	2.302e+37	2.28e-05
3033	diHPCARP_Ib.mpttptmmd	4.324e+44	9.99	9.99	2.295e+37	2.27e-05
3034	diHPCARP_Ib.tmmppptpd	6.860e+43	8.91	8.91	2.224e+37	2.2e-05
3035	diHPCARP_Ib.tmtmppmpd	9.830e+43	9.12	9.12	2.215e+37	2.19e-05
3036	diHPCARP_Ib.tppmmttmd	2.313e+44	9.64	9.64	2.189e+37	2.17e-05
3037	diHPCARP_Ib.mpptmmpmd	1.662e+44	9.46	9.46	2.138e+37	2.11e-05
3038	diHPCARP_Ib.tmmmpptpd	6.583e+43	8.92	8.92	2.106e+37	2.08e-05
3039	diHPCARP_Ib.pttpttppd	2.462e+44	9.71	9.71	2.086e+37	2.06e-05
3040	diHPCARP_Ib.tmmpppppd	4.105e+43	8.65	8.65	2.045e+37	2.02e-05
3041	diHPCARP_Ib.mttmmmmmmmd	4.044e+45	11.40	11.40	2.012e+37	1.99e-05
3042	diHPCARP_Ib.mpmtmmppd	1.498e+44	9.44	9.44	1.995e+37	1.97e-05
3043	diHPCARP_Ib.mptmmtppd	5.605e+44	10.23	10.23	1.978e+37	1.96e-05
3044	diHPCARP_Ib.tmppptpmd	2.403e+44	9.73	9.73	1.963e+37	1.94e-05
3045	diHPCARP_Ib.pmtmpmtmd	3.507e+44	9.96	9.96	1.953e+37	1.93e-05
3046	diHPCARP_Ib.mttppmmmpd	1.855e+44	9.58	9.58	1.946e+37	1.93e-05
3047	diHPCARP_Ib.tmppttppd	4.740e+43	8.77	8.77	1.928e+37	1.91e-05
3048	diHPCARP_Ib.mmttmppmd	2.968e+44	9.87	9.87	1.913e+37	1.89e-05
3049	diHPCARP_Ib.mptpppppd	3.841e+44	10.03	10.03	1.911e+37	1.89e-05
3050	diHPCARP_Ib.pmmptmtpd	3.539e+43	8.61	8.61	1.884e+37	1.86e-05
3051	diHPCARP_Ib.mmttppmpd	1.563e+44	9.50	9.50	1.871e+37	1.85e-05
3052	diHPCARP_Ib.mtttppppd	1.925e+44	9.63	9.63	1.871e+37	1.85e-05
3053	diHPCARP_Ib.mtmmmmmmpd	4.770e+43	8.80	8.80	1.864e+37	1.84e-05
3054	diHPCARP_Ib.mmtpppmmd	3.080e+44	9.91	9.91	1.851e+37	1.83e-05
3055	diHPCARP_Ib.mmmmpmpd	7.724e+43	9.09	9.09	1.845e+37	1.82e-05
3056	diHPCARP_Ib.tmppptppd	2.660e+44	9.85	9.85	1.761e+37	1.74e-05
3057	diHPCARP_Ib.tpptmtmmd	9.305e+44	10.60	10.60	1.755e+37	1.74e-05
3058	diHPCARP_Ib.mmttmppmd	1.877e+44	9.65	9.65	1.746e+37	1.73e-05
3059	diHPCARP_Ib.mttpppmmd	8.240e+44	10.53	10.53	1.744e+37	1.72e-05
3060	diHPCARP_Ib.mmttmpppd	8.855e+44	10.58	10.58	1.742e+37	1.72e-05
3061	diHPCARP_Ib.mptppppmd	3.304e+44	10.02	10.02	1.664e+37	1.65e-05
3062	diHPCARP_Ib.mptmppmmd	8.736e+43	9.22	9.22	1.664e+37	1.65e-05
3063	diHPCARP_Ib.tpptppppd	1.598e+44	9.60	9.60	1.634e+37	1.62e-05
3064	diHPCARP_Ib.tppmptmpd	5.837e+43	9.00	9.00	1.627e+37	1.61e-05
3065	diHPCARP_Ib.tpmtpttmd	3.449e+44	10.07	10.07	1.597e+37	1.58e-05
3066	diHPCARP_Ib.tpptpttmd	2.591e+44	9.90	9.90	1.596e+37	1.58e-05
3067	diHPCARP_Ib.mpttpttmd	6.126e+44	10.42	10.42	1.572e+37	1.55e-05
3068	diHPCARP_Ib.mmpptmtpd	3.198e+43	8.66	8.66	1.570e+37	1.55e-05
3069	diHPCARP_Ib.tmttppppd	2.048e+44	9.77	9.77	1.562e+37	1.54e-05
3070	diHPCARP_Ib.pmmptppd	3.914e+43	8.79	8.79	1.553e+37	1.54e-05
3071	diHPCARP_Ib.pmpptmppd	1.642e+43	8.27	8.27	1.544e+37	1.53e-05
3072	diHPCARP_Ib.mtmmmmmmd	1.572e+44	9.62	9.62	1.539e+37	1.52e-05
3073	diHPCARP_Ib.tpmtptmpd	2.205e+44	9.84	9.84	1.509e+37	1.49e-05

3074	diHPCARP_Ib.tpmtmtpmd	8.832e+44	10.67	10.67	1.485e+37	1.47e-05
3075	diHPCARP_Ib.pmpptmtpd	2.534e+43	8.57	8.57	1.451e+37	1.44e-05
3076	diHPCARP_Ib.mpptppmmd	7.734e+43	9.25	9.25	1.417e+37	1.4e-05
3077	diHPCARP_Ib.mtmppptpd	7.888e+43	9.26	9.26	1.413e+37	1.4e-05
3078	diHPCARP_Ib.ptptmttmd	1.085e+44	9.45	9.45	1.406e+37	1.39e-05
3079	diHPCARP_Ib.tppmmtpmd	6.485e+43	9.15	9.15	1.403e+37	1.39e-05
3080	diHPCARP_Ib.mmpmpmtmd	5.392e+43	9.05	9.05	1.367e+37	1.35e-05
3081	diHPCARP_Ib.tpmppmmd	7.511e+43	9.25	9.25	1.362e+37	1.35e-05
3082	diHPCARP_Ib.mttmppppd	6.888e+43	9.20	9.20	1.361e+37	1.35e-05
3083	diHPCARP_Ib.ptptmmmmmd	1.169e+44	9.52	9.52	1.357e+37	1.34e-05
3084	diHPCARP_Ib.mpptpmpmd	3.977e+43	8.89	8.89	1.338e+37	1.32e-05
3085	diHPCARP_Ib.mmtpppppd	6.345e+43	9.16	9.16	1.338e+37	1.32e-05
3086	diHPCARP_Ib.mpttptmpd	5.567e+44	10.47	10.47	1.314e+37	1.3e-05
3087	diHPCARP_Ib.mmmppmmpmd	3.601e+43	8.84	8.84	1.312e+37	1.3e-05
3088	diHPCARP_Ib.mmtmmpppd	3.124e+44	10.15	10.15	1.255e+37	1.24e-05
3089	diHPCARP_Ib.mpttmtmmd	4.812e+44	10.42	10.42	1.237e+37	1.22e-05
3090	diHPCARP_Ib.tmpmtmpmd	3.425e+44	10.22	10.22	1.233e+37	1.22e-05
3091	diHPCARP_Ib.pmmppptpd	4.584e+43	9.03	9.03	1.217e+37	1.2e-05
3092	diHPCARP_Ib.tpmmtppd	6.567e+43	9.24	9.24	1.213e+37	1.2e-05
3093	diHPCARP_Ib.tmpmtppmd	1.079e+45	10.91	10.91	1.212e+37	1.2e-05
3094	diHPCARP_Ib.tptmppmpd	1.543e+44	9.75	9.75	1.211e+37	1.2e-05
3095	diHPCARP_Ib.mmmtpmmpd	4.827e+44	10.44	10.44	1.204e+37	1.19e-05
3096	diHPCARP_Ib.pmmmmppmd	1.121e+44	9.57	9.57	1.195e+37	1.18e-05
3097	diHPCARP_Ib.mptmmmpmd	3.126e+44	10.18	10.18	1.195e+37	1.18e-05
3098	diHPCARP_Ib.ptttmtmpd	1.385e+44	9.73	9.73	1.122e+37	1.11e-05
3099	diHPCARP_Ib.tmttppppd	2.089e+44	9.98	9.98	1.116e+37	1.1e-05
3100	diHPCARP_Ib.pppmmtpd	1.860e+43	8.55	8.55	1.094e+37	1.08e-05
3101	diHPCARP_Ib.tmmmpmpd	2.541e+43	8.74	8.74	1.092e+37	1.08e-05
3102	diHPCARP_Ib.mppppppmd	5.108e+43	9.16	9.16	1.083e+37	1.07e-05
3103	diHPCARP_Ib.mttppmmmd	5.911e+44	10.62	10.62	1.081e+37	1.07e-05
3104	diHPCARP_Ib.tpttmtpd	3.663e+45	11.72	11.72	1.063e+37	1.05e-05
3105	diHPCARP_Ib.tpmtptmmd	7.952e+44	10.81	10.81	1.062e+37	1.05e-05
3106	diHPCARP_Ib.mmtmmptmd	4.727e+44	10.50	10.50	1.056e+37	1.04e-05
3107	diHPCARP_Ib.mmpmpmpmd	4.922e+43	9.16	9.16	1.054e+37	1.04e-05
3108	diHPCARP_Ib.tpmtpttmd	7.650e+44	10.79	10.79	1.051e+37	1.04e-05
3109	diHPCARP_Ib.mtptmmmmmd	1.716e+44	9.92	9.92	1.027e+37	1.02e-05
3110	diHPCARP_Ib.mmmtpmmpmd	3.769e+44	10.42	10.42	9.733e+36	9.63e-06
3111	diHPCARP_Ib.tppmpmmpmd	4.624e+43	9.17	9.17	9.676e+36	9.57e-06
3112	diHPCARP_Ib.tpmppptpd	3.930e+43	9.08	9.08	9.559e+36	9.46e-06
3113	diHPCARP_Ib.tpmppmtmd	6.471e+43	9.38	9.38	9.475e+36	9.37e-06
3114	diHPCARP_Ib.mptppptmd	2.743e+44	10.25	10.25	9.432e+36	9.33e-06
3115	diHPCARP_Ib.tppmmpppd	7.451e+43	9.47	9.47	9.418e+36	9.32e-06
3116	diHPCARP_Ib.mttmmmpd	1.020e+44	9.66	9.66	9.410e+36	9.31e-06
3117	diHPCARP_Ib.mpptpttmd	8.925e+43	9.59	9.59	9.173e+36	9.07e-06
3118	diHPCARP_Ib.tptmmpmpd	3.956e+44	10.48	10.48	9.150e+36	9.05e-06
3119	diHPCARP_Ib.tmpmtmmpd	5.981e+44	10.74	10.74	9.039e+36	8.94e-06
3120	diHPCARP_Ib.mpmmpptmd	6.470e+43	9.44	9.44	8.545e+36	8.45e-06
3121	diHPCARP_Ib.mmmtpmtmd	3.709e+44	10.49	10.49	8.477e+36	8.38e-06
3122	diHPCARP_Ib.tmpptppd	4.695e+44	10.63	10.63	8.451e+36	8.36e-06
3123	diHPCARP_Ib.mttmpmmpd	2.020e+44	10.13	10.13	8.384e+36	8.29e-06
3124	diHPCARP_Ib.tttmmmpmd	1.755e+44	10.05	10.05	8.330e+36	8.24e-06
3125	diHPCARP_Ib.tpttppppd	2.865e+44	10.35	10.35	8.214e+36	8.12e-06
3126	diHPCARP_Ib.mmttppppd	4.291e+44	10.60	10.60	8.098e+36	8.01e-06
3127	diHPCARP_Ib.mmmppmmpd	2.370e+43	8.88	8.88	8.090e+36	8e-06
3128	diHPCARP_Ib.mppmmmtmd	7.562e+43	9.57	9.57	8.059e+36	7.97e-06
3129	diHPCARP_Ib.tpptptmpd	2.092e+44	10.18	10.18	8.050e+36	7.96e-06
3130	diHPCARP_Ib.tpmtptppd	1.609e+44	10.02	10.02	8.036e+36	7.95e-06
3131	diHPCARP_Ib.pmtmmmpmd	2.939e+44	10.40	10.40	7.835e+36	7.75e-06
3132	diHPCARP_Ib.tpmtmttmd	5.378e+44	10.79	10.79	7.470e+36	7.39e-06
3133	diHPCARP_Ib.tpmmpmpd	5.606e+43	9.45	9.45	7.352e+36	7.27e-06
3134	diHPCARP_Ib.mpttppmpd	4.079e+44	10.63	10.63	7.337e+36	7.26e-06
3135	diHPCARP_Ib.tptppptpd	4.244e+44	10.67	10.67	7.158e+36	7.08e-06
3136	diHPCARP_Ib.tpttmmpd	1.038e+45	11.20	11.20	7.148e+36	7.07e-06
3137	diHPCARP_Ib.tmttppmpd	1.566e+44	10.08	10.08	7.070e+36	6.99e-06
3138	diHPCARP_Ib.mtptppptpd	2.798e+44	10.43	10.43	7.016e+36	6.94e-06
3139	diHPCARP_Ib.tpmtmtmpd	2.174e+44	10.29	10.29	6.937e+36	6.86e-06
3140	diHPCARP_Ib.mpmmtpppd	1.088e+44	9.89	9.89	6.808e+36	6.73e-06
3141	diHPCARP_Ib.tpttppmpd	4.375e+44	10.75	10.75	6.463e+36	6.39e-06
3142	diHPCARP_Ib.mtptmmmpd	1.146e+44	9.95	9.95	6.446e+36	6.38e-06
3143	diHPCARP_Ib.mpttppmmd	2.297e+44	10.38	10.38	6.328e+36	6.26e-06
3144	diHPCARP_Ib.mpptmmpd	1.058e+44	9.92	9.92	6.283e+36	6.22e-06
3145	diHPCARP_Ib.mtmppttmd	3.992e+44	10.72	10.72	6.236e+36	6.17e-06

3146	diHPCARP_Ib.ptptmtmpd	2.101e+44	10.35	10.35	6.081e+36	6.01e-06
3147	diHPCARP_Ib.pttmmpmpd	2.456e+44	10.45	10.45	5.986e+36	5.92e-06
3148	diHPCARP_Ib.tpmppptpd	3.471e+43	9.29	9.29	5.931e+36	5.87e-06
3149	diHPCARP_Ib.tmpptpmpd	4.835e+44	10.87	10.87	5.823e+36	5.76e-06
3150	diHPCARP_Ib.tpptmpmpd	1.993e+44	10.36	10.36	5.701e+36	5.64e-06
3151	diHPCARP_Ib.tpttmpppd	2.713e+44	10.54	10.54	5.651e+36	5.59e-06
3152	diHPCARP_Ib.mmpptpmpd	6.552e+44	11.09	11.09	5.452e+36	5.39e-06
3153	diHPCARP_Ib.mmpmtmpmd	5.332e+44	10.97	10.97	5.433e+36	5.37e-06
3154	diHPCARP_Ib.tptmmpppd	1.446e+44	10.21	10.21	5.288e+36	5.23e-06
3155	diHPCARP_Ib.tttmmmtmd	1.763e+44	10.33	10.33	5.264e+36	5.21e-06
3156	diHPCARP_Ib.mppmntpmd	7.069e+43	9.79	9.79	5.243e+36	5.19e-06
3157	diHPCARP_Ib.tpmtmtmpd	3.782e+44	10.80	10.80	5.141e+36	5.09e-06
3158	diHPCARP_Ib.tpmmmpppd	5.692e+44	11.05	11.05	5.038e+36	4.98e-06
3159	diHPCARP_Ib.tpmmmmtmd	1.773e+43	9.03	9.03	4.688e+36	4.64e-06
3160	diHPCARP_Ib.tmpmtmpmd	1.604e+44	10.35	10.35	4.650e+36	4.6e-06
3161	diHPCARP_Ib.tmpmtmpmd	2.848e+44	10.69	10.69	4.639e+36	4.59e-06
3162	diHPCARP_Ib.ptmpmpmpd	8.202e+43	9.96	9.96	4.580e+36	4.53e-06
3163	diHPCARP_Ib.tmtmpmpd	1.513e+44	10.35	10.35	4.399e+36	4.35e-06
3164	diHPCARP_Ib.pttmntppd	2.077e+44	10.54	10.54	4.378e+36	4.33e-06
3165	diHPCARP_Ib.mmpptpmpd	4.402e+44	10.99	10.99	4.358e+36	4.31e-06
3166	diHPCARP_Ib.mttpmmmmd	1.514e+44	10.35	10.35	4.345e+36	4.3e-06
3167	diHPCARP_Ib.mmpmmmtmd	8.255e+43	10.02	10.02	4.121e+36	4.08e-06
3168	diHPCARP_Ib.mttmpmmmd	1.780e+44	10.49	10.49	4.081e+36	4.04e-06
3169	diHPCARP_Ib.mpmmtmpmd	3.380e+43	9.51	9.51	3.976e+36	3.93e-06
3170	diHPCARP_Ib.pmpmmpppd	3.097e+43	9.47	9.47	3.887e+36	3.84e-06
3171	diHPCARP_Ib.tpmpppppd	3.784e+43	9.61	9.61	3.770e+36	3.73e-06
3172	diHPCARP_Ib.tmpptmpmd	2.813e+44	10.81	10.81	3.736e+36	3.7e-06
3173	diHPCARP_Ib.mpttpttpd	9.214e+44	11.54	11.54	3.620e+36	3.58e-06
3174	diHPCARP_Ib.ttpmpmpd	3.597e+43	9.61	9.61	3.585e+36	3.55e-06
3175	diHPCARP_Ib.mttmmmmmpd	1.278e+44	10.38	10.38	3.487e+36	3.45e-06
3176	diHPCARP_Ib.ptmtmpmpd	6.022e+43	9.94	9.94	3.438e+36	3.4e-06
3177	diHPCARP_Ib.pmttpmpmd	4.345e+44	11.12	11.12	3.432e+36	3.39e-06
3178	diHPCARP_Ib.mttmpmpd	3.674e+44	11.04	11.04	3.359e+36	3.32e-06
3179	diHPCARP_Ib.mppmtmpmd	4.449e+44	11.16	11.16	3.320e+36	3.28e-06
3180	diHPCARP_Ib.mpttmppmd	5.313e+44	11.26	11.26	3.316e+36	3.28e-06
3181	diHPCARP_Ib.pmpptmpd	2.315e+43	9.40	9.40	3.289e+36	3.25e-06
3182	diHPCARP_Ib.tpmpppppd	4.820e+43	9.84	9.84	3.261e+36	3.23e-06
3183	diHPCARP_Ib.mpmmtmpmd	2.682e+43	9.50	9.50	3.241e+36	3.21e-06
3184	diHPCARP_Ib.mpmmmppmd	1.282e+44	10.45	10.45	3.152e+36	3.12e-06
3185	diHPCARP_Ib.ptppptmpd	5.885e+43	10.00	10.00	3.063e+36	3.03e-06
3186	diHPCARP_Ib.mpmmmmpmd	1.775e+44	10.66	10.66	3.051e+36	3.02e-06
3187	diHPCARP_Ib.mmmtpmpd	3.230e+44	11.02	11.02	3.030e+36	3e-06
3188	diHPCARP_Ib.mmmppppmd	2.588e+43	9.52	9.52	3.016e+36	2.98e-06
3189	diHPCARP_Ib.mpttptmpd	5.307e+44	11.33	11.33	2.972e+36	2.94e-06
3190	diHPCARP_Ib.mpmmtmpmd	3.637e+43	9.74	9.74	2.926e+36	2.89e-06
3191	diHPCARP_Ib.tpmpppppd	3.505e+43	9.72	9.72	2.899e+36	2.87e-06
3192	diHPCARP_Ib.mmpmtmpmd	3.184e+44	11.04	11.04	2.892e+36	2.86e-06
3193	diHPCARP_Ib.mptmtmpmd	6.945e+44	11.52	11.52	2.833e+36	2.8e-06
3194	diHPCARP_Ib.tpmppppmd	4.982e+43	9.95	9.95	2.796e+36	2.77e-06
3195	diHPCARP_Ib.mpttppppd	3.166e+44	11.06	11.06	2.775e+36	2.74e-06
3196	diHPCARP_Ib.mmpppptmpd	1.629e+44	10.67	10.67	2.742e+36	2.71e-06
3197	diHPCARP_Ib.ppmptmpd	3.178e+44	11.07	11.07	2.728e+36	2.7e-06
3198	diHPCARP_Ib.tppmmmtmd	4.191e+44	11.27	11.27	2.573e+36	2.55e-06
3199	diHPCARP_Ib.mtttppmpd	1.592e+44	10.70	10.70	2.538e+36	2.51e-06
3200	diHPCARP_Ib.tpmmntmpd	5.059e+43	10.03	10.03	2.489e+36	2.46e-06
3201	diHPCARP_Ib.mptmmppmd	3.031e+44	11.11	11.11	2.463e+36	2.44e-06
3202	diHPCARP_Ib.tpmtppppd	1.707e+45	12.14	12.14	2.430e+36	2.4e-06
3203	diHPCARP_Ib.tpttpttpd	6.738e+44	11.60	11.60	2.398e+36	2.37e-06
3204	diHPCARP_Ib.mtpmmmmmd	1.693e+44	10.80	10.80	2.292e+36	2.27e-06
3205	diHPCARP_Ib.pmmmtppmd	2.301e+43	9.63	9.63	2.234e+36	2.21e-06
3206	diHPCARP_Ib.mpmmtmpmd	6.426e+43	10.25	10.25	2.196e+36	2.17e-06
3207	diHPCARP_Ib.mpttppppd	2.124e+44	10.97	10.97	2.175e+36	2.15e-06
3208	diHPCARP_Ib.mmttppppd	4.551e+44	11.42	11.42	2.167e+36	2.14e-06
3209	diHPCARP_Ib.mpttppmpd	2.114e+44	10.97	10.97	2.162e+36	2.14e-06
3210	diHPCARP_Ib.mmpmmntmpd	7.009e+43	10.32	10.32	2.113e+36	2.09e-06
3211	diHPCARP_Ib.mtppppppd	8.723e+43	10.46	10.46	2.087e+36	2.06e-06
3212	diHPCARP_Ib.mppmtmpmd	1.468e+44	10.79	10.79	2.011e+36	1.99e-06
3213	diHPCARP_Ib.mmmtpmpd	3.888e+44	11.38	11.38	1.986e+36	1.96e-06
3214	diHPCARP_Ib.pmttmmpmd	4.373e+44	11.46	11.46	1.968e+36	1.95e-06
3215	diHPCARP_Ib.tptmmmpd	1.012e+45	11.96	11.96	1.957e+36	1.94e-06
3216	diHPCARP_Ib.mpmmmntmpd	1.322e+44	10.75	10.75	1.938e+36	1.92e-06
3217	diHPCARP_Ib.tppppptmpd	1.499e+44	10.84	10.84	1.897e+36	1.88e-06

3218	diHPCARP_Ib.pmntmptmd	2.443e+43	9.76	9.76	1.887e+36	1.87e-06
3219	diHPCARP_Ib.mtppmmpmd	2.384e+44	11.13	11.13	1.851e+36	1.83e-06
3220	diHPCARP_Ib.mtmtppmmd	2.659e+44	11.20	11.20	1.832e+36	1.81e-06
3221	diHPCARP_Ib.mmppttmd	1.298e+44	10.78	10.78	1.812e+36	1.79e-06
3222	diHPCARP_Ib.tmpppmtmd	8.202e+43	10.51	10.51	1.801e+36	1.78e-06
3223	diHPCARP_Ib.ptpppttmd	8.556e+43	10.56	10.56	1.746e+36	1.73e-06
3224	diHPCARP_Ib.tmpptmpd	2.705e+44	11.26	11.26	1.686e+36	1.67e-06
3225	diHPCARP_Ib.mpmtmptmd	3.918e+43	10.13	10.13	1.627e+36	1.61e-06
3226	diHPCARP_Ib.mppmmptmd	1.573e+44	10.96	10.96	1.626e+36	1.61e-06
3227	diHPCARP_Ib.mtpppmmd	6.395e+43	10.43	10.43	1.604e+36	1.59e-06
3228	diHPCARP_Ib.tppppptpd	7.656e+43	10.55	10.55	1.591e+36	1.57e-06
3229	diHPCARP_Ib.tttppptpd	4.283e+43	10.22	10.22	1.532e+36	1.52e-06
3230	diHPCARP_Ib.mtmmpmmd	7.663e+44	11.95	11.95	1.512e+36	1.5e-06
3231	diHPCARP_Ib.ttpmtptpd	2.168e+44	11.22	11.22	1.462e+36	1.45e-06
3232	diHPCARP_Ib.mppmmpmmd	5.816e+43	10.45	10.45	1.423e+36	1.41e-06
3233	diHPCARP_Ib.mtttppmmd	4.025e+44	11.61	11.61	1.393e+36	1.38e-06
3234	diHPCARP_Ib.tmntppppd	5.645e+44	11.82	11.82	1.391e+36	1.38e-06
3235	diHPCARP_Ib.mtppppmpd	5.786e+43	10.47	10.47	1.369e+36	1.35e-06
3236	diHPCARP_Ib.mppmmntmd	1.880e+44	11.20	11.20	1.299e+36	1.29e-06
3237	diHPCARP_Ib.mtttmmpmd	1.977e+44	11.24	11.24	1.276e+36	1.26e-06
3238	diHPCARP_Ib.mmtmmpmmd	1.168e+44	10.93	10.93	1.267e+36	1.25e-06
3239	diHPCARP_Ib.mptmmtmd	3.677e+44	11.63	11.63	1.241e+36	1.23e-06
3240	diHPCARP_Ib.ptmptppd	1.574e+44	11.13	11.13	1.232e+36	1.22e-06
3241	diHPCARP_Ib.ptmpttmd	7.170e+43	10.66	10.66	1.230e+36	1.22e-06
3242	diHPCARP_Ib.tmpmmtmd	5.073e+43	10.45	10.45	1.229e+36	1.22e-06
3243	diHPCARP_Ib.tmntpoptpd	3.555e+44	11.63	11.63	1.189e+36	1.18e-06
3244	diHPCARP_Ib.ptptmmpmd	7.698e+43	10.73	10.73	1.167e+36	1.15e-06
3245	diHPCARP_Ib.mppoptmmd	5.163e+43	10.50	10.50	1.161e+36	1.15e-06
3246	diHPCARP_Ib.mtmmtmmpmd	3.911e+44	11.73	11.73	1.112e+36	1.1e-06
3247	diHPCARP_Ib.mppmmtmmd	4.687e+43	10.48	10.48	1.082e+36	1.07e-06
3248	diHPCARP_Ib.mppptmmpmd	1.971e+44	11.34	11.34	1.078e+36	1.07e-06
3249	diHPCARP_Ib.mppmmpmmd	9.160e+43	10.94	10.94	9.790e+35	9.68e-07
3250	diHPCARP_Ib.tmpmtmtpd	2.166e+44	11.47	11.47	9.589e+35	9.48e-07
3251	diHPCARP_Ib.mmtmtpmmd	5.932e+44	12.08	12.08	9.473e+35	9.37e-07
3252	diHPCARP_Ib.mppmmpmmd	7.640e+43	10.86	10.86	9.354e+35	9.25e-07
3253	diHPCARP_Ib.ttmmpmmpd	1.016e+44	11.05	11.05	9.134e+35	9.03e-07
3254	diHPCARP_Ib.tppptppmd	1.741e+44	11.40	11.40	8.634e+35	8.54e-07
3255	diHPCARP_Ib.mtmtppmmd	8.024e+43	10.94	10.94	8.600e+35	8.51e-07
3256	diHPCARP_Ib.mmpmpttmd	1.525e+44	11.35	11.35	8.252e+35	8.16e-07
3257	diHPCARP_Ib.tppmmpmmd	9.546e+43	11.14	11.14	7.360e+35	7.28e-07
3258	diHPCARP_Ib.tmpppmmd	9.092e+43	11.12	11.12	7.247e+35	7.17e-07
3259	diHPCARP_Ib.pmpptmmpd	1.426e+43	10.02	10.02	7.211e+35	7.13e-07
3260	diHPCARP_Ib.mppppmmd	2.156e+44	11.64	11.64	7.197e+35	7.12e-07
3261	diHPCARP_Ib.mtmmtmmpd	8.089e+43	11.06	11.06	7.083e+35	7.01e-07
3262	diHPCARP_Ib.pmpmtmmpd	2.647e+44	11.83	11.83	6.368e+35	6.3e-07
3263	diHPCARP_Ib.pmpppmmpd	2.046e+43	10.31	10.31	6.316e+35	6.25e-07
3264	diHPCARP_Ib.pmntpmpmd	3.172e+44	11.97	11.97	6.065e+35	6e-07
3265	diHPCARP_Ib.mppmtmmpd	3.572e+43	10.71	10.71	5.602e+35	5.54e-07
3266	diHPCARP_Ib.mtmtmptmd	3.253e+44	12.04	12.04	5.520e+35	5.46e-07
3267	diHPCARP_Ib.tppmmpmmd	6.995e+43	11.13	11.13	5.443e+35	5.38e-07
3268	diHPCARP_Ib.mmtmtpmmd	2.780e+44	11.99	11.99	5.128e+35	5.07e-07
3269	diHPCARP_Ib.mtmppmmpd	7.126e+43	11.19	11.19	4.990e+35	4.94e-07
3270	diHPCARP_Ib.mppmmpmmd	2.394e+44	11.92	11.92	4.925e+35	4.87e-07
3271	diHPCARP_Ib.mmpmpppmd	7.222e+43	11.22	11.22	4.876e+35	4.82e-07
3272	diHPCARP_Ib.ttmmpmtpd	1.998e+44	11.84	11.84	4.739e+35	4.69e-07
3273	diHPCARP_Ib.tppmmpmtpd	2.295e+44	11.93	11.93	4.715e+35	4.66e-07
3274	diHPCARP_Ib.tmntppmmd	2.717e+44	12.07	12.07	4.388e+35	4.34e-07
3275	diHPCARP_Ib.tppmtpppmd	2.973e+44	12.13	12.13	4.341e+35	4.29e-07
3276	diHPCARP_Ib.tttppmmpd	4.948e+44	12.44	12.44	4.284e+35	4.24e-07
3277	diHPCARP_Ib.tpmtppptpd	1.008e+45	12.87	12.87	4.260e+35	4.21e-07
3278	diHPCARP_Ib.tmpppptmd	1.418e+44	11.71	11.71	4.176e+35	4.13e-07
3279	diHPCARP_Ib.pmntpoptmd	2.245e+44	11.99	11.99	4.160e+35	4.11e-07
3280	diHPCARP_Ib.pmpmtmtpd	1.796e+44	11.89	11.89	3.890e+35	3.85e-07
3281	diHPCARP_Ib.ptmtppmmd	1.130e+44	11.64	11.64	3.765e+35	3.72e-07
3282	diHPCARP_Ib.mmpmmpmmd	4.922e+43	11.15	11.15	3.709e+35	3.67e-07
3283	diHPCARP_Ib.pmpppmtpd	1.076e+44	11.65	11.65	3.482e+35	3.44e-07
3284	diHPCARP_Ib.ttmppmmtmd	6.595e+43	11.43	11.43	3.084e+35	3.05e-07
3285	diHPCARP_Ib.mppmtppmmd	2.598e+44	12.27	12.27	2.980e+35	2.95e-07
3286	diHPCARP_Ib.mppmmpmmd	1.607e+43	10.63	10.63	2.882e+35	2.85e-07
3287	diHPCARP_Ib.pmpppmmpd	1.482e+44	11.96	11.96	2.856e+35	2.83e-07
3288	diHPCARP_Ib.tmmpmmpd	4.049e+43	11.25	11.25	2.602e+35	2.57e-07
3289	diHPCARP_Ib.ttpmmpmmd	1.030e+44	11.81	11.81	2.552e+35	2.52e-07

3290	diHPCARP_Ib.ttptmpppd	3.105e+44	12.47	12.47	2.550e+35	2.52e-07
3291	diHPCARP_Ib.mmptmtmmd	8.927e+43	11.74	11.74	2.502e+35	2.48e-07
3292	diHPCARP_Ib.mtpmppmpd	2.095e+43	10.90	10.90	2.389e+35	2.36e-07
3293	diHPCARP_Ib.tpppppppd	1.237e+44	12.01	12.01	2.194e+35	2.17e-07
3294	diHPCARP_Ib.mtpmppmmd	2.198e+43	10.98	10.98	2.194e+35	2.17e-07
3295	diHPCARP_Ib.pmmppmmd	1.198e+43	10.71	10.71	1.880e+35	1.86e-07
3296	diHPCARP_Ib.mpmtppmmd	1.377e+44	12.17	12.17	1.880e+35	1.86e-07
3297	diHPCARP_Ib.mmpmmtmmd	4.005e+43	11.44	11.44	1.858e+35	1.84e-07
3298	diHPCARP_Ib.ptmtmmpd	1.182e+44	12.19	12.19	1.566e+35	1.55e-07
3299	diHPCARP_Ib.mpppmtmmd	1.957e+44	12.52	12.52	1.486e+35	1.47e-07
3300	diHPCARP_Ib.tttppmpd	6.094e+43	11.85	11.85	1.419e+35	1.4e-07
3301	diHPCARP_Ib.ptppmmd	3.344e+43	11.52	11.52	1.355e+35	1.34e-07
3302	diHPCARP_Ib.mpmtptmmd	1.981e+44	12.58	12.58	1.352e+35	1.34e-07
3303	diHPCARP_Ib.mpmtpttmd	3.411e+44	12.91	12.91	1.351e+35	1.34e-07
3304	diHPCARP_Ib.tmpmtpmmd	9.255e+43	12.16	12.16	1.282e+35	1.27e-07
3305	diHPCARP_Ib.mpmtppmpd	5.602e+44	13.24	13.24	1.261e+35	1.25e-07
3306	diHPCARP_Ib.mtmtppmmd	5.816e+44	13.29	13.29	1.209e+35	1.2e-07
3307	diHPCARP_Ib.mpmtpttmd	1.745e+44	12.60	12.60	1.164e+35	1.15e-07
3308	diHPCARP_Ib.tpmtppmpd	1.662e+44	12.59	12.59	1.126e+35	1.11e-07
3309	diHPCARP_Ib.pmpmtpmmd	1.179e+44	12.44	12.44	1.021e+35	1.01e-07
3310	diHPCARP_Ib.pmpmtpmmd	2.954e+43	11.69	11.69	9.069e+34	8.97e-08
3311	diHPCARP_Ib.tppmmpmmd	6.474e+43	12.27	12.27	7.406e+34	7.33e-08
3312	diHPCARP_Ib.mmpmtpmmd	3.748e+43	11.98	11.98	7.031e+34	6.95e-08
3313	diHPCARP_Ib.tttmtpd	1.348e+44	12.79	12.79	6.543e+34	6.47e-08
3314	diHPCARP_Ib.tttmtpmpd	1.195e+44	12.76	12.76	6.038e+34	5.97e-08
3315	diHPCARP_Ib.tttmtpmpd	1.836e+44	13.16	13.16	4.790e+34	4.74e-08
3316	diHPCARP_Ib.tttmmpmpd	5.970e+43	12.57	12.57	4.159e+34	4.11e-08
3317	diHPCARP_Ib.ptmmpmmpd	5.615e+43	12.54	12.54	4.130e+34	4.09e-08
3318	diHPCARP_Ib.tttmtpd	2.627e+44	13.46	13.46	4.100e+34	4.06e-08
3319	diHPCARP_Ib.pmpmtpmmd	5.702e+43	12.58	12.58	3.887e+34	3.85e-08
3320	diHPCARP_Ib.ttttppmpd	2.862e+44	13.55	13.55	3.880e+34	3.84e-08
3321	diHPCARP_Ib.ttpmmpmpd	1.362e+43	11.77	11.77	3.659e+34	3.62e-08
3322	diHPCARP_Ib.tttmppppd	2.347e+44	13.55	13.55	3.150e+34	3.12e-08
3323	diHPCARP_Ib.tttmmpmmd	1.677e+44	13.58	13.58	2.139e+34	2.12e-08
3324	diHPCARP_Ib.tttmtpd	3.148e+44	14.10	14.10	1.680e+34	1.66e-08
3325	diHPCARP_Ib.tmtmpppd	4.275e+44	14.34	14.34	1.524e+34	1.51e-08
3326	diHPCARP_Ib.tttmppppd	5.783e+44	14.74	14.74	1.053e+34	1.04e-08
3327	diHPCARP_Ib.mppmmpmmd	2.498e+43	12.90	12.90	9.999e+33	9.89e-09
3328	diHPCARP_Ib.tmtppmpd	4.479e+44	14.62	14.62	9.957e+33	9.85e-09
3329	diHPCARP_Ib.ttmppmmpd	5.228e+43	13.42	13.42	8.788e+33	8.69e-09
3330	diHPCARP_Ib.mmpmmtmd	8.561e+44	15.13	15.13	8.153e+33	8.06e-09
3331	diHPCARP_Ib.tppmmpd	5.780e+43	13.53	13.53	8.112e+33	8.02e-09
3332	diHPCARP_Ib.ttttppppd	6.619e+44	14.99	14.99	7.952e+33	7.87e-09
3333	diHPCARP_Ib.mmpmtpmmd	9.843e+43	13.89	13.89	7.533e+33	7.45e-09
3334	diHPCARP_Ib.ttttptpd	8.144e+44	15.20	15.20	6.864e+33	6.79e-09
3335	diHPCARP_Ib.tmpmmpmpd	1.426e+44	14.50	14.50	3.886e+33	3.84e-09
3336	diHPCARP_Ib.tttmmpppd	3.688e+44	15.25	15.25	2.859e+33	2.83e-09
3337	diHPCARP_Ib.mmpmmpmmd	1.986e+44	15.83	15.83	5.847e+32	5.78e-10
3338	diHPCARP_Ib.mmpmmtmd	1.180e+44	15.56	15.56	5.447e+32	5.39e-10
3339	diHPCARP_Ib.mmpmmpmmd	2.025e+44	16.00	16.00	4.473e+32	4.42e-10
3340	diHPCARP_Ib.mmpmmtmmd	1.127e+44	16.78	16.78	6.731e+31	6.66e-11
3341	diHPCARP_Ib.mmpmmtmmd	4.963e+43	17.16	17.16	1.567e+31	1.55e-11
3342	diHPCARP_Ib.ptptmmd	1.029e+43	23.59	23.59	6.764e+25	6.69e-17
3343	diHPCARP_Ib.tptptmmd	1.106e+44	27.73	27.73	6.913e+23	6.84e-19
3344	diHPCARP_Ib.mtptmmd	1.443e+44	28.12	28.12	4.751e+23	4.7e-19
3345	diHPCARP_Ib.tptptmpd	9.994e+43	27.96	27.96	4.271e+23	4.22e-19
3346	diHPCARP_Ib.ptptmmd	8.459e+43	28.22	28.22	2.339e+23	2.31e-19
3347	diHPCARP_Ib.ptptmpd	5.981e+43	29.62	29.62	1.584e+22	1.57e-20
3348	Total				1.011e+44	100

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(2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)

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Population analysis at 300K. Vibrational scaling: 0.971.

3356 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)

3357 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

3358 %: contribution to the population (with current data set assumed 100%)

3359 Compound Qtot Erel Erel2 n*Q*MB %

3360 -----

3361 diHPCARP_Ic.pppppptpd 3.438e+43 0.24 0.24 2.289e+43 32.7

3362	diHPCARP_Ic.mmtmptmmd	1.632e+43	0.00	0.00	1.632e+43	23.3
3363	diHPCARP_Ic.pptmppmmd	2.292e+43	0.76	0.76	6.443e+42	9.21
3364	diHPCARP_Ic.pmtmntmmd	1.075e+43	0.60	0.60	3.962e+42	5.67
3365	diHPCARP_Ic.pptpmtpmmd	2.217e+43	1.27	1.27	2.617e+42	3.74
3366	diHPCARP_Ic.ppmmntpmmd	2.670e+43	1.45	1.45	2.332e+42	3.33
3367	diHPCARP_Ic.pttmntmmd	1.202e+43	1.09	1.09	1.929e+42	2.76
3368	diHPCARP_Ic.mmppttpd	2.836e+43	1.72	1.72	1.578e+42	2.26
3369	diHPCARP_Ic.pmppttpd	1.235e+43	1.37	1.37	1.236e+42	1.77
3370	diHPCARP_Ic.pptmptpd	1.270e+44	2.83	2.83	1.094e+42	1.56
3371	diHPCARP_Ic.mttmptmmd	1.296e+43	1.51	1.51	1.032e+42	1.48
3372	diHPCARP_Ic.tpppmntpd	2.735e+43	2.07	2.07	8.464e+41	1.21
3373	diHPCARP_Ic.tptmmntmmd	3.194e+43	2.39	2.39	5.818e+41	0.832
3374	diHPCARP_Ic.ppmmntpmmd	9.024e+42	1.69	1.69	5.328e+41	0.762
3375	diHPCARP_Ic.pmmmpmmd	2.187e+43	2.55	2.55	3.022e+41	0.432
3376	diHPCARP_Ic.pmtmptmmd	2.645e+43	2.67	2.67	3.013e+41	0.431
3377	diHPCARP_Ic.pptmpppd	5.714e+44	4.57	4.57	2.678e+41	0.383
3378	diHPCARP_Ic.pmpmptpd	6.617e+43	3.42	3.42	2.150e+41	0.307
3379	diHPCARP_Ic.pppppmmd	3.275e+43	3.00	3.00	2.148e+41	0.307
3380	diHPCARP_Ic.tmmmmntmmd	2.525e+43	2.93	2.93	1.851e+41	0.265
3381	diHPCARP_Ic.pmpmptpmmd	5.271e+43	3.40	3.40	1.766e+41	0.253
3382	diHPCARP_Ic.pptpmtmmd	1.495e+44	4.07	4.07	1.613e+41	0.231
3383	diHPCARP_Ic.mmtpptmmd	3.809e+43	3.32	3.32	1.462e+41	0.209
3384	diHPCARP_Ic.pppppttpd	5.444e+43	3.53	3.53	1.456e+41	0.208
3385	diHPCARP_Ic.tmtmptmmd	3.914e+43	3.35	3.35	1.411e+41	0.202
3386	diHPCARP_Ic.pptpmtpmmd	1.323e+43	2.72	2.72	1.388e+41	0.198
3387	diHPCARP_Ic.tmtmmpmmd	1.846e+43	2.94	2.94	1.336e+41	0.191
3388	diHPCARP_Ic.pptppptpd	6.325e+43	3.71	3.71	1.262e+41	0.18
3389	diHPCARP_Ic.mttppptpd	2.477e+43	3.16	3.16	1.245e+41	0.178
3390	diHPCARP_Ic.pptpppppd	1.126e+44	4.12	4.12	1.131e+41	0.162
3391	diHPCARP_Ic.pptpppmmd	3.480e+43	3.42	3.42	1.115e+41	0.159
3392	diHPCARP_Ic.pttpmtpmmd	3.424e+43	3.48	3.48	9.982e+40	0.143
3393	diHPCARP_Ic.pptpppppd	2.988e+44	4.79	4.79	9.714e+40	0.139
3394	diHPCARP_Ic.ptmmntpmmd	2.742e+43	3.39	3.39	9.266e+40	0.133
3395	diHPCARP_Ic.pmtpppppd	3.180e+43	3.49	3.49	9.157e+40	0.131
3396	diHPCARP_Ic.pptppptpd	9.671e+43	4.20	4.20	8.442e+40	0.121
3397	diHPCARP_Ic.tmtmmpmmd	8.285e+43	4.18	4.18	7.441e+40	0.106
3398	diHPCARP_Ic.mttppptmmd	4.940e+43	3.99	3.99	6.118e+40	0.0875
3399	diHPCARP_Ic.pmtpmtmmd	2.162e+43	3.53	3.53	5.824e+40	0.0833
3400	diHPCARP_Ic.pptmmpmmd	3.813e+43	3.88	3.88	5.700e+40	0.0815
3401	diHPCARP_Ic.tttmntmmd	1.833e+43	3.52	3.52	5.040e+40	0.0721
3402	diHPCARP_Ic.pptppmmd	7.797e+43	4.39	4.39	4.931e+40	0.0705
3403	diHPCARP_Ic.pptpmtppd	1.078e+44	4.62	4.62	4.639e+40	0.0663
3404	diHPCARP_Ic.pptppptpd	1.818e+44	4.94	4.94	4.571e+40	0.0654
3405	diHPCARP_Ic.pptpmpmmd	2.022e+44	5.01	5.01	4.504e+40	0.0644
3406	diHPCARP_Ic.tmmmpmmd	2.217e+43	3.70	3.70	4.503e+40	0.0644
3407	diHPCARP_Ic.pptpmpmmd	1.780e+44	4.97	4.97	4.261e+40	0.0609
3408	diHPCARP_Ic.pmtmnttpd	3.477e+44	5.38	5.38	4.219e+40	0.0603
3409	diHPCARP_Ic.pppmptpmmd	1.231e+44	4.76	4.76	4.175e+40	0.0597
3410	diHPCARP_Ic.tmntmmpmmd	6.514e+43	4.39	4.39	4.140e+40	0.0592
3411	diHPCARP_Ic.mmttptmmd	1.043e+44	4.71	4.71	3.843e+40	0.0549
3412	diHPCARP_Ic.pptpmtpmmd	1.420e+44	4.92	4.92	3.693e+40	0.0528
3413	diHPCARP_Ic.tmtmmpmmd	2.402e+44	5.26	5.26	3.567e+40	0.051
3414	diHPCARP_Ic.tpppptpd	6.084e+43	4.44	4.44	3.546e+40	0.0507
3415	diHPCARP_Ic.mttppptpd	6.835e+43	4.51	4.51	3.531e+40	0.0505
3416	diHPCARP_Ic.pppmntmmd	1.022e+44	4.78	4.78	3.395e+40	0.0485
3417	diHPCARP_Ic.mttppptpd	8.372e+43	4.66	4.66	3.388e+40	0.0485
3418	diHPCARP_Ic.tppmptpd	1.189e+44	4.88	4.88	3.287e+40	0.047
3419	diHPCARP_Ic.pmmtpmmd	6.735e+43	4.55	4.55	3.270e+40	0.0468
3420	diHPCARP_Ic.ppppppppd	1.549e+44	5.05	5.05	3.253e+40	0.0465
3421	diHPCARP_Ic.pmtmmpmmd	9.853e+42	3.41	3.41	3.212e+40	0.0459
3422	diHPCARP_Ic.ptpmpmmd	5.776e+43	4.48	4.48	3.162e+40	0.0452
3423	diHPCARP_Ic.pmpmptmmd	1.542e+43	3.69	3.69	3.161e+40	0.0452
3424	diHPCARP_Ic.pptpppppd	2.358e+44	5.38	5.38	2.851e+40	0.0408
3425	diHPCARP_Ic.pptppmmd	4.417e+43	4.39	4.39	2.811e+40	0.0402
3426	diHPCARP_Ic.pmtpmtpmmd	4.010e+43	4.33	4.33	2.791e+40	0.0399
3427	diHPCARP_Ic.mtmmpmmd	2.452e+43	4.06	4.06	2.699e+40	0.0386
3428	diHPCARP_Ic.mmpppmmd	3.163e+43	4.23	4.23	2.642e+40	0.0378
3429	diHPCARP_Ic.tptmmpmmd	2.649e+44	5.50	5.50	2.627e+40	0.0376
3430	diHPCARP_Ic.pmmppmmd	2.792e+43	4.17	4.17	2.539e+40	0.0363
3431	diHPCARP_Ic.mtttptmmd	5.674e+43	4.60	4.60	2.532e+40	0.0362
3432	diHPCARP_Ic.ptttmtmmd	2.319e+44	5.45	5.45	2.501e+40	0.0358
3433	diHPCARP_Ic.ppttptpmmd	3.427e+44	5.68	5.68	2.492e+40	0.0356

3434	diHPCARP_Ic.ptmmpmmpd	1.977e+43	3.98	3.98	2.479e+40	0.0355
3435	diHPCARP_Ic.pptpmtppd	1.689e+43	3.91	3.91	2.387e+40	0.0341
3436	diHPCARP_Ic.mttmpmtmd	5.709e+43	4.65	4.65	2.335e+40	0.0334
3437	diHPCARP_Ic.pptpmttmd	9.544e+43	4.96	4.96	2.309e+40	0.033
3438	diHPCARP_Ic.tpttmmpd	9.862e+44	6.36	6.36	2.286e+40	0.0327
3439	diHPCARP_Ic.tmtppmmpd	9.500e+43	4.98	4.98	2.245e+40	0.0321
3440	diHPCARP_Ic.ptpmpppmd	2.296e+43	4.14	4.14	2.225e+40	0.0318
3441	diHPCARP_Ic.ppppmtppd	1.162e+44	5.11	5.11	2.212e+40	0.0316
3442	diHPCARP_Ic.pptpmtmmd	1.200e+44	5.15	5.15	2.141e+40	0.0306
3443	diHPCARP_Ic.pmpppmmpd	3.735e+43	4.46	4.46	2.117e+40	0.0303
3444	diHPCARP_Ic.tptmntmmd	1.467e+44	5.27	5.27	2.115e+40	0.0302
3445	diHPCARP_Ic.pttpmttmd	8.690e+43	5.00	5.00	1.990e+40	0.0285
3446	diHPCARP_Ic.ppttppmmd	5.607e+43	4.74	4.74	1.979e+40	0.0283
3447	diHPCARP_Ic.mttmntmmd	2.189e+43	4.19	4.19	1.956e+40	0.028
3448	diHPCARP_Ic.tttmptmmd	1.784e+43	4.08	4.08	1.916e+40	0.0274
3449	diHPCARP_Ic.tptmptmmd	8.306e+43	5.00	5.00	1.897e+40	0.0271
3450	diHPCARP_Ic.pmpmmttmd	1.982e+43	4.15	4.15	1.882e+40	0.0269
3451	diHPCARP_Ic.mmppptmmd	6.323e+43	4.86	4.86	1.813e+40	0.0259
3452	diHPCARP_Ic.pppmmtmmd	2.851e+43	4.39	4.39	1.808e+40	0.0258
3453	diHPCARP_Ic.ppptpmtmd	2.985e+44	5.80	5.80	1.790e+40	0.0256
3454	diHPCARP_Ic.mmpmmttmd	1.964e+43	4.18	4.18	1.783e+40	0.0255
3455	diHPCARP_Ic.ppppptmmd	9.678e+43	5.13	5.13	1.779e+40	0.0254
3456	diHPCARP_Ic.mtttptmmd	1.049e+44	5.18	5.18	1.759e+40	0.0251
3457	diHPCARP_Ic.pmttmtmmd	6.855e+43	4.93	4.93	1.744e+40	0.0249
3458	diHPCARP_Ic.pmtmpttmd	1.532e+44	5.44	5.44	1.671e+40	0.0239
3459	diHPCARP_Ic.ppppptmmd	1.373e+44	5.37	5.37	1.670e+40	0.0239
3460	diHPCARP_Ic.pppmptmmd	3.744e+43	4.63	4.63	1.593e+40	0.0228
3461	diHPCARP_Ic.mmtmntmmd	2.086e+43	4.30	4.30	1.534e+40	0.0219
3462	diHPCARP_Ic.tptmptmmd	3.540e+43	4.64	4.64	1.481e+40	0.0212
3463	diHPCARP_Ic.mtppttmd	3.893e+43	4.69	4.69	1.481e+40	0.0212
3464	diHPCARP_Ic.mmppttmd	1.666e+44	5.56	5.56	1.473e+40	0.0211
3465	diHPCARP_Ic.ppttmtmmd	3.028e+44	5.93	5.93	1.454e+40	0.0208
3466	diHPCARP_Ic.tmtpptmmd	3.795e+44	6.07	6.07	1.434e+40	0.0205
3467	diHPCARP_Ic.tptpmpppd	1.123e+44	5.36	5.36	1.387e+40	0.0198
3468	diHPCARP_Ic.mtmmpmtpmd	5.037e+43	4.89	4.89	1.370e+40	0.0196
3469	diHPCARP_Ic.tpmmpmtpmd	2.554e+43	4.49	4.49	1.363e+40	0.0195
3470	diHPCARP_Ic.ptttmtmmd	6.893e+43	5.13	5.13	1.272e+40	0.0182
3471	diHPCARP_Ic.mmmmpmtpmd	1.813e+44	5.71	5.71	1.259e+40	0.018
3472	diHPCARP_Ic.tptpmmmpd	5.922e+43	5.05	5.05	1.243e+40	0.0178
3473	diHPCARP_Ic.mttmptmmd	2.885e+43	4.63	4.63	1.231e+40	0.0176
3474	diHPCARP_Ic.ptmppmmpd	9.948e+42	3.99	3.99	1.228e+40	0.0176
3475	diHPCARP_Ic.pmtmptmmd	1.595e+44	5.65	5.65	1.220e+40	0.0174
3476	diHPCARP_Ic.ptmmpmmpd	2.609e+43	4.58	4.58	1.202e+40	0.0172
3477	diHPCARP_Ic.pppppmmpd	7.186e+43	5.21	5.21	1.155e+40	0.0165
3478	diHPCARP_Ic.mmmmpmtpmd	1.580e+44	5.68	5.68	1.146e+40	0.0164
3479	diHPCARP_Ic.tmmmpmtpmd	1.601e+44	5.70	5.70	1.130e+40	0.0162
3480	diHPCARP_Ic.ttpmmpmmpd	4.060e+43	4.89	4.89	1.120e+40	0.016
3481	diHPCARP_Ic.pppmppppd	2.203e+44	5.90	5.90	1.107e+40	0.0158
3482	diHPCARP_Ic.tptpmtmmd	5.032e+43	5.05	5.05	1.058e+40	0.0151
3483	diHPCARP_Ic.mmppptmmd	1.790e+44	5.81	5.81	1.056e+40	0.0151
3484	diHPCARP_Ic.tpttppppd	3.151e+44	6.15	6.15	1.046e+40	0.015
3485	diHPCARP_Ic.ptmmtmtpmd	5.605e+43	5.12	5.12	1.042e+40	0.0149
3486	diHPCARP_Ic.tptpmtmmd	7.952e+43	5.34	5.34	1.022e+40	0.0146
3487	diHPCARP_Ic.pmttmtmmd	4.214e+43	4.98	4.98	9.889e+39	0.0141
3488	diHPCARP_Ic.tptpmtmmd	5.829e+43	5.21	5.21	9.402e+39	0.0134
3489	diHPCARP_Ic.pptppmmpd	2.835e+43	4.78	4.78	9.352e+39	0.0134
3490	diHPCARP_Ic.tttpptmmd	5.130e+43	5.13	5.13	9.333e+39	0.0133
3491	diHPCARP_Ic.ptmtmtmmd	3.800e+43	4.96	4.96	9.193e+39	0.0131
3492	diHPCARP_Ic.pmtpptmmd	1.378e+44	5.76	5.76	8.805e+39	0.0126
3493	diHPCARP_Ic.ppmmpmmpd	2.426e+43	4.75	4.75	8.353e+39	0.0119
3494	diHPCARP_Ic.mtttptppd	1.720e+44	5.94	5.94	8.075e+39	0.0115
3495	diHPCARP_Ic.ttmmpmtpmd	6.799e+43	5.41	5.41	7.743e+39	0.0111
3496	diHPCARP_Ic.pmpmtpmmd	3.536e+43	5.03	5.03	7.665e+39	0.011
3497	diHPCARP_Ic.pmpmmtmmd	2.875e+43	4.91	4.91	7.567e+39	0.0108
3498	diHPCARP_Ic.pptmptmmd	1.624e+44	5.97	5.97	7.226e+39	0.0103
3499	diHPCARP_Ic.pmpmtpmmd	8.370e+42	4.22	4.22	7.081e+39	0.0101
3500	diHPCARP_Ic.tptmmpmmpd	1.492e+44	5.95	5.95	6.924e+39	0.0099
3501	diHPCARP_Ic.mtmmpmtpmd	7.881e+43	5.57	5.57	6.853e+39	0.0098
3502	diHPCARP_Ic.pmttppmmpd	4.987e+43	5.31	5.31	6.757e+39	0.00966
3503	diHPCARP_Ic.pttmmtppd	1.113e+44	5.79	5.79	6.728e+39	0.00962
3504	diHPCARP_Ic.pmtpptmmd	8.677e+43	5.65	5.65	6.672e+39	0.00954
3505	diHPCARP_Ic.ttmmpmmpd	1.896e+43	4.74	4.74	6.656e+39	0.00952

3506	diHPCARP_Ic.pppmptmd	1.632e+44	6.03	6.03	6.617e+39	0.00946
3507	diHPCARP_Ic.ptppptpd	1.311e+43	4.53	4.53	6.514e+39	0.00932
3508	diHPCARP_Ic.ptttmtpd	1.958e+44	6.16	6.16	6.376e+39	0.00912
3509	diHPCARP_Ic.pmtmmtpd	3.127e+43	5.07	5.07	6.361e+39	0.0091
3510	diHPCARP_Ic.ptttmttd	1.946e+44	6.16	6.16	6.312e+39	0.00903
3511	diHPCARP_Ic.ppnmmttmd	2.430e+44	6.30	6.30	6.274e+39	0.00897
3512	diHPCARP_Ic.ptttmtpd	1.316e+44	5.93	5.93	6.251e+39	0.00894
3513	diHPCARP_Ic.pmtppptpd	2.814e+44	6.40	6.40	6.133e+39	0.00877
3514	diHPCARP_Ic.pptmtmpd	8.543e+43	5.69	5.69	6.081e+39	0.0087
3515	diHPCARP_Ic.tpppmmmmd	2.569e+43	4.98	4.98	6.056e+39	0.00866
3516	diHPCARP_Ic.ptmmmttd	8.082e+43	5.67	5.67	6.009e+39	0.00859
3517	diHPCARP_Ic.mmpptmmd	5.726e+43	5.47	5.47	5.933e+39	0.00848
3518	diHPCARP_Ic.mtttptmd	1.222e+44	5.92	5.92	5.931e+39	0.00848
3519	diHPCARP_Ic.tpmptmpd	3.287e+43	5.14	5.14	5.915e+39	0.00846
3520	diHPCARP_Ic.tptpmtpd	2.051e+44	6.26	6.26	5.617e+39	0.00803
3521	diHPCARP_Ic.ppttptmpd	1.013e+44	5.84	5.84	5.605e+39	0.00802
3522	diHPCARP_Ic.ptmtmmd	3.442e+44	6.59	6.59	5.480e+39	0.00784
3523	diHPCARP_Ic.mmpptmmd	2.039e+44	6.28	6.28	5.427e+39	0.00776
3524	diHPCARP_Ic.pmtppptpd	1.377e+44	6.05	6.05	5.389e+39	0.00771
3525	diHPCARP_Ic.ptmmpmpmd	3.440e+43	5.22	5.22	5.375e+39	0.00769
3526	diHPCARP_Ic.tmmmmtpd	1.634e+44	6.15	6.15	5.367e+39	0.00768
3527	diHPCARP_Ic.mttmptpd	1.064e+44	5.90	5.90	5.362e+39	0.00767
3528	diHPCARP_Ic.mmmmmtpd	7.199e+43	5.68	5.68	5.280e+39	0.00755
3529	diHPCARP_Ic.mmpmptmpd	5.714e+43	5.54	5.54	5.277e+39	0.00755
3530	diHPCARP_Ic.tmtmmmpd	1.280e+44	6.02	6.02	5.269e+39	0.00753
3531	diHPCARP_Ic.tmtppppd	7.964e+43	5.75	5.75	5.188e+39	0.00742
3532	diHPCARP_Ic.pptpmtmd	4.107e+43	5.36	5.36	5.106e+39	0.0073
3533	diHPCARP_Ic.pmpmtmpd	5.743e+43	5.57	5.57	5.051e+39	0.00722
3534	diHPCARP_Ic.pmtppmmd	7.161e+43	5.70	5.70	5.024e+39	0.00718
3535	diHPCARP_Ic.ptppmpmd	1.917e+43	4.94	4.94	4.839e+39	0.00692
3536	diHPCARP_Ic.tptpmpd	1.733e+44	6.27	6.27	4.709e+39	0.00673
3537	diHPCARP_Ic.tptmtpd	1.112e+44	6.00	6.00	4.703e+39	0.00672
3538	diHPCARP_Ic.tmtmptpd	7.390e+43	5.76	5.76	4.686e+39	0.0067
3539	diHPCARP_Ic.mttmptpd	4.361e+43	5.45	5.45	4.652e+39	0.00665
3540	diHPCARP_Ic.tmmmmtpd	1.951e+44	6.35	6.35	4.631e+39	0.00662
3541	diHPCARP_Ic.pmtppmpd	6.662e+43	5.71	5.71	4.578e+39	0.00655
3542	diHPCARP_Ic.mtpmpmpd	1.177e+43	4.69	4.69	4.540e+39	0.00649
3543	diHPCARP_Ic.mpppmtpd	6.382e+43	5.70	5.70	4.499e+39	0.00643
3544	diHPCARP_Ic.tppmmtpd	1.142e+43	4.68	4.68	4.465e+39	0.00639
3545	diHPCARP_Ic.pptppptmd	1.164e+44	6.07	6.07	4.417e+39	0.00632
3546	diHPCARP_Ic.tttptpmd	1.112e+44	6.05	6.05	4.342e+39	0.00621
3547	diHPCARP_Ic.ttpmmpmd	4.920e+43	5.57	5.57	4.309e+39	0.00616
3548	diHPCARP_Ic.mmtppptpd	8.045e+43	5.86	5.86	4.301e+39	0.00615
3549	diHPCARP_Ic.pmpmtmpd	2.721e+43	5.24	5.24	4.133e+39	0.00591
3550	diHPCARP_Ic.mmpptmpd	3.650e+43	5.42	5.42	4.107e+39	0.00587
3551	diHPCARP_Ic.mttppptpd	1.793e+44	6.37	6.37	4.104e+39	0.00587
3552	diHPCARP_Ic.mtmmtmpd	4.490e+43	5.55	5.55	4.097e+39	0.00586
3553	diHPCARP_Ic.pptppmmpd	6.474e+43	5.77	5.77	4.069e+39	0.00582
3554	diHPCARP_Ic.mptppmpd	1.210e+43	4.77	4.77	4.031e+39	0.00576
3555	diHPCARP_Ic.ptmmmtppd	7.037e+43	5.84	5.84	3.898e+39	0.00557
3556	diHPCARP_Ic.tmmmpmpd	8.834e+43	5.99	5.99	3.849e+39	0.0055
3557	diHPCARP_Ic.pmmmpmpd	7.024e+43	5.85	5.85	3.838e+39	0.00549
3558	diHPCARP_Ic.pmttptmmd	2.754e+44	6.67	6.67	3.794e+39	0.00542
3559	diHPCARP_Ic.ptmmmtmpd	2.524e+43	5.25	5.25	3.784e+39	0.00541
3560	diHPCARP_Ic.ttmmpmpd	4.181e+43	5.55	5.55	3.769e+39	0.00539
3561	diHPCARP_Ic.pptpmpd	2.220e+44	6.55	6.55	3.764e+39	0.00538
3562	diHPCARP_Ic.tpppmtmd	5.457e+45	8.46	8.46	3.725e+39	0.00533
3563	diHPCARP_Ic.tpmmtmpd	2.220e+43	5.18	5.18	3.715e+39	0.00531
3564	diHPCARP_Ic.ttpmmpmd	1.984e+43	5.13	5.13	3.653e+39	0.00522
3565	diHPCARP_Ic.pmtppmpd	3.857e+43	5.52	5.52	3.652e+39	0.00522
3566	diHPCARP_Ic.tptpmpd	1.064e+44	6.16	6.16	3.491e+39	0.00499
3567	diHPCARP_Ic.mpmmpmpd	4.433e+43	5.65	5.65	3.414e+39	0.00488
3568	diHPCARP_Ic.pptmtpmd	1.708e+44	6.46	6.46	3.373e+39	0.00482
3569	diHPCARP_Ic.pmttptmpd	1.928e+44	6.55	6.55	3.271e+39	0.00468
3570	diHPCARP_Ic.pmttptpd	1.900e+44	6.54	6.54	3.263e+39	0.00467
3571	diHPCARP_Ic.mppmptmd	5.763e+43	5.83	5.83	3.247e+39	0.00464
3572	diHPCARP_Ic.ptmmpmpd	2.849e+43	5.41	5.41	3.246e+39	0.00464
3573	diHPCARP_Ic.tmtmmpmd	1.861e+44	6.53	6.53	3.244e+39	0.00464
3574	diHPCARP_Ic.ppptpmpd	6.920e+44	7.32	7.32	3.236e+39	0.00463
3575	diHPCARP_Ic.pptmtpmpd	2.720e+43	5.40	5.40	3.143e+39	0.00449
3576	diHPCARP_Ic.ttmmpmpd	1.680e+43	5.13	5.13	3.083e+39	0.00441
3577	diHPCARP_Ic.mpmmpmpd	1.109e+43	4.90	4.90	3.001e+39	0.00429

3578	diHPCARP_Ic.ptpmmppmd	9.027e+42	4.78	4.78	2.953e+39	0.00422
3579	diHPCARP_Ic.mmtppptpd	6.507e+43	5.97	5.97	2.932e+39	0.00419
3580	diHPCARP_Ic.ptmmptmpd	3.845e+43	5.67	5.67	2.847e+39	0.00407
3581	diHPCARP_Ic.tmmmpmtmd	1.804e+44	6.59	6.59	2.842e+39	0.00406
3582	diHPCARP_Ic.tmtppptpd	4.026e+44	7.07	7.07	2.832e+39	0.00405
3583	diHPCARP_Ic.ppmmtmmd	6.571e+43	5.99	5.99	2.831e+39	0.00405
3584	diHPCARP_Ic.mtmppmpmd	1.578e+43	5.15	5.15	2.803e+39	0.00401
3585	diHPCARP_Ic.tpttmtmpd	1.286e+44	6.41	6.41	2.772e+39	0.00396
3586	diHPCARP_Ic.tmpppptpd	5.176e+43	5.86	5.86	2.767e+39	0.00396
3587	diHPCARP_Ic.pmpptmtd	4.630e+43	5.81	5.81	2.712e+39	0.00388
3588	diHPCARP_Ic.pmttmtppd	5.136e+44	7.25	7.25	2.698e+39	0.00386
3589	diHPCARP_Ic.pmtppmpmd	6.345e+43	6.00	6.00	2.686e+39	0.00384
3590	diHPCARP_Ic.mtmmtmpd	7.151e+43	6.08	6.08	2.671e+39	0.00382
3591	diHPCARP_Ic.tmtppptpd	3.318e+44	7.01	7.01	2.582e+39	0.00369
3592	diHPCARP_Ic.mptmmtmmd	4.807e+43	5.86	5.86	2.580e+39	0.00369
3593	diHPCARP_Ic.tpttmtmpd	4.570e+44	7.21	7.21	2.538e+39	0.00363
3594	diHPCARP_Ic.pttptmtd	6.727e+43	6.08	6.08	2.510e+39	0.00359
3595	diHPCARP_Ic.mmttpttpd	1.008e+44	6.32	6.32	2.495e+39	0.00357
3596	diHPCARP_Ic.ptptpmpmd	4.598e+43	5.86	5.86	2.493e+39	0.00356
3597	diHPCARP_Ic.pmttptppd	3.881e+44	7.14	7.14	2.445e+39	0.0035
3598	diHPCARP_Ic.pmmmpmmd	4.471e+43	5.86	5.86	2.410e+39	0.00345
3599	diHPCARP_Ic.tpttptmpd	3.160e+44	7.04	7.04	2.354e+39	0.00337
3600	diHPCARP_Ic.pmtppmpmd	3.586e+43	5.77	5.77	2.259e+39	0.00323
3601	diHPCARP_Ic.pmpptmtd	5.678e+43	6.04	6.04	2.249e+39	0.00322
3602	diHPCARP_Ic.mtmtpmpd	6.329e+43	6.11	6.11	2.241e+39	0.0032
3603	diHPCARP_Ic.tmmptmtd	6.542e+43	6.13	6.13	2.241e+39	0.0032
3604	diHPCARP_Ic.tttptmtd	5.038e+43	5.98	5.98	2.201e+39	0.00315
3605	diHPCARP_Ic.tmmppmtd	1.086e+44	6.45	6.45	2.189e+39	0.00313
3606	diHPCARP_Ic.pttptmpd	4.725e+43	5.95	5.95	2.169e+39	0.0031
3607	diHPCARP_Ic.mtmtpmpd	4.491e+43	5.93	5.93	2.149e+39	0.00307
3608	diHPCARP_Ic.tttppmtd	4.065e+43	5.88	5.88	2.100e+39	0.003
3609	diHPCARP_Ic.tppmpmpmd	2.478e+44	6.97	6.97	2.088e+39	0.00299
3610	diHPCARP_Ic.tpttmmmd	1.128e+44	6.50	6.50	2.085e+39	0.00298
3611	diHPCARP_Ic.ptpmpmpmd	9.463e+42	5.02	5.02	2.069e+39	0.00296
3612	diHPCARP_Ic.mtmmpptpd	5.731e+43	6.10	6.10	2.065e+39	0.00295
3613	diHPCARP_Ic.tppppptpd	1.168e+44	6.53	6.53	2.044e+39	0.00292
3614	diHPCARP_Ic.ptppmttd	2.428e+43	5.60	5.60	2.009e+39	0.00287
3615	diHPCARP_Ic.tmtptmpd	1.882e+44	6.84	6.84	1.955e+39	0.0028
3616	diHPCARP_Ic.ttmmtmtd	6.504e+43	6.21	6.21	1.951e+39	0.00279
3617	diHPCARP_Ic.mtmtpmpd	5.740e+43	6.14	6.14	1.934e+39	0.00277
3618	diHPCARP_Ic.mmtmtmpd	1.430e+44	6.69	6.69	1.918e+39	0.00274
3619	diHPCARP_Ic.tppmmmpmd	7.371e+43	6.31	6.31	1.859e+39	0.00266
3620	diHPCARP_Ic.pmmmpmtd	6.170e+43	6.21	6.21	1.856e+39	0.00265
3621	diHPCARP_Ic.tppptmpmd	3.987e+44	7.32	7.32	1.839e+39	0.00263
3622	diHPCARP_Ic.ptntpmpmd	3.231e+43	5.83	5.83	1.816e+39	0.0026
3623	diHPCARP_Ic.ptttppmpd	4.550e+43	6.04	6.04	1.799e+39	0.00257
3624	diHPCARP_Ic.tpptmmtpd	7.596e+43	6.35	6.35	1.789e+39	0.00256
3625	diHPCARP_Ic.tpptmmtmd	8.836e+44	7.82	7.82	1.772e+39	0.00253
3626	diHPCARP_Ic.tmmmmmmmd	5.664e+43	6.19	6.19	1.761e+39	0.00252
3627	diHPCARP_Ic.tmtppptpd	2.050e+44	6.96	6.96	1.745e+39	0.00249
3628	diHPCARP_Ic.pmtptmpd	2.780e+43	5.77	5.77	1.732e+39	0.00248
3629	diHPCARP_Ic.mmtptmpd	1.281e+44	6.69	6.69	1.720e+39	0.00246
3630	diHPCARP_Ic.tmtptmmd	2.778e+44	7.17	7.17	1.668e+39	0.00238
3631	diHPCARP_Ic.pmtmtmmd	7.949e+43	6.43	6.43	1.638e+39	0.00234
3632	diHPCARP_Ic.ppptptppd	1.156e+44	6.67	6.67	1.594e+39	0.00228
3633	diHPCARP_Ic.mmtptppd	1.904e+44	6.97	6.97	1.591e+39	0.00227
3634	diHPCARP_Ic.pttppmpmd	8.341e+43	6.48	6.48	1.587e+39	0.00227
3635	diHPCARP_Ic.tmmmtmmd	3.166e+44	7.28	7.28	1.582e+39	0.00226
3636	diHPCARP_Ic.ptppmmtpd	5.307e+43	6.22	6.22	1.558e+39	0.00223
3637	diHPCARP_Ic.tmtmmmpmd	6.607e+43	6.35	6.35	1.554e+39	0.00222
3638	diHPCARP_Ic.mmtptmmd	1.371e+44	6.79	6.79	1.551e+39	0.00222
3639	diHPCARP_Ic.tmpmptpd	2.231e+43	5.72	5.72	1.511e+39	0.00216
3640	diHPCARP_Ic.tmmppmtd	1.105e+44	6.69	6.69	1.478e+39	0.00211
3641	diHPCARP_Ic.tmttmtmpd	1.353e+44	6.82	6.82	1.461e+39	0.00209
3642	diHPCARP_Ic.mttptmpd	1.090e+44	6.69	6.69	1.457e+39	0.00208
3643	diHPCARP_Ic.tttptmpd	2.130e+44	7.09	7.09	1.449e+39	0.00207
3644	diHPCARP_Ic.mmtptmpd	2.149e+44	7.11	7.11	1.410e+39	0.00202
3645	diHPCARP_Ic.tttptmmd	5.638e+43	6.34	6.34	1.367e+39	0.00195
3646	diHPCARP_Ic.tptmptmpd	5.375e+43	6.32	6.32	1.347e+39	0.00193
3647	diHPCARP_Ic.mppppmpd	1.348e+44	6.87	6.87	1.342e+39	0.00192
3648	diHPCARP_Ic.pptmtmmd	8.191e+43	6.58	6.58	1.327e+39	0.0019
3649	diHPCARP_Ic.pptmptmpd	4.056e+43	6.16	6.16	1.322e+39	0.00189

3650	diHPCARP_Ic.tptmtpd	3.852e+44	7.50	7.50	1.316e+39	0.00188
3651	diHPCARP_Ic.ptmtmtpd	7.381e+43	6.52	6.52	1.316e+39	0.00188
3652	diHPCARP_Ic.tppmtpd	4.286e+43	6.20	6.20	1.299e+39	0.00186
3653	diHPCARP_Ic.pptmmtpd	3.654e+43	6.11	6.11	1.295e+39	0.00185
3654	diHPCARP_Ic.tptmtpmd	2.199e+44	7.18	7.18	1.291e+39	0.00185
3655	diHPCARP_Ic.ttmtpmtd	9.684e+43	6.69	6.69	1.288e+39	0.00184
3656	diHPCARP_Ic.tttptmtd	8.631e+43	6.63	6.63	1.288e+39	0.00184
3657	diHPCARP_Ic.mtmtpmtd	1.848e+44	7.08	7.08	1.282e+39	0.00183
3658	diHPCARP_Ic.pmpmtpd	7.936e+43	6.58	6.58	1.274e+39	0.00182
3659	diHPCARP_Ic.tptmtpmd	6.990e+43	6.51	6.51	1.270e+39	0.00182
3660	diHPCARP_Ic.ptmmtpmtd	7.412e+43	6.54	6.54	1.268e+39	0.00181
3661	diHPCARP_Ic.pptmtpmtd	1.941e+45	8.50	8.50	1.254e+39	0.00179
3662	diHPCARP_Ic.mttptmtd	2.715e+44	7.33	7.33	1.246e+39	0.00178
3663	diHPCARP_Ic.mppmtpd	3.507e+43	6.11	6.11	1.245e+39	0.00178
3664	diHPCARP_Ic.mmmtpmtd	3.177e+43	6.05	6.05	1.245e+39	0.00178
3665	diHPCARP_Ic.pppptmtd	8.681e+43	6.66	6.66	1.223e+39	0.00175
3666	diHPCARP_Ic.tppmtpmtd	4.151e+43	6.25	6.25	1.156e+39	0.00165
3667	diHPCARP_Ic.tptmtpmd	2.645e+44	7.36	7.36	1.146e+39	0.00164
3668	diHPCARP_Ic.pptptmtd	2.534e+44	7.34	7.34	1.145e+39	0.00164
3669	diHPCARP_Ic.ttmtpmtd	1.178e+44	6.88	6.88	1.143e+39	0.00163
3670	diHPCARP_Ic.tmmtpmtd	1.386e+44	6.99	6.99	1.125e+39	0.00161
3671	diHPCARP_Ic.tppmtpmtd	3.545e+43	6.18	6.18	1.110e+39	0.00159
3672	diHPCARP_Ic.tmtmtpmtd	1.619e+44	7.09	7.09	1.105e+39	0.00158
3673	diHPCARP_Ic.tmtptmtd	6.754e+44	7.94	7.94	1.102e+39	0.00158
3674	diHPCARP_Ic.mtppmtd	1.174e+43	5.53	5.53	1.095e+39	0.00157
3675	diHPCARP_Ic.ptmmtpmtd	6.580e+43	6.57	6.57	1.084e+39	0.00155
3676	diHPCARP_Ic.tppmtpmtd	9.214e+44	8.15	8.15	1.067e+39	0.00153
3677	diHPCARP_Ic.mmtmtpmtd	1.441e+44	7.04	7.04	1.066e+39	0.00152
3678	diHPCARP_Ic.tmmtpmtd	7.580e+44	8.04	8.04	1.053e+39	0.00151
3679	diHPCARP_Ic.tptptmtd	2.839e+44	7.46	7.46	1.053e+39	0.00151
3680	diHPCARP_Ic.mmmtpmtd	4.434e+43	6.35	6.35	1.050e+39	0.0015
3681	diHPCARP_Ic.pppmtpmtd	1.254e+44	6.97	6.97	1.045e+39	0.00149
3682	diHPCARP_Ic.mppmtpd	2.686e+43	6.06	6.06	1.037e+39	0.00148
3683	diHPCARP_Ic.mtptmtd	3.840e+43	6.27	6.27	1.036e+39	0.00148
3684	diHPCARP_Ic.tptmtpmtd	1.109e+44	6.92	6.92	1.011e+39	0.00145
3685	diHPCARP_Ic.pmmtpmtd	7.119e+43	6.66	6.66	9.995e+38	0.00143
3686	diHPCARP_Ic.mptmtpmtd	6.893e+43	6.64	6.64	9.958e+38	0.00142
3687	diHPCARP_Ic.ttmtpmtd	1.143e+43	5.58	5.58	9.821e+38	0.0014
3688	diHPCARP_Ic.tmtptmtd	3.454e+44	7.61	7.61	9.802e+38	0.0014
3689	diHPCARP_Ic.tptmtpd	4.355e+44	7.76	7.76	9.728e+38	0.00139
3690	diHPCARP_Ic.pptmtpmtd	1.691e+44	7.19	7.19	9.714e+38	0.00139
3691	diHPCARP_Ic.mptmtpmtd	1.068e+44	6.92	6.92	9.694e+38	0.00139
3692	diHPCARP_Ic.mtppmtd	1.549e+43	5.77	5.77	9.678e+38	0.00138
3693	diHPCARP_Ic.mmtmtpd	1.883e+44	7.27	7.27	9.582e+38	0.00137
3694	diHPCARP_Ic.tppmtpmtd	1.883e+44	7.27	7.27	9.475e+38	0.00135
3695	diHPCARP_Ic.mtmtpmtd	2.859e+44	7.53	7.53	9.338e+38	0.00134
3696	diHPCARP_Ic.pppmtpmtd	3.537e+43	6.29	6.29	9.308e+38	0.00133
3697	diHPCARP_Ic.tmtptmtd	5.967e+43	6.60	6.60	9.307e+38	0.00133
3698	diHPCARP_Ic.tptmtpmtd	1.180e+44	7.01	7.01	9.226e+38	0.00132
3699	diHPCARP_Ic.tppmtpmtd	2.758e+44	7.52	7.52	9.189e+38	0.00131
3700	diHPCARP_Ic.tttmtpmtd	7.397e+43	6.74	6.74	9.027e+38	0.00129
3701	diHPCARP_Ic.mptmtpmtd	3.602e+43	6.32	6.32	8.979e+38	0.00128
3702	diHPCARP_Ic.ttmtpmtd	6.217e+43	6.65	6.65	8.969e+38	0.00128
3703	diHPCARP_Ic.pmtmtpmtd	1.660e+44	7.25	7.25	8.716e+38	0.00125
3704	diHPCARP_Ic.tmmtpmtd	2.449e+44	7.48	7.48	8.713e+38	0.00125
3705	diHPCARP_Ic.ptmtpmtd	6.999e+43	6.73	6.73	8.701e+38	0.00124
3706	diHPCARP_Ic.tppmtpmtd	1.526e+44	7.20	7.20	8.632e+38	0.00123
3707	diHPCARP_Ic.pppmtpd	5.099e+44	7.93	7.93	8.504e+38	0.00122
3708	diHPCARP_Ic.pppmtpmtd	8.557e+43	6.87	6.87	8.472e+38	0.00121
3709	diHPCARP_Ic.mmtmtpmtd	1.345e+44	7.14	7.14	8.389e+38	0.0012
3710	diHPCARP_Ic.mmtmtpmtd	1.810e+44	7.33	7.33	8.339e+38	0.00119
3711	diHPCARP_Ic.tppmtpd	5.295e+43	6.60	6.60	8.305e+38	0.00119
3712	diHPCARP_Ic.pptmtpmtd	1.259e+45	8.49	8.49	8.156e+38	0.00117
3713	diHPCARP_Ic.tmtmtpmtd	1.158e+44	7.07	7.07	8.150e+38	0.00117
3714	diHPCARP_Ic.pptmtpmtd	6.709e+44	8.12	8.12	8.086e+38	0.00116
3715	diHPCARP_Ic.mmmtpmtd	1.155e+44	7.08	7.08	8.083e+38	0.00116
3716	diHPCARP_Ic.mmmtpmtd	2.132e+44	7.45	7.45	7.978e+38	0.00114
3717	diHPCARP_Ic.pmmtpmtd	2.456e+43	6.17	6.17	7.915e+38	0.00113
3718	diHPCARP_Ic.pmtmtpd	9.536e+43	6.98	6.98	7.815e+38	0.00112
3719	diHPCARP_Ic.mtppmtd	3.180e+43	6.34	6.34	7.699e+38	0.0011
3720	diHPCARP_Ic.mtmtpmtd	1.294e+44	7.17	7.17	7.682e+38	0.0011
3721	diHPCARP_Ic.tppmtpmtd	6.062e+43	6.73	6.73	7.545e+38	0.00108

3722	diHPCARP_Ic.tmmmpptpd	3.423e+44	7.78	7.78	7.400e+38	0.00106
3723	diHPCARP_Ic.mtttmtmpd	7.669e+43	6.89	6.89	7.343e+38	0.00105
3724	diHPCARP_Ic.ptptpptpd	2.670e+44	7.64	7.64	7.313e+38	0.00105
3725	diHPCARP_Ic.ptpppmtmd	4.237e+43	6.55	6.55	7.158e+38	0.00102
3726	diHPCARP_Ic.mttpmtmmd	6.902e+43	6.85	6.85	7.043e+38	0.00101
3727	diHPCARP_Ic.ttpmtmtpd	1.903e+44	7.46	7.46	7.036e+38	0.00101
3728	diHPCARP_Ic.ttmtmmpmd	6.242e+43	6.80	6.80	6.986e+38	0.000999
3729	diHPCARP_Ic.pmpmpmpmd	6.983e+43	6.87	6.87	6.963e+38	0.000996
3730	diHPCARP_Ic.ttpmmmtmd	1.339e+44	7.26	7.26	6.941e+38	0.000993
3731	diHPCARP_Ic.ttmmmtmmd	9.272e+43	7.04	7.04	6.924e+38	0.00099
3732	diHPCARP_Ic.tptpptpd	2.744e+44	7.69	7.69	6.893e+38	0.000986
3733	diHPCARP_Ic.pppmpmtmd	7.592e+43	6.92	6.92	6.872e+38	0.000983
3734	diHPCARP_Ic.ppptpmpd	9.934e+43	7.08	7.08	6.856e+38	0.00098
3735	diHPCARP_Ic.pmmmtmtpd	5.231e+43	6.71	6.71	6.722e+38	0.000961
3736	diHPCARP_Ic.tppmpptpd	1.961e+43	6.13	6.13	6.711e+38	0.00096
3737	diHPCARP_Ic.tmtmptppd	4.144e+44	7.95	7.95	6.669e+38	0.000954
3738	diHPCARP_Ic.mpmtptmpd	5.088e+43	6.70	6.70	6.663e+38	0.000953
3739	diHPCARP_Ic.pmtmptmpd	7.414e+43	6.93	6.93	6.659e+38	0.000952
3740	diHPCARP_Ic.tmmmmmtmd	4.055e+44	7.94	7.94	6.636e+38	0.000949
3741	diHPCARP_Ic.tppmmmtmd	4.814e+44	8.05	8.05	6.581e+38	0.000941
3742	diHPCARP_Ic.mmmmmmtmd	1.729e+44	7.44	7.44	6.525e+38	0.000933
3743	diHPCARP_Ic.tmmmmmtmd	6.943e+44	8.28	8.28	6.479e+38	0.000926
3744	diHPCARP_Ic.tmmmtmtpd	2.942e+44	7.79	7.79	6.255e+38	0.000894
3745	diHPCARP_Ic.mtmmpmtmd	2.672e+44	7.73	7.73	6.196e+38	0.000886
3746	diHPCARP_Ic.pmmmpmpmd	5.237e+43	6.77	6.77	6.174e+38	0.000883
3747	diHPCARP_Ic.pttpptmpd	7.766e+43	7.00	7.00	6.164e+38	0.000881
3748	diHPCARP_Ic.pmtmmtmpd	2.978e+43	6.45	6.45	5.995e+38	0.000857
3749	diHPCARP_Ic.mmttptppd	1.720e+44	7.50	7.50	5.946e+38	0.00085
3750	diHPCARP_Ic.tmmmtmmd	6.773e+44	8.33	8.33	5.823e+38	0.000833
3751	diHPCARP_Ic.tmtmmtmpd	2.941e+44	7.83	7.83	5.815e+38	0.000831
3752	diHPCARP_Ic.mmpmmtmpd	1.216e+43	5.93	5.93	5.778e+38	0.000826
3753	diHPCARP_Ic.pttppmpmd	1.604e+43	6.10	6.10	5.728e+38	0.000819
3754	diHPCARP_Ic.ttttptpmd	1.559e+44	7.47	7.47	5.640e+38	0.000807
3755	diHPCARP_Ic.ppttptppd	1.588e+44	7.48	7.48	5.629e+38	0.000805
3756	diHPCARP_Ic.ptttptmpd	1.433e+44	7.42	7.42	5.603e+38	0.000801
3757	diHPCARP_Ic.pmttmtmpd	5.831e+43	6.90	6.90	5.510e+38	0.000788
3758	diHPCARP_Ic.tppmpmpmd	1.004e+44	7.23	7.23	5.463e+38	0.000781
3759	diHPCARP_Ic.mmttmtmpd	4.324e+44	8.10	8.10	5.434e+38	0.000777
3760	diHPCARP_Ic.pmmmpmpmd	3.757e+43	6.65	6.65	5.419e+38	0.000775
3761	diHPCARP_Ic.tttmptmpd	5.526e+43	6.88	6.88	5.399e+38	0.000772
3762	diHPCARP_Ic.tpptmttpd	1.621e+45	8.89	8.89	5.385e+38	0.00077
3763	diHPCARP_Ic.pmttppmpd	1.372e+44	7.43	7.43	5.304e+38	0.000758
3764	diHPCARP_Ic.pttppmpmd	2.563e+43	6.43	6.43	5.289e+38	0.000756
3765	diHPCARP_Ic.pmmtpmpd	1.879e+44	7.62	7.62	5.243e+38	0.00075
3766	diHPCARP_Ic.tppmpmpd	3.451e+43	6.62	6.62	5.230e+38	0.000748
3767	diHPCARP_Ic.pmtmtpd	5.387e+43	6.89	6.89	5.165e+38	0.000739
3768	diHPCARP_Ic.mtmtpmpd	4.737e+43	6.81	6.81	5.153e+38	0.000737
3769	diHPCARP_Ic.tmtmtpd	3.250e+44	7.96	7.96	5.151e+38	0.000737
3770	diHPCARP_Ic.tpptpmpd	2.566e+44	7.84	7.84	5.006e+38	0.000716
3771	diHPCARP_Ic.tmmmmmpmd	6.891e+43	7.06	7.06	4.996e+38	0.000714
3772	diHPCARP_Ic.tptpmtmmd	2.230e+44	7.76	7.76	4.972e+38	0.000711
3773	diHPCARP_Ic.pmtppmtmd	9.519e+43	7.26	7.26	4.921e+38	0.000704
3774	diHPCARP_Ic.tmmmmmpd	7.720e+43	7.15	7.15	4.806e+38	0.000687
3775	diHPCARP_Ic.ttpptmmd	1.315e+44	7.47	7.47	4.782e+38	0.000684
3776	diHPCARP_Ic.tmmppmmd	3.056e+44	7.97	7.97	4.744e+38	0.000678
3777	diHPCARP_Ic.pppmmtmpd	5.239e+43	6.93	6.93	4.700e+38	0.000672
3778	diHPCARP_Ic.ppppmtmd	6.172e+43	7.04	7.04	4.603e+38	0.000658
3779	diHPCARP_Ic.mmtppmtmd	1.634e+44	7.62	7.62	4.592e+38	0.000657
3780	diHPCARP_Ic.tptmttpd	8.295e+44	8.59	8.59	4.584e+38	0.000655
3781	diHPCARP_Ic.tmttptmpd	4.095e+44	8.17	8.17	4.556e+38	0.000651
3782	diHPCARP_Ic.tmtptmmd	9.801e+43	7.34	7.34	4.441e+38	0.000635
3783	diHPCARP_Ic.mmpmptmmd	2.061e+43	6.41	6.41	4.411e+38	0.000631
3784	diHPCARP_Ic.tmmtpmtmd	2.309e+44	7.85	7.85	4.409e+38	0.00063
3785	diHPCARP_Ic.pmpmptmmd	6.555e+43	7.10	7.10	4.409e+38	0.00063
3786	diHPCARP_Ic.mmtmtpd	3.126e+44	8.05	8.05	4.293e+38	0.000614
3787	diHPCARP_Ic.tppmmtmd	3.914e+43	6.82	6.82	4.196e+38	0.0006
3788	diHPCARP_Ic.mmpppmpd	1.346e+43	6.19	6.19	4.184e+38	0.000598
3789	diHPCARP_Ic.tptmmpmd	8.072e+43	7.27	7.27	4.064e+38	0.000581
3790	diHPCARP_Ic.tmtptmpd	1.151e+44	7.48	7.48	4.061e+38	0.000581
3791	diHPCARP_Ic.mtmptmpd	1.152e+44	7.49	7.49	4.035e+38	0.000577
3792	diHPCARP_Ic.pptmptppd	1.283e+44	7.56	7.56	3.973e+38	0.000568
3793	diHPCARP_Ic.pttmtmpd	1.393e+43	6.26	6.26	3.850e+38	0.000551

3794	diHPCARP_Ic.mpttmtmpd	1.404e+44	7.64	7.64	3.837e+38	0.000549
3795	diHPCARP_Ic.tnmtpttpd	1.001e+45	8.81	8.81	3.798e+38	0.000543
3796	diHPCARP_Ic.tpptmmpmd	1.428e+44	7.68	7.68	3.623e+38	0.000518
3797	diHPCARP_Ic.mmttmtppd	3.250e+44	8.18	8.18	3.601e+38	0.000515
3798	diHPCARP_Ic.tpppptpmd	1.787e+44	7.83	7.83	3.550e+38	0.000508
3799	diHPCARP_Ic.tpppmtppd	4.020e+44	8.32	8.32	3.517e+38	0.000503
3800	diHPCARP_Ic.ptppmtpd	2.669e+43	6.70	6.70	3.512e+38	0.000502
3801	diHPCARP_Ic.mttmmtmpd	5.013e+43	7.08	7.08	3.501e+38	0.000501
3802	diHPCARP_Ic.pmtmmmmmd	1.267e+43	6.27	6.27	3.435e+38	0.000491
3803	diHPCARP_Ic.tpttptppd	3.872e+44	8.31	8.31	3.407e+38	0.000487
3804	diHPCARP_Ic.ptppmmpmd	1.572e+43	6.41	6.41	3.370e+38	0.000482
3805	diHPCARP_Ic.ttttmmmpd	5.080e+43	7.11	7.11	3.344e+38	0.000478
3806	diHPCARP_Ic.pptpmtmd	1.491e+44	7.75	7.75	3.343e+38	0.000478
3807	diHPCARP_Ic.ppmmmppd	1.083e+44	7.57	7.57	3.333e+38	0.000477
3808	diHPCARP_Ic.tmpptmpd	3.909e+44	8.33	8.33	3.327e+38	0.000476
3809	diHPCARP_Ic.tpmmpmpmd	3.170e+44	8.21	8.21	3.309e+38	0.000473
3810	diHPCARP_Ic.mtttmmmmmd	3.269e+44	8.23	8.23	3.288e+38	0.00047
3811	diHPCARP_Ic.mtmtmtmpd	6.145e+43	7.24	7.24	3.272e+38	0.000468
3812	diHPCARP_Ic.pmmtpmtmd	2.958e+44	8.18	8.18	3.262e+38	0.000466
3813	diHPCARP_Ic.mtptppmpd	2.265e+44	8.02	8.02	3.247e+38	0.000464
3814	diHPCARP_Ic.mtmtptppd	8.610e+43	7.47	7.47	3.128e+38	0.000447
3815	diHPCARP_Ic.mmpmpttmd	3.789e+43	6.98	6.98	3.113e+38	0.000445
3816	diHPCARP_Ic.tpmmpmpmd	8.049e+43	7.43	7.43	3.104e+38	0.000444
3817	diHPCARP_Ic.mptmmtmpd	3.370e+44	8.29	8.29	3.090e+38	0.000442
3818	diHPCARP_Ic.tpptmtmpd	3.388e+44	8.29	8.29	3.074e+38	0.00044
3819	diHPCARP_Ic.tpttmtmtmd	1.658e+44	7.87	7.87	3.059e+38	0.000437
3820	diHPCARP_Ic.ptmpmttmd	9.520e+43	7.54	7.54	3.052e+38	0.000436
3821	diHPCARP_Ic.tptmptppd	3.034e+44	8.23	8.23	3.048e+38	0.000436
3822	diHPCARP_Ic.tptmtppd	5.156e+44	8.55	8.55	3.027e+38	0.000433
3823	diHPCARP_Ic.ttttmtmtmd	8.335e+43	7.47	7.47	3.017e+38	0.000431
3824	diHPCARP_Ic.mtmtmtmpd	9.280e+43	7.54	7.54	2.988e+38	0.000427
3825	diHPCARP_Ic.tmtpttpd	5.064e+44	8.55	8.55	2.974e+38	0.000425
3826	diHPCARP_Ic.tpttpmtpd	3.875e+44	8.40	8.40	2.958e+38	0.000423
3827	diHPCARP_Ic.ttttmmmpmd	1.331e+44	7.77	7.77	2.933e+38	0.000419
3828	diHPCARP_Ic.ttptptpmd	2.714e+44	8.20	8.20	2.883e+38	0.000412
3829	diHPCARP_Ic.ttptmtppd	7.989e+43	7.48	7.48	2.863e+38	0.000409
3830	diHPCARP_Ic.tttptppd	2.915e+44	8.26	8.26	2.821e+38	0.000403
3831	diHPCARP_Ic.tpttpttpd	3.709e+44	8.40	8.40	2.807e+38	0.000401
3832	diHPCARP_Ic.mpttptmpd	1.618e+44	7.91	7.91	2.796e+38	0.0004
3833	diHPCARP_Ic.mtttmtmtmd	2.732e+44	8.23	8.23	2.776e+38	0.000397
3834	diHPCARP_Ic.mmmmtmtmd	4.138e+44	8.47	8.47	2.773e+38	0.000396
3835	diHPCARP_Ic.mtptpmpmd	7.635e+43	7.47	7.47	2.753e+38	0.000394
3836	diHPCARP_Ic.tppmpttmd	4.183e+44	8.50	8.50	2.705e+38	0.000387
3837	diHPCARP_Ic.tpptpttmd	8.207e+44	8.91	8.91	2.666e+38	0.000381
3838	diHPCARP_Ic.ttmmnttpd	1.379e+44	7.85	7.85	2.658e+38	0.00038
3839	diHPCARP_Ic.tmpmptmpd	1.882e+43	6.66	6.66	2.644e+38	0.000378
3840	diHPCARP_Ic.tppmmpmpmd	1.840e+44	8.03	8.03	2.606e+38	0.000373
3841	diHPCARP_Ic.pmmmtmtmd	8.839e+43	7.59	7.59	2.599e+38	0.000372
3842	diHPCARP_Ic.tpppmtppd	2.818e+44	8.29	8.29	2.594e+38	0.000371
3843	diHPCARP_Ic.mmttpttmd	2.575e+44	8.24	8.24	2.574e+38	0.000368
3844	diHPCARP_Ic.mmttmtmtmd	2.793e+44	8.29	8.29	2.558e+38	0.000366
3845	diHPCARP_Ic.mmmmtmtppd	3.853e+44	8.48	8.48	2.554e+38	0.000365
3846	diHPCARP_Ic.mmmtpttmd	2.614e+44	8.25	8.25	2.554e+38	0.000365
3847	diHPCARP_Ic.ptmtptmpd	4.604e+43	7.22	7.22	2.551e+38	0.000365
3848	diHPCARP_Ic.tnmtpttmd	5.877e+44	8.74	8.74	2.505e+38	0.000358
3849	diHPCARP_Ic.ptmmmmmpmd	2.957e+43	6.96	6.96	2.499e+38	0.000357
3850	diHPCARP_Ic.tpmtmtmpd	9.100e+44	9.02	9.02	2.446e+38	0.00035
3851	diHPCARP_Ic.tmpppmmpd	2.929e+44	8.35	8.35	2.424e+38	0.000347
3852	diHPCARP_Ic.tmppttmd	8.875e+43	7.64	7.64	2.412e+38	0.000345
3853	diHPCARP_Ic.mptmmpmpd	5.536e+43	7.37	7.37	2.362e+38	0.000338
3854	diHPCARP_Ic.tttmmpmpmd	4.373e+43	7.24	7.24	2.332e+38	0.000333
3855	diHPCARP_Ic.tpmmmpppd	1.230e+44	7.86	7.86	2.327e+38	0.000333
3856	diHPCARP_Ic.tptmntppd	3.542e+44	8.49	8.49	2.317e+38	0.000331
3857	diHPCARP_Ic.tmtptmpd	1.057e+45	9.15	9.15	2.295e+38	0.000328
3858	diHPCARP_Ic.mtppmpmpmd	2.925e+43	7.01	7.01	2.280e+38	0.000326
3859	diHPCARP_Ic.pmmppmmmd	2.343e+43	6.88	6.88	2.277e+38	0.000326
3860	diHPCARP_Ic.tmpmmmmmpd	1.647e+43	6.67	6.67	2.271e+38	0.000325
3861	diHPCARP_Ic.tttmptpmd	9.384e+43	7.72	7.72	2.245e+38	0.000321
3862	diHPCARP_Ic.tpptmmmpmd	1.934e+44	8.15	8.15	2.243e+38	0.000321
3863	diHPCARP_Ic.mmmpttppd	1.150e+44	7.85	7.85	2.184e+38	0.000312
3864	diHPCARP_Ic.tptpmttmd	4.622e+44	8.70	8.70	2.135e+38	0.000305
3865	diHPCARP_Ic.pmtppttmd	3.132e+44	8.47	8.47	2.124e+38	0.000304

3866	diHPCARP_Ic.tttptmtmd	2.765e+44	8.41	8.41	2.077e+38	0.000297
3867	diHPCARP_Ic.ptttppmpmd	8.017e+43	7.68	7.68	2.054e+38	0.000294
3868	diHPCARP_Ic.tmmmtmmmd	1.732e+44	8.14	8.14	2.040e+38	0.000292
3869	diHPCARP_Ic.tpnmmtpmd	3.900e+44	8.63	8.63	2.030e+38	0.00029
3870	diHPCARP_Ic.tpnmmmpmd	1.934e+44	8.21	8.21	2.022e+38	0.000289
3871	diHPCARP_Ic.mtttmtmpmd	1.471e+44	8.05	8.05	2.018e+38	0.000289
3872	diHPCARP_Ic.mmmppptmd	5.412e+43	7.45	7.45	2.014e+38	0.000288
3873	diHPCARP_Ic.tmmmtpppd	1.507e+44	8.06	8.06	2.013e+38	0.000288
3874	diHPCARP_Ic.mttpttmd	1.997e+44	8.24	8.24	1.991e+38	0.000285
3875	diHPCARP_Ic.tppmpttpd	3.083e+44	8.50	8.50	1.985e+38	0.000284
3876	diHPCARP_Ic.pppptmpd	3.613e+43	7.23	7.23	1.961e+38	0.00028
3877	diHPCARP_Ic.mtmmpppmd	1.904e+43	6.85	6.85	1.942e+38	0.000278
3878	diHPCARP_Ic.tptpttmd	3.599e+44	8.61	8.61	1.921e+38	0.000275
3879	diHPCARP_Ic.pmtppmmpd	4.693e+43	7.40	7.40	1.908e+38	0.000273
3880	diHPCARP_Ic.ttttppmd	1.484e+44	8.09	8.09	1.902e+38	0.000272
3881	diHPCARP_Ic.mmmmmmpmd	7.038e+43	7.64	7.64	1.899e+38	0.000272
3882	diHPCARP_Ic.mmmmpmtmd	8.681e+43	7.77	7.77	1.885e+38	0.00027
3883	diHPCARP_Ic.mtppppmpmd	3.548e+43	7.25	7.25	1.868e+38	0.000267
3884	diHPCARP_Ic.pmmtpmmmd	1.058e+44	7.90	7.90	1.863e+38	0.000266
3885	diHPCARP_Ic.mmmmmmtmd	1.481e+44	8.10	8.10	1.857e+38	0.000266
3886	diHPCARP_Ic.mmmmmtppd	1.036e+44	7.89	7.89	1.846e+38	0.000264
3887	diHPCARP_Ic.mtptmmmpmd	1.749e+44	8.21	8.21	1.840e+38	0.000263
3888	diHPCARP_Ic.ptmmpttmd	3.791e+44	8.67	8.67	1.838e+38	0.000263
3889	diHPCARP_Ic.tppppptpd	3.897e+44	8.69	8.69	1.830e+38	0.000262
3890	diHPCARP_Ic.pmmptmpd	8.553e+43	7.80	7.80	1.772e+38	0.000253
3891	diHPCARP_Ic.pmmptmpd	6.371e+43	7.64	7.64	1.718e+38	0.000246
3892	diHPCARP_Ic.mmpmpptpd	4.073e+43	7.38	7.38	1.701e+38	0.000243
3893	diHPCARP_Ic.mmtmmtpd	1.560e+44	8.19	8.19	1.689e+38	0.000241
3894	diHPCARP_Ic.mmpptppd	4.573e+43	7.46	7.46	1.687e+38	0.000241
3895	diHPCARP_Ic.tttpttmd	7.922e+43	7.79	7.79	1.687e+38	0.000241
3896	diHPCARP_Ic.tttmmmpd	4.672e+43	7.47	7.47	1.679e+38	0.00024
3897	diHPCARP_Ic.tmtpttmd	9.800e+43	7.92	7.92	1.678e+38	0.00024
3898	diHPCARP_Ic.pmmtpppmd	4.192e+43	7.41	7.41	1.677e+38	0.00024
3899	diHPCARP_Ic.pmpptmpd	1.186e+43	6.66	6.66	1.669e+38	0.000239
3900	diHPCARP_Ic.mtppmttd	4.091e+43	7.41	7.41	1.640e+38	0.000234
3901	diHPCARP_Ic.ttmmtmtmd	6.331e+43	7.67	7.67	1.631e+38	0.000233
3902	diHPCARP_Ic.ptmtptmd	5.895e+43	7.64	7.64	1.604e+38	0.000229
3903	diHPCARP_Ic.tmmmttmd	9.230e+44	9.28	9.28	1.602e+38	0.000229
3904	diHPCARP_Ic.mmpmpptmd	1.644e+43	6.89	6.89	1.566e+38	0.000224
3905	diHPCARP_Ic.mppmmptmd	1.052e+44	8.02	8.02	1.511e+38	0.000216
3906	diHPCARP_Ic.mttppmpd	6.115e+43	7.70	7.70	1.508e+38	0.000216
3907	diHPCARP_Ic.ptppmtmd	1.357e+43	6.81	6.81	1.491e+38	0.000213
3908	diHPCARP_Ic.tttptppd	3.048e+44	8.66	8.66	1.489e+38	0.000213
3909	diHPCARP_Ic.ptttmtmd	8.637e+43	7.92	7.92	1.475e+38	0.000211
3910	diHPCARP_Ic.mppmmtpd	4.148e+43	7.48	7.48	1.474e+38	0.000211
3911	diHPCARP_Ic.tmtpttmd	2.935e+44	8.65	8.65	1.455e+38	0.000208
3912	diHPCARP_Ic.tpnmmtpd	1.567e+44	8.28	8.28	1.446e+38	0.000207
3913	diHPCARP_Ic.ppnmmtpd	8.019e+43	7.89	7.89	1.443e+38	0.000206
3914	diHPCARP_Ic.mmtmmmpmd	3.547e+43	7.40	7.40	1.439e+38	0.000206
3915	diHPCARP_Ic.pmtpttmd	1.216e+44	8.14	8.14	1.438e+38	0.000206
3916	diHPCARP_Ic.mmpmpmpd	6.045e+44	9.10	9.10	1.430e+38	0.000204
3917	diHPCARP_Ic.tmtmptmd	1.891e+44	8.40	8.40	1.428e+38	0.000204
3918	diHPCARP_Ic.tmtmmtmd	1.642e+44	8.33	8.33	1.411e+38	0.000202
3919	diHPCARP_Ic.tpnmmmpmd	5.048e+43	7.62	7.62	1.410e+38	0.000202
3920	diHPCARP_Ic.tmmppptmd	9.333e+43	7.99	7.99	1.409e+38	0.000202
3921	diHPCARP_Ic.mptmmtmd	5.856e+43	7.71	7.71	1.404e+38	0.000201
3922	diHPCARP_Ic.ttmmttmd	1.230e+44	8.16	8.16	1.401e+38	0.0002
3923	diHPCARP_Ic.mppmtmpd	5.714e+44	9.08	9.08	1.379e+38	0.000197
3924	diHPCARP_Ic.tttppmtmd	5.300e+44	9.04	9.04	1.372e+38	0.000196
3925	diHPCARP_Ic.mptmptmd	8.499e+43	7.95	7.95	1.366e+38	0.000195
3926	diHPCARP_Ic.mmtpttmd	5.784e+44	9.10	9.10	1.361e+38	0.000195
3927	diHPCARP_Ic.tpnmmmtmd	1.192e+44	8.17	8.17	1.341e+38	0.000192
3928	diHPCARP_Ic.tmtpppmd	1.327e+44	8.23	8.23	1.335e+38	0.000191
3929	diHPCARP_Ic.ttpmptmd	4.817e+43	7.63	7.63	1.331e+38	0.00019
3930	diHPCARP_Ic.tpmtpmd	3.851e+44	8.87	8.87	1.330e+38	0.00019
3931	diHPCARP_Ic.tttmmtmd	2.204e+44	8.54	8.54	1.327e+38	0.00019
3932	diHPCARP_Ic.tmmmpmtmd	1.254e+44	8.20	8.20	1.324e+38	0.000189
3933	diHPCARP_Ic.tttpttmd	2.310e+44	8.57	8.57	1.324e+38	0.000189
3934	diHPCARP_Ic.pmmppmtpd	2.270e+43	7.19	7.19	1.304e+38	0.000186
3935	diHPCARP_Ic.mptpmmpd	2.000e+44	8.51	8.51	1.274e+38	0.000182
3936	diHPCARP_Ic.tmmmpmpd	2.662e+43	7.31	7.31	1.268e+38	0.000181
3937	diHPCARP_Ic.mptptmpd	1.279e+44	8.24	8.24	1.267e+38	0.000181

3938	diHPCARP_Ic.tmtmpttpd	1.436e+44	8.31	8.31	1.262e+38	0.00018
3939	diHPCARP_Ic.mmtpppmmd	8.793e+43	8.02	8.02	1.255e+38	0.00018
3940	diHPCARP_Ic.tpptpttpd	1.559e+44	8.37	8.37	1.245e+38	0.000178
3941	diHPCARP_Ic.ppttptmmd	3.888e+44	8.92	8.92	1.242e+38	0.000178
3942	diHPCARP_Ic.mtmtpttmd	3.896e+44	8.92	8.92	1.238e+38	0.000177
3943	diHPCARP_Ic.mtpmmmpmd	4.869e+43	7.69	7.69	1.222e+38	0.000175
3944	diHPCARP_Ic.tpptptmpd	3.972e+43	7.58	7.58	1.199e+38	0.000171
3945	diHPCARP_Ic.ttttptmmd	7.406e+43	7.95	7.95	1.191e+38	0.00017
3946	diHPCARP_Ic.pppmpttmd	6.175e+43	7.85	7.85	1.174e+38	0.000168
3947	diHPCARP_Ic.pmmmtmmd	8.105e+43	8.02	8.02	1.173e+38	0.000168
3948	diHPCARP_Ic.mttptmtpd	1.329e+44	8.31	8.31	1.166e+38	0.000167
3949	diHPCARP_Ic.mtppttmd	1.062e+44	8.18	8.18	1.162e+38	0.000166
3950	diHPCARP_Ic.mpptmtpmd	8.405e+43	8.05	8.05	1.146e+38	0.000164
3951	diHPCARP_Ic.tmmmtmtd	5.020e+44	9.12	9.12	1.140e+38	0.000163
3952	diHPCARP_Ic.mtmtmtd	1.223e+44	8.28	8.28	1.140e+38	0.000163
3953	diHPCARP_Ic.ttpptppmd	2.882e+43	7.44	7.44	1.098e+38	0.000157
3954	diHPCARP_Ic.pttpmmmpd	2.731e+43	7.41	7.41	1.097e+38	0.000157
3955	diHPCARP_Ic.mpppppppd	2.938e+43	7.45	7.45	1.092e+38	0.000156
3956	diHPCARP_Ic.tppptmmd	1.276e+44	8.33	8.33	1.088e+38	0.000156
3957	diHPCARP_Ic.pmmppppmd	3.371e+43	7.55	7.55	1.074e+38	0.000154
3958	diHPCARP_Ic.pmtmtd	2.097e+44	8.65	8.65	1.052e+38	0.00015
3959	diHPCARP_Ic.tttmtpd	1.069e+44	8.25	8.25	1.046e+38	0.00015
3960	diHPCARP_Ic.tmmmpmtd	1.463e+44	8.44	8.44	1.040e+38	0.000149
3961	diHPCARP_Ic.mtpmmpmd	1.431e+43	7.05	7.05	1.039e+38	0.000149
3962	diHPCARP_Ic.mttppppmd	3.359e+43	7.57	7.57	1.034e+38	0.000148
3963	diHPCARP_Ic.tmpptmmd	1.124e+44	8.29	8.29	1.026e+38	0.000147
3964	diHPCARP_Ic.pppmpttpd	8.035e+43	8.09	8.09	1.023e+38	0.000146
3965	diHPCARP_Ic.pmmmtmtpd	3.239e+43	7.55	7.55	1.017e+38	0.000145
3966	diHPCARP_Ic.mttmtpmd	1.241e+44	8.36	8.36	1.011e+38	0.000145
3967	diHPCARP_Ic.ptmpmmpmd	4.651e+43	7.78	7.78	9.999e+37	0.000143
3968	diHPCARP_Ic.tttmtpd	7.884e+44	9.47	9.47	9.956e+37	0.000142
3969	diHPCARP_Ic.ppmmtmmpd	1.342e+44	8.42	8.42	9.842e+37	0.000141
3970	diHPCARP_Ic.mtpptpmd	1.767e+44	8.59	8.59	9.814e+37	0.00014
3971	diHPCARP_Ic.tmmptmtd	1.296e+44	8.40	8.40	9.812e+37	0.00014
3972	diHPCARP_Ic.tttmtpd	2.206e+44	8.72	8.72	9.774e+37	0.00014
3973	diHPCARP_Ic.mtpmtpmd	1.961e+44	8.65	8.65	9.742e+37	0.000139
3974	diHPCARP_Ic.mmmmtmtd	5.059e+44	9.22	9.22	9.738e+37	0.000139
3975	diHPCARP_Ic.mpttptpmd	7.922e+44	9.49	9.49	9.666e+37	0.000138
3976	diHPCARP_Ic.tpptptppd	3.599e+44	9.03	9.03	9.430e+37	0.000135
3977	diHPCARP_Ic.pppmmpmd	1.514e+44	8.53	8.53	9.304e+37	0.000133
3978	diHPCARP_Ic.tmmmtppd	1.929e+44	8.67	8.67	9.275e+37	0.000133
3979	diHPCARP_Ic.ttpmmmpmd	3.830e+43	7.71	7.71	9.245e+37	0.000132
3980	diHPCARP_Ic.mppmtpmd	1.608e+43	7.20	7.20	9.149e+37	0.000131
3981	diHPCARP_Ic.tmppttpd	4.125e+44	9.14	9.14	9.125e+37	0.00013
3982	diHPCARP_Ic.ptmptmpd	3.660e+43	7.69	7.69	9.105e+37	0.00013
3983	diHPCARP_Ic.mmtmtpmd	1.703e+44	8.63	8.63	8.809e+37	0.000126
3984	diHPCARP_Ic.tmmmtppd	2.013e+44	8.73	8.73	8.747e+37	0.000125
3985	diHPCARP_Ic.tmppttmd	2.698e+44	8.91	8.91	8.676e+37	0.000124
3986	diHPCARP_Ic.mtmtppmd	2.047e+43	7.38	7.38	8.543e+37	0.000122
3987	diHPCARP_Ic.pmmptpmd	1.413e+43	7.16	7.16	8.543e+37	0.000122
3988	diHPCARP_Ic.tpttptmd	6.944e+44	9.49	9.49	8.535e+37	0.000122
3989	diHPCARP_Ic.tppptmpd	4.402e+43	7.85	7.85	8.430e+37	0.000121
3990	diHPCARP_Ic.ppppppppd	4.532e+43	7.88	7.88	8.297e+37	0.000119
3991	diHPCARP_Ic.mmpmtmtpd	8.919e+43	8.29	8.29	8.084e+37	0.000116
3992	diHPCARP_Ic.tttmmmpmd	6.876e+43	8.14	8.14	8.036e+37	0.000115
3993	diHPCARP_Ic.pmmppmtd	1.881e+43	7.37	7.37	8.000e+37	0.000114
3994	diHPCARP_Ic.tptmtd	1.008e+45	9.75	9.75	7.942e+37	0.000114
3995	diHPCARP_Ic.ptmtpmtd	3.546e+43	7.77	7.77	7.798e+37	0.000112
3996	diHPCARP_Ic.tppmtpd	2.493e+44	8.93	8.93	7.751e+37	0.000111
3997	diHPCARP_Ic.tmpmmpmd	1.038e+44	8.42	8.42	7.595e+37	0.000109
3998	diHPCARP_Ic.mptmmpd	2.366e+44	8.92	8.92	7.556e+37	0.000108
3999	diHPCARP_Ic.tppmtpd	2.556e+44	8.99	8.99	7.224e+37	0.000103
4000	diHPCARP_Ic.tmttppmd	5.996e+44	9.50	9.50	7.212e+37	0.000103
4001	diHPCARP_Ic.tmtmtpmd	1.942e+44	8.83	8.83	7.139e+37	0.000102
4002	diHPCARP_Ic.mptmmpmd	4.166e+44	9.29	9.29	7.059e+37	0.000101
4003	diHPCARP_Ic.tmmmtmtd	1.303e+44	8.61	8.61	7.010e+37	0.0001
4004	diHPCARP_Ic.mppmtpmd	9.228e+43	8.40	8.40	6.996e+37	0.0001
4005	diHPCARP_Ic.pmmtpmmpd	1.054e+44	8.48	8.48	6.974e+37	9.97e-05
4006	diHPCARP_Ic.mptmmpd	2.066e+44	8.90	8.90	6.803e+37	9.73e-05
4007	diHPCARP_Ic.tpmtpmtd	1.013e+44	8.48	8.48	6.712e+37	9.6e-05
4008	diHPCARP_Ic.pttptpmd	1.019e+44	8.50	8.50	6.574e+37	9.4e-05
4009	diHPCARP_Ic.mmmmpmtpd	1.060e+44	8.52	8.52	6.538e+37	9.35e-05

4010	diHPCARP_Ic.mmtpmmpd	3.091e+44	9.16	9.16	6.512e+37	9.31e-05
4011	diHPCARP_Ic.mmpmtmpd	2.556e+44	9.06	9.06	6.439e+37	9.21e-05
4012	diHPCARP_Ic.ptpmpptpd	2.280e+43	7.62	7.62	6.401e+37	9.15e-05
4013	diHPCARP_Ic.ptppmtmd	4.509e+43	8.03	8.03	6.390e+37	9.14e-05
4014	diHPCARP_Ic.tmmpttmd	9.722e+43	8.50	8.50	6.277e+37	8.98e-05
4015	diHPCARP_Ic.tmmtmppd	2.285e+44	9.01	9.01	6.247e+37	8.93e-05
4016	diHPCARP_Ic.pmtptmmd	1.225e+44	8.64	8.64	6.207e+37	8.88e-05
4017	diHPCARP_Ic.ttttmmd	1.603e+44	8.81	8.81	6.118e+37	8.75e-05
4018	diHPCARP_Ic.mtmpttmd	1.657e+44	8.83	8.83	6.085e+37	8.7e-05
4019	diHPCARP_Ic.mmmtmppd	2.015e+44	8.95	8.95	6.047e+37	8.65e-05
4020	diHPCARP_Ic.tmmpttpd	1.301e+44	8.70	8.70	6.027e+37	8.62e-05
4021	diHPCARP_Ic.tpmmtmpd	3.267e+44	9.25	9.25	5.934e+37	8.48e-05
4022	diHPCARP_Ic.mtpttmd	6.195e+43	8.26	8.26	5.914e+37	8.46e-05
4023	diHPCARP_Ic.tmmpttmd	1.322e+44	8.72	8.72	5.901e+37	8.44e-05
4024	diHPCARP_Ic.mppmtmd	6.954e+43	8.34	8.34	5.847e+37	8.36e-05
4025	diHPCARP_Ic.pmtmpmpd	9.650e+43	8.54	8.54	5.842e+37	8.35e-05
4026	diHPCARP_Ic.mtpttmd	7.642e+43	8.40	8.40	5.809e+37	8.31e-05
4027	diHPCARP_Ic.tmmtmppd	1.739e+44	8.89	8.89	5.809e+37	8.31e-05
4028	diHPCARP_Ic.mmtptmmd	1.457e+44	8.80	8.80	5.637e+37	8.06e-05
4029	diHPCARP_Ic.ttpmtmd	2.838e+43	7.84	7.84	5.548e+37	7.93e-05
4030	diHPCARP_Ic.mtmmpmpd	2.990e+43	7.89	7.89	5.365e+37	7.67e-05
4031	diHPCARP_Ic.tmmpttmd	3.334e+44	9.33	9.33	5.338e+37	7.63e-05
4032	diHPCARP_Ic.ptmmpmpd	1.350e+43	7.42	7.42	5.274e+37	7.54e-05
4033	diHPCARP_Ic.pmmpttmd	1.024e+44	8.63	8.63	5.259e+37	7.52e-05
4034	diHPCARP_Ic.pmmmpmpd	2.636e+43	7.84	7.84	5.101e+37	7.29e-05
4035	diHPCARP_Ic.pmmpttmd	8.582e+43	8.55	8.55	5.089e+37	7.28e-05
4036	diHPCARP_Ic.tpmmtmpd	3.327e+44	9.36	9.36	5.059e+37	7.23e-05
4037	diHPCARP_Ic.mtptmpmpd	3.583e+43	8.04	8.04	5.008e+37	7.16e-05
4038	diHPCARP_Ic.tttpttmd	9.819e+43	8.65	8.65	4.918e+37	7.03e-05
4039	diHPCARP_Ic.mtptmpmpd	1.658e+44	8.97	8.97	4.833e+37	6.91e-05
4040	diHPCARP_Ic.tttmtmpd	1.142e+45	10.12	10.12	4.832e+37	6.91e-05
4041	diHPCARP_Ic.tmmpttmd	1.753e+44	9.01	9.01	4.804e+37	6.87e-05
4042	diHPCARP_Ic.tttmmpmpd	5.246e+43	8.30	8.30	4.697e+37	6.72e-05
4043	diHPCARP_Ic.tmmtmppd	5.776e+43	8.36	8.36	4.691e+37	6.71e-05
4044	diHPCARP_Ic.tpmmtmpd	2.954e+44	9.34	9.34	4.647e+37	6.64e-05
4045	diHPCARP_Ic.tmtpttmd	4.704e+44	9.62	9.62	4.642e+37	6.64e-05
4046	diHPCARP_Ic.tmppttmd	4.292e+43	8.19	8.19	4.627e+37	6.62e-05
4047	diHPCARP_Ic.tmtmmtmd	5.664e+43	8.36	8.36	4.615e+37	6.6e-05
4048	diHPCARP_Ic.tppmtmpd	6.482e+43	8.44	8.44	4.615e+37	6.6e-05
4049	diHPCARP_Ic.mtptmpmpd	2.257e+44	9.18	9.18	4.597e+37	6.57e-05
4050	diHPCARP_Ic.pmmmttmd	1.024e+44	8.72	8.72	4.568e+37	6.53e-05
4051	diHPCARP_Ic.mptmpmpd	1.111e+44	8.78	8.78	4.487e+37	6.42e-05
4052	diHPCARP_Ic.ttppttmd	7.457e+44	9.92	9.92	4.462e+37	6.38e-05
4053	diHPCARP_Ic.ttppttmd	1.231e+44	8.85	8.85	4.420e+37	6.32e-05
4054	diHPCARP_Ic.pppmpmpd	3.657e+44	9.50	9.50	4.383e+37	6.27e-05
4055	diHPCARP_Ic.mptmmtmd	6.704e+44	9.87	9.87	4.344e+37	6.21e-05
4056	diHPCARP_Ic.mttpttmd	8.536e+43	8.64	8.64	4.327e+37	6.19e-05
4057	diHPCARP_Ic.pmtmpmpd	8.809e+43	8.66	8.66	4.299e+37	6.15e-05
4058	diHPCARP_Ic.tttmmtmd	2.146e+44	9.20	9.20	4.269e+37	6.1e-05
4059	diHPCARP_Ic.tppmttmd	1.780e+45	10.47	10.47	4.224e+37	6.04e-05
4060	diHPCARP_Ic.ttpmmtmpd	1.594e+43	7.66	7.66	4.203e+37	6.01e-05
4061	diHPCARP_Ic.tptmttmd	9.713e+44	10.11	10.11	4.196e+37	6e-05
4062	diHPCARP_Ic.ptmpttmd	5.852e+44	9.81	9.81	4.169e+37	5.96e-05
4063	diHPCARP_Ic.tmtpttmd	1.515e+44	9.01	9.01	4.105e+37	5.87e-05
4064	diHPCARP_Ic.ttppttmd	4.027e+43	8.23	8.23	4.097e+37	5.86e-05
4065	diHPCARP_Ic.tpmmttmd	2.542e+44	9.33	9.33	4.069e+37	5.82e-05
4066	diHPCARP_Ic.pppmpmpd	5.513e+43	8.42	8.42	4.040e+37	5.78e-05
4067	diHPCARP_Ic.tttmmtppd	2.997e+44	9.43	9.43	4.029e+37	5.76e-05
4068	diHPCARP_Ic.pttmptmpd	1.379e+44	8.98	8.98	3.953e+37	5.65e-05
4069	diHPCARP_Ic.mmtptmpd	3.630e+43	8.19	8.19	3.940e+37	5.63e-05
4070	diHPCARP_Ic.tptmttmd	5.568e+44	9.82	9.82	3.919e+37	5.6e-05
4071	diHPCARP_Ic.mtmppmpd	2.868e+43	8.05	8.05	3.900e+37	5.58e-05
4072	diHPCARP_Ic.ttppttmd	6.444e+44	9.92	9.92	3.832e+37	5.48e-05
4073	diHPCARP_Ic.tmmpttmd	1.981e+44	9.22	9.22	3.828e+37	5.47e-05
4074	diHPCARP_Ic.mppmmpmpd	1.657e+44	9.13	9.13	3.725e+37	5.33e-05
4075	diHPCARP_Ic.tpppttmd	6.721e+43	8.59	8.59	3.709e+37	5.3e-05
4076	diHPCARP_Ic.tmtpttmd	5.245e+44	9.82	9.82	3.701e+37	5.29e-05
4077	diHPCARP_Ic.mtppmmpd	4.532e+43	8.36	8.36	3.663e+37	5.24e-05
4078	diHPCARP_Ic.mptmtmpd	2.008e+44	9.26	9.26	3.592e+37	5.14e-05
4079	diHPCARP_Ic.mttpttmd	2.888e+44	9.49	9.49	3.541e+37	5.06e-05
4080	diHPCARP_Ic.ttppttmd	3.202e+43	8.20	8.20	3.408e+37	4.87e-05
4081	diHPCARP_Ic.mmtmpttmd	1.593e+44	9.16	9.16	3.385e+37	4.84e-05

4082	diHPCARP_Ic.pmmmtmpmd	2.934e+43	8.15	8.15	3.363e+37	4.81e-05
4083	diHPCARP_Ic.mptmmmpmd	2.141e+44	9.34	9.34	3.361e+37	4.81e-05
4084	diHPCARP_Ic.mtptmtmd	6.993e+44	10.05	10.05	3.348e+37	4.79e-05
4085	diHPCARP_Ic.tpptppppd	1.808e+44	9.26	9.26	3.273e+37	4.68e-05
4086	diHPCARP_Ic.mpptmtmpd	5.900e+43	8.59	8.59	3.254e+37	4.65e-05
4087	diHPCARP_Ic.pmtppmmmd	6.244e+43	8.63	8.63	3.230e+37	4.62e-05
4088	diHPCARP_Ic.mpmtpttmd	4.044e+44	9.74	9.74	3.228e+37	4.62e-05
4089	diHPCARP_Ic.tmtmpmmd	5.600e+43	8.57	8.57	3.185e+37	4.55e-05
4090	diHPCARP_Ic.pttppmmd	4.585e+43	8.46	8.46	3.171e+37	4.53e-05
4091	diHPCARP_Ic.tmtppmpd	2.148e+44	9.38	9.38	3.132e+37	4.48e-05
4092	diHPCARP_Ic.mppmppppd	2.063e+43	7.99	7.99	3.097e+37	4.43e-05
4093	diHPCARP_Ic.tpptmtppd	8.238e+44	10.20	10.20	3.080e+37	4.4e-05
4094	diHPCARP_Ic.mpppmtmpd	9.191e+43	8.89	8.89	3.072e+37	4.39e-05
4095	diHPCARP_Ic.mptpmpmmd	8.006e+43	8.82	8.82	2.999e+37	4.29e-05
4096	diHPCARP_Ic.tmpmpmmd	2.939e+43	8.23	8.23	2.984e+37	4.27e-05
4097	diHPCARP_Ic.tmtmpmpd	3.834e+43	8.39	8.39	2.979e+37	4.26e-05
4098	diHPCARP_Ic.pmpmtmmd	1.230e+44	9.08	9.08	2.975e+37	4.25e-05
4099	diHPCARP_Ic.ttpmmppd	6.089e+43	8.67	8.67	2.922e+37	4.18e-05
4100	diHPCARP_Ic.mpttmmppd	6.116e+44	10.05	10.05	2.919e+37	4.17e-05
4101	diHPCARP_Ic.mmmmtmmmpd	1.317e+44	9.14	9.14	2.908e+37	4.16e-05
4102	diHPCARP_Ic.tppmpttpd	3.599e+44	9.74	9.74	2.900e+37	4.15e-05
4103	diHPCARP_Ic.mtmmttppd	2.036e+44	9.41	9.41	2.853e+37	4.08e-05
4104	diHPCARP_Ic.tpptptmmd	2.136e+44	9.45	9.45	2.785e+37	3.98e-05
4105	diHPCARP_Ic.tmmppmpmd	2.153e+44	9.46	9.46	2.778e+37	3.97e-05
4106	diHPCARP_Ic.mmtpppppd	2.028e+44	9.43	9.43	2.756e+37	3.94e-05
4107	diHPCARP_Ic.ttmppmpd	2.618e+43	8.21	8.21	2.754e+37	3.94e-05
4108	diHPCARP_Ic.tmtpppppd	1.414e+44	9.22	9.22	2.714e+37	3.88e-05
4109	diHPCARP_Ic.tppmpmmd	1.937e+44	9.41	9.41	2.685e+37	3.84e-05
4110	diHPCARP_Ic.mpppmmmd	9.669e+43	9.00	9.00	2.673e+37	3.82e-05
4111	diHPCARP_Ic.pmttppmpd	6.228e+43	8.75	8.75	2.629e+37	3.76e-05
4112	diHPCARP_Ic.mppmmmtpd	3.526e+44	9.79	9.79	2.606e+37	3.73e-05
4113	diHPCARP_Ic.tmmptmpd	9.676e+43	9.02	9.02	2.593e+37	3.71e-05
4114	diHPCARP_Ic.mpttmtmpd	2.370e+44	9.56	9.56	2.578e+37	3.69e-05
4115	diHPCARP_Ic.mppmttmd	8.569e+44	10.33	10.33	2.548e+37	3.64e-05
4116	diHPCARP_Ic.mmmmpmmmpd	9.987e+43	9.05	9.05	2.544e+37	3.64e-05
4117	diHPCARP_Ic.mppmtmpd	4.011e+44	9.89	9.89	2.522e+37	3.61e-05
4118	diHPCARP_Ic.tpmttmd	1.040e+45	10.46	10.46	2.504e+37	3.58e-05
4119	diHPCARP_Ic.tpmttmd	6.186e+44	10.15	10.15	2.499e+37	3.57e-05
4120	diHPCARP_Ic.ptmtptmd	3.391e+44	9.79	9.79	2.498e+37	3.57e-05
4121	diHPCARP_Ic.tmtmtppd	2.815e+44	9.68	9.68	2.491e+37	3.56e-05
4122	diHPCARP_Ic.tpptmtmd	3.668e+44	9.84	9.84	2.485e+37	3.55e-05
4123	diHPCARP_Ic.ttttptppd	4.905e+44	10.02	10.02	2.474e+37	3.54e-05
4124	diHPCARP_Ic.mmpmptppd	2.590e+43	8.27	8.27	2.441e+37	3.49e-05
4125	diHPCARP_Ic.ttpmttmd	3.213e+44	9.78	9.78	2.431e+37	3.48e-05
4126	diHPCARP_Ic.tmmpppppd	1.877e+44	9.46	9.46	2.429e+37	3.47e-05
4127	diHPCARP_Ic.mtpmpmtpd	1.161e+44	9.17	9.17	2.420e+37	3.46e-05
4128	diHPCARP_Ic.pmmpttmd	2.327e+44	9.59	9.59	2.403e+37	3.44e-05
4129	diHPCARP_Ic.mtppmtmmd	2.708e+43	8.32	8.32	2.360e+37	3.37e-05
4130	diHPCARP_Ic.pmttptmd	1.504e+44	9.35	9.35	2.318e+37	3.31e-05
4131	diHPCARP_Ic.mtttmttmd	1.185e+44	9.21	9.21	2.305e+37	3.3e-05
4132	diHPCARP_Ic.mtppppppd	5.834e+43	8.79	8.79	2.301e+37	3.29e-05
4133	diHPCARP_Ic.tpppppppd	9.854e+43	9.10	9.10	2.297e+37	3.28e-05
4134	diHPCARP_Ic.tmmppmmd	7.919e+43	8.99	8.99	2.245e+37	3.21e-05
4135	diHPCARP_Ic.ttttpttmd	6.706e+44	10.26	10.26	2.241e+37	3.2e-05
4136	diHPCARP_Ic.ttpmppppd	1.974e+43	8.18	8.18	2.187e+37	3.13e-05
4137	diHPCARP_Ic.mpmptmmd	1.395e+45	10.71	10.71	2.183e+37	3.12e-05
4138	diHPCARP_Ic.pmmmtmpmd	1.577e+44	9.42	9.42	2.176e+37	3.11e-05
4139	diHPCARP_Ic.pmpmttmd	1.800e+44	9.50	9.50	2.168e+37	3.1e-05
4140	diHPCARP_Ic.pmpmmtpd	2.094e+43	8.22	8.22	2.165e+37	3.1e-05
4141	diHPCARP_Ic.tppmmpppd	2.130e+44	9.61	9.61	2.123e+37	3.04e-05
4142	diHPCARP_Ic.mtpmpmmpd	4.974e+43	8.75	8.75	2.116e+37	3.03e-05
4143	diHPCARP_Ic.ttpmpttmd	1.169e+44	9.26	9.26	2.113e+37	3.02e-05
4144	diHPCARP_Ic.ttpmtmmd	8.051e+43	9.04	9.04	2.085e+37	2.98e-05
4145	diHPCARP_Ic.ptttmmmpd	4.427e+43	8.69	8.69	2.065e+37	2.95e-05
4146	diHPCARP_Ic.pmmpttmd	2.064e+44	9.64	9.64	1.955e+37	2.8e-05
4147	diHPCARP_Ic.mptmmtmpd	1.163e+44	9.30	9.30	1.951e+37	2.79e-05
4148	diHPCARP_Ic.mptmmmpd	3.447e+44	9.95	9.95	1.939e+37	2.77e-05
4149	diHPCARP_Ic.mmttmtptd	2.918e+44	9.85	9.85	1.933e+37	2.76e-05
4150	diHPCARP_Ic.tpptptpd	8.156e+44	10.47	10.47	1.933e+37	2.76e-05
4151	diHPCARP_Ic.mptmttmd	8.576e+44	10.50	10.50	1.926e+37	2.75e-05
4152	diHPCARP_Ic.ptptmttmd	9.941e+43	9.22	9.22	1.918e+37	2.74e-05
4153	diHPCARP_Ic.tmppttmd	3.084e+44	9.90	9.90	1.909e+37	2.73e-05

4154	diHPCARP_Ic.tpttppppd	1.803e+44	9.58	9.58	1.889e+37	2.7e-05
4155	diHPCARP_Ic.mpmnptmmd	1.615e+44	9.52	9.52	1.887e+37	2.7e-05
4156	diHPCARP_Ic.tmpmmtttd	4.025e+43	8.71	8.71	1.827e+37	2.61e-05
4157	diHPCARP_Ic.mppptmpppd	1.180e+44	9.35	9.35	1.826e+37	2.61e-05
4158	diHPCARP_Ic.mtppmppmd	4.695e+43	8.80	8.80	1.822e+37	2.6e-05
4159	diHPCARP_Ic.tmpmptttd	8.892e+43	9.18	9.18	1.820e+37	2.6e-05
4160	diHPCARP_Ic.ttpmmttd	1.981e+44	9.66	9.66	1.815e+37	2.6e-05
4161	diHPCARP_Ic.tppmppppd	8.136e+43	9.14	9.14	1.801e+37	2.58e-05
4162	diHPCARP_Ic.mpmptmmd	4.576e+43	8.80	8.80	1.792e+37	2.56e-05
4163	diHPCARP_Ic.mmmptmmd	4.302e+43	8.77	8.77	1.762e+37	2.52e-05
4164	diHPCARP_Ic.tttmptttd	2.898e+44	9.92	9.92	1.730e+37	2.47e-05
4165	diHPCARP_Ic.tpmptttd	8.877e+43	9.21	9.21	1.726e+37	2.47e-05
4166	diHPCARP_Ic.mmtmttmd	4.737e+44	10.22	10.22	1.708e+37	2.44e-05
4167	diHPCARP_Ic.mtppptmpd	1.988e+43	8.33	8.33	1.705e+37	2.44e-05
4168	diHPCARP_Ic.pmmptttd	6.391e+43	9.03	9.03	1.702e+37	2.43e-05
4169	diHPCARP_Ic.tmmptttd	1.164e+44	9.38	9.38	1.695e+37	2.42e-05
4170	diHPCARP_Ic.tttmtttd	2.593e+44	9.87	9.87	1.663e+37	2.38e-05
4171	diHPCARP_Ic.tpmptttd	1.449e+44	9.53	9.53	1.659e+37	2.37e-05
4172	diHPCARP_Ic.mttmmttd	7.636e+43	9.15	9.15	1.653e+37	2.36e-05
4173	diHPCARP_Ic.ptmpmmttd	1.596e+43	8.22	8.22	1.648e+37	2.36e-05
4174	diHPCARP_Ic.tpmmtttd	1.187e+45	10.80	10.80	1.609e+37	2.3e-05
4175	diHPCARP_Ic.tpmmttmd	5.948e+43	9.02	9.02	1.585e+37	2.27e-05
4176	diHPCARP_Ic.ttpptmmd	2.431e+43	8.51	8.51	1.547e+37	2.21e-05
4177	diHPCARP_Ic.tmmptmmd	2.180e+44	9.82	9.82	1.537e+37	2.2e-05
4178	diHPCARP_Ic.tttmttmd	3.720e+44	10.15	10.15	1.503e+37	2.15e-05
4179	diHPCARP_Ic.mmttppmmd	1.596e+44	9.65	9.65	1.494e+37	2.14e-05
4180	diHPCARP_Ic.tmttpttd	2.849e+44	9.99	9.99	1.491e+37	2.13e-05
4181	diHPCARP_Ic.mppptmtpd	6.646e+43	9.13	9.13	1.478e+37	2.11e-05
4182	diHPCARP_Ic.mmttpttd	6.664e+43	9.14	9.14	1.470e+37	2.1e-05
4183	diHPCARP_Ic.mmmptmtpd	1.211e+45	10.87	10.87	1.455e+37	2.08e-05
4184	diHPCARP_Ic.ttpmtmtd	5.562e+43	9.04	9.04	1.453e+37	2.08e-05
4185	diHPCARP_Ic.ttpptmmd	4.995e+43	8.98	8.98	1.439e+37	2.06e-05
4186	diHPCARP_Ic.tpmmtmtd	9.474e+43	9.36	9.36	1.428e+37	2.04e-05
4187	diHPCARP_Ic.ptmmtmtd	6.934e+43	9.18	9.18	1.422e+37	2.03e-05
4188	diHPCARP_Ic.mttmmtmtd	3.071e+43	8.71	8.71	1.395e+37	1.99e-05
4189	diHPCARP_Ic.mmttpppttd	1.803e+44	9.76	9.76	1.389e+37	1.99e-05
4190	diHPCARP_Ic.pmttmmtd	7.582e+43	9.25	9.25	1.384e+37	1.98e-05
4191	diHPCARP_Ic.tpmmtttd	5.952e+44	10.48	10.48	1.382e+37	1.98e-05
4192	diHPCARP_Ic.tppmmtmtd	2.356e+44	9.93	9.93	1.367e+37	1.96e-05
4193	diHPCARP_Ic.mptmpttd	1.441e+44	9.65	9.65	1.350e+37	1.93e-05
4194	diHPCARP_Ic.ptttppmmd	1.024e+44	9.45	9.45	1.341e+37	1.92e-05
4195	diHPCARP_Ic.tpmmtmtd	6.127e+43	9.14	9.14	1.341e+37	1.92e-05
4196	diHPCARP_Ic.mmmmtmtd	2.727e+44	10.04	10.04	1.333e+37	1.91e-05
4197	diHPCARP_Ic.tttmmtmtd	1.520e+44	9.69	9.69	1.321e+37	1.89e-05
4198	diHPCARP_Ic.mtppmmttd	1.254e+44	9.58	9.58	1.316e+37	1.88e-05
4199	diHPCARP_Ic.mppmmtmtd	3.906e+43	8.90	8.90	1.294e+37	1.85e-05
4200	diHPCARP_Ic.ttpptmtd	1.646e+44	9.75	9.75	1.289e+37	1.84e-05
4201	diHPCARP_Ic.ttmmtmtd	5.035e+43	9.05	9.05	1.281e+37	1.83e-05
4202	diHPCARP_Ic.mmttmtmtd	7.664e+44	10.69	10.69	1.252e+37	1.79e-05
4203	diHPCARP_Ic.mmtmppppd	1.880e+45	11.23	11.23	1.231e+37	1.76e-05
4204	diHPCARP_Ic.mmmtppttd	1.177e+44	9.59	9.59	1.224e+37	1.75e-05
4205	diHPCARP_Ic.mmtpppppd	3.699e+44	10.27	10.27	1.217e+37	1.74e-05
4206	diHPCARP_Ic.tmmptttd	1.304e+44	9.65	9.65	1.213e+37	1.73e-05
4207	diHPCARP_Ic.mpmmtmtd	4.413e+43	9.01	9.01	1.211e+37	1.73e-05
4208	diHPCARP_Ic.mppmmtmtd	4.797e+44	10.44	10.44	1.183e+37	1.69e-05
4209	diHPCARP_Ic.tptmppppd	1.268e+44	9.65	9.65	1.177e+37	1.68e-05
4210	diHPCARP_Ic.ttpmpttd	1.213e+44	9.63	9.63	1.174e+37	1.68e-05
4211	diHPCARP_Ic.pttptttd	1.810e+44	9.88	9.88	1.141e+37	1.63e-05
4212	diHPCARP_Ic.tttmmttd	5.839e+43	9.21	9.21	1.139e+37	1.63e-05
4213	diHPCARP_Ic.mtptmmtmd	8.618e+43	9.45	9.45	1.134e+37	1.62e-05
4214	diHPCARP_Ic.tmmppmtd	5.497e+43	9.18	9.18	1.127e+37	1.61e-05
4215	diHPCARP_Ic.ttpmmttd	2.830e+43	8.79	8.79	1.124e+37	1.61e-05
4216	diHPCARP_Ic.pmpmmtmtd	8.641e+42	8.08	8.08	1.116e+37	1.6e-05
4217	diHPCARP_Ic.mmmptttd	6.961e+43	9.33	9.33	1.115e+37	1.59e-05
4218	diHPCARP_Ic.pmttptmtd	3.269e+44	10.25	10.25	1.112e+37	1.59e-05
4219	diHPCARP_Ic.ttpppmtd	1.177e+44	9.65	9.65	1.106e+37	1.58e-05
4220	diHPCARP_Ic.pttmpttd	6.229e+43	9.28	9.28	1.086e+37	1.55e-05
4221	diHPCARP_Ic.mmtmmtmtd	2.029e+44	9.98	9.98	1.084e+37	1.55e-05
4222	diHPCARP_Ic.mmtmmttd	3.758e+44	10.35	10.35	1.082e+37	1.55e-05
4223	diHPCARP_Ic.tppppmtd	2.358e+44	10.09	10.09	1.056e+37	1.51e-05
4224	diHPCARP_Ic.mptmpppd	1.530e+44	9.84	9.84	1.043e+37	1.49e-05
4225	diHPCARP_Ic.ptptmmttd	1.752e+44	9.92	9.92	1.042e+37	1.49e-05

4226	diHPCARP_Ic.mptpptppd	7.394e+43	9.41	9.41	1.039e+37	1.49e-05
4227	diHPCARP_Ic.tmtptppd	2.340e+44	10.10	10.10	1.029e+37	1.47e-05
4228	diHPCARP_Ic.pppmmpd	1.198e+44	9.71	9.71	1.014e+37	1.45e-05
4229	diHPCARP_Ic.mtppppmpd	3.011e+43	8.89	8.89	1.012e+37	1.45e-05
4230	diHPCARP_Ic.mtppmtpd	3.794e+43	9.04	9.04	9.832e+36	1.41e-05
4231	diHPCARP_Ic.mmttptpmd	1.486e+44	9.87	9.87	9.629e+36	1.38e-05
4232	diHPCARP_Ic.tmpmmpd	1.114e+44	9.70	9.70	9.581e+36	1.37e-05
4233	diHPCARP_Ic.mppmtmtpd	1.391e+44	9.84	9.84	9.502e+36	1.36e-05
4234	diHPCARP_Ic.mtttmtppd	3.842e+44	10.45	10.45	9.440e+36	1.35e-05
4235	diHPCARP_Ic.mttmpppmd	3.331e+43	8.99	8.99	9.367e+36	1.34e-05
4236	diHPCARP_Ic.ttmppppmd	3.134e+43	8.97	8.97	9.205e+36	1.32e-05
4237	diHPCARP_Ic.pmmmtmtpmd	4.033e+43	9.12	9.12	9.169e+36	1.31e-05
4238	diHPCARP_Ic.mppmtpd	5.058e+43	9.25	9.25	9.164e+36	1.31e-05
4239	diHPCARP_Ic.tpppppmd	2.357e+44	10.17	10.17	9.164e+36	1.31e-05
4240	diHPCARP_Ic.mmmmpmmpd	7.320e+43	9.48	9.48	9.106e+36	1.3e-05
4241	diHPCARP_Ic.mtppmtpd	4.822e+43	9.23	9.23	9.105e+36	1.3e-05
4242	diHPCARP_Ic.mtppmtmd	2.279e+44	10.16	10.16	9.024e+36	1.29e-05
4243	diHPCARP_Ic.ptpmmtpd	7.566e+43	9.51	9.51	8.876e+36	1.27e-05
4244	diHPCARP_Ic.ptmmmpd	2.702e+43	8.92	8.92	8.634e+36	1.23e-05
4245	diHPCARP_Ic.mmmmmmpmd	3.017e+44	10.36	10.36	8.617e+36	1.23e-05
4246	diHPCARP_Ic.mmtmtpmd	8.169e+44	10.95	10.95	8.597e+36	1.23e-05
4247	diHPCARP_Ic.pmmtpmtpd	2.137e+44	10.17	10.17	8.306e+36	1.19e-05
4248	diHPCARP_Ic.pmmmpmmpd	3.032e+43	9.01	9.01	8.281e+36	1.18e-05
4249	diHPCARP_Ic.mtmtmmpd	7.652e+43	9.56	9.56	8.270e+36	1.18e-05
4250	diHPCARP_Ic.mppmtmmd	2.876e+43	8.99	8.99	8.170e+36	1.17e-05
4251	diHPCARP_Ic.mmttppmpd	8.611e+44	11.02	11.02	8.133e+36	1.16e-05
4252	diHPCARP_Ic.mtttmtmd	4.581e+44	10.65	10.65	7.966e+36	1.14e-05
4253	diHPCARP_Ic.mppmmpd	6.373e+43	9.48	9.48	7.964e+36	1.14e-05
4254	diHPCARP_Ic.ptppptpd	6.547e+43	9.50	9.50	7.891e+36	1.13e-05
4255	diHPCARP_Ic.ptpmmtpd	3.115e+43	9.06	9.06	7.787e+36	1.11e-05
4256	diHPCARP_Ic.pmmtpptpd	1.496e+44	10.00	10.00	7.775e+36	1.11e-05
4257	diHPCARP_Ic.pmtmmtpd	1.394e+44	9.96	9.96	7.722e+36	1.1e-05
4258	diHPCARP_Ic.mppmtpd	2.619e+44	10.34	10.34	7.706e+36	1.1e-05
4259	diHPCARP_Ic.mptmtmtpd	1.885e+44	10.15	10.15	7.580e+36	1.08e-05
4260	diHPCARP_Ic.tmpmtmtpd	9.448e+43	9.74	9.74	7.528e+36	1.08e-05
4261	diHPCARP_Ic.mtppmmpd	2.231e+43	8.88	8.88	7.518e+36	1.07e-05
4262	diHPCARP_Ic.mptmmpd	1.188e+44	9.88	9.88	7.502e+36	1.07e-05
4263	diHPCARP_Ic.tptmtpd	1.214e+44	9.90	9.90	7.399e+36	1.06e-05
4264	diHPCARP_Ic.mppmmpd	2.423e+44	10.32	10.32	7.345e+36	1.05e-05
4265	diHPCARP_Ic.ptptmtpd	8.824e+43	9.72	9.72	7.338e+36	1.05e-05
4266	diHPCARP_Ic.pmmmtmmd	6.297e+43	9.53	9.53	7.239e+36	1.04e-05
4267	diHPCARP_Ic.tmtmpppmd	1.972e+44	10.21	10.21	7.201e+36	1.03e-05
4268	diHPCARP_Ic.ttpmtpmd	8.430e+43	9.71	9.71	7.132e+36	1.02e-05
4269	diHPCARP_Ic.ptmtpmtpd	1.805e+44	10.17	10.17	7.057e+36	1.01e-05
4270	diHPCARP_Ic.mppmmpmd	6.470e+43	9.56	9.56	7.013e+36	1e-05
4271	diHPCARP_Ic.ptttptpd	3.800e+44	10.62	10.62	6.999e+36	1e-05
4272	diHPCARP_Ic.mmtmmpd	3.659e+44	10.61	10.61	6.789e+36	9.71e-06
4273	diHPCARP_Ic.mtpppmpd	2.715e+43	9.06	9.06	6.789e+36	9.71e-06
4274	diHPCARP_Ic.tmpmtpmd	9.336e+43	9.80	9.80	6.750e+36	9.65e-06
4275	diHPCARP_Ic.tpppppmd	1.034e+44	9.87	9.87	6.705e+36	9.59e-06
4276	diHPCARP_Ic.tttmtpd	8.698e+43	9.76	9.76	6.703e+36	9.58e-06
4277	diHPCARP_Ic.mmpmtpd	5.658e+43	9.51	9.51	6.692e+36	9.57e-06
4278	diHPCARP_Ic.tppmmpd	4.574e+43	9.40	9.40	6.534e+36	9.34e-06
4279	diHPCARP_Ic.mttmtpd	2.625e+44	10.45	10.45	6.389e+36	9.14e-06
4280	diHPCARP_Ic.mptmmpmd	1.128e+44	9.95	9.95	6.314e+36	9.03e-06
4281	diHPCARP_Ic.mmmmpmtpd	8.628e+43	9.80	9.80	6.226e+36	8.9e-06
4282	diHPCARP_Ic.tmtppppd	2.599e+44	10.46	10.46	6.189e+36	8.85e-06
4283	diHPCARP_Ic.mtppmmpd	6.580e+43	9.66	9.66	6.066e+36	8.67e-06
4284	diHPCARP_Ic.tppmtpmd	2.173e+43	9.01	9.01	5.946e+36	8.5e-06
4285	diHPCARP_Ic.mtppmtpd	1.462e+44	10.15	10.15	5.872e+36	8.4e-06
4286	diHPCARP_Ic.tppmmpd	6.708e+43	9.69	9.69	5.862e+36	8.38e-06
4287	diHPCARP_Ic.ttpppptpd	2.480e+44	10.49	10.49	5.698e+36	8.15e-06
4288	diHPCARP_Ic.tppppmpd	5.294e+43	9.58	9.58	5.598e+36	8.01e-06
4289	diHPCARP_Ic.mtppmmpd	5.218e+43	9.57	9.57	5.598e+36	8e-06
4290	diHPCARP_Ic.mpppppmpd	9.782e+43	9.94	9.94	5.590e+36	7.99e-06
4291	diHPCARP_Ic.mmtmmpd	3.770e+44	10.75	10.75	5.537e+36	7.92e-06
4292	diHPCARP_Ic.mmtmtpmd	3.793e+44	10.78	10.78	5.321e+36	7.61e-06
4293	diHPCARP_Ic.tptmtpd	2.707e+44	10.58	10.58	5.274e+36	7.54e-06
4294	diHPCARP_Ic.ttpmtpd	3.302e+44	10.71	10.71	5.246e+36	7.5e-06
4295	diHPCARP_Ic.tppmtpd	3.336e+44	10.72	10.72	5.159e+36	7.38e-06
4296	diHPCARP_Ic.pmtmmpd	1.248e+44	10.14	10.14	5.140e+36	7.35e-06
4297	diHPCARP_Ic.tppmmpd	5.897e+43	9.70	9.70	5.070e+36	7.25e-06

4298	diHPCARP_Ic.ptptpttmd	1.181e+45	11.49	11.49	5.029e+36	7.19e-06
4299	diHPCARP_Ic.mmpmmtmpmd	1.153e+43	8.73	8.73	5.016e+36	7.17e-06
4300	diHPCARP_Ic.tmpmmttmd	6.846e+43	9.81	9.81	4.883e+36	6.98e-06
4301	diHPCARP_Ic.mmmmtptmd	4.736e+43	9.60	9.60	4.814e+36	6.88e-06
4302	diHPCARP_Ic.mmtmptpmd	5.725e+43	9.72	9.72	4.760e+36	6.81e-06
4303	diHPCARP_Ic.tpmmtppd	1.195e+44	10.16	10.16	4.732e+36	6.77e-06
4304	diHPCARP_Ic.tpmptppd	1.346e+44	10.24	10.24	4.707e+36	6.73e-06
4305	diHPCARP_Ic.mmpmtmmd	8.201e+43	9.94	9.94	4.687e+36	6.7e-06
4306	diHPCARP_Ic.mptmpttmd	3.188e+44	10.76	10.76	4.641e+36	6.64e-06
4307	diHPCARP_Ic.tttppmpd	5.967e+43	9.77	9.77	4.572e+36	6.54e-06
4308	diHPCARP_Ic.tttmmpd	2.773e+44	10.69	10.69	4.530e+36	6.48e-06
4309	diHPCARP_Ic.mpppmmpd	1.291e+44	10.24	10.24	4.490e+36	6.42e-06
4310	diHPCARP_Ic.mppmpmpd	4.518e+43	9.61	9.61	4.485e+36	6.41e-06
4311	diHPCARP_Ic.mpmmtmpmd	9.455e+43	10.06	10.06	4.472e+36	6.4e-06
4312	diHPCARP_Ic.mmttppd	2.457e+44	10.65	10.65	4.257e+36	6.09e-06
4313	diHPCARP_Ic.mppmpmmd	3.567e+43	9.51	9.51	4.208e+36	6.02e-06
4314	diHPCARP_Ic.tpttppd	3.355e+44	10.85	10.85	4.185e+36	5.98e-06
4315	diHPCARP_Ic.pttmmpd	1.629e+44	10.42	10.42	4.156e+36	5.94e-06
4316	diHPCARP_Ic.pmtmmmpd	4.500e+43	9.66	9.66	4.150e+36	5.93e-06
4317	diHPCARP_Ic.mmmppptmd	8.865e+43	10.07	10.07	4.091e+36	5.85e-06
4318	diHPCARP_Ic.tttmmtmd	2.462e+44	10.68	10.68	4.080e+36	5.83e-06
4319	diHPCARP_Ic.mppmtmmd	5.978e+44	11.22	11.22	3.995e+36	5.71e-06
4320	diHPCARP_Ic.mtmmpmd	8.431e+43	10.05	10.05	3.993e+36	5.71e-06
4321	diHPCARP_Ic.tppppmpd	8.721e+43	10.08	10.08	3.947e+36	5.64e-06
4322	diHPCARP_Ic.mttmmpd	1.692e+44	10.48	10.48	3.940e+36	5.63e-06
4323	diHPCARP_Ic.mppmtmmd	8.732e+43	10.09	10.09	3.891e+36	5.56e-06
4324	diHPCARP_Ic.tmtppmpd	7.573e+43	10.01	10.01	3.882e+36	5.55e-06
4325	diHPCARP_Ic.pttppd	7.492e+43	10.01	10.01	3.843e+36	5.5e-06
4326	diHPCARP_Ic.tmtppmpd	3.739e+43	9.60	9.60	3.811e+36	5.45e-06
4327	diHPCARP_Ic.mppmtmpmd	2.615e+44	10.77	10.77	3.737e+36	5.34e-06
4328	diHPCARP_Ic.ptpmmpd	2.357e+43	9.34	9.34	3.729e+36	5.33e-06
4329	diHPCARP_Ic.pttppmpd	3.149e+43	9.51	9.51	3.727e+36	5.33e-06
4330	diHPCARP_Ic.mtptmtpd	1.167e+44	10.29	10.29	3.708e+36	5.3e-06
4331	diHPCARP_Ic.tmppttmd	1.185e+45	11.68	11.68	3.701e+36	5.29e-06
4332	diHPCARP_Ic.tptppmpd	2.248e+44	10.69	10.69	3.692e+36	5.28e-06
4333	diHPCARP_Ic.mtmmtppd	1.760e+44	10.54	10.54	3.684e+36	5.27e-06
4334	diHPCARP_Ic.tmtppmpd	1.229e+44	10.34	10.34	3.596e+36	5.14e-06
4335	diHPCARP_Ic.mtpmmtmmd	3.537e+43	9.60	9.60	3.581e+36	5.12e-06
4336	diHPCARP_Ic.tpmmtppd	2.507e+44	10.77	10.77	3.570e+36	5.1e-06
4337	diHPCARP_Ic.pmtpmmtmd	8.582e+43	10.14	10.14	3.518e+36	5.03e-06
4338	diHPCARP_Ic.tppptmpd	4.982e+43	9.85	9.85	3.325e+36	4.75e-06
4339	diHPCARP_Ic.pmpptmpd	1.060e+44	10.30	10.30	3.317e+36	4.74e-06
4340	diHPCARP_Ic.ttmmpmpd	5.753e+43	9.95	9.95	3.247e+36	4.64e-06
4341	diHPCARP_Ic.pmpptmmd	2.332e+43	9.42	9.42	3.203e+36	4.58e-06
4342	diHPCARP_Ic.tmpmtpmd	3.757e+43	9.71	9.71	3.151e+36	4.51e-06
4343	diHPCARP_Ic.ptpmmpmmd	8.079e+43	10.18	10.18	3.122e+36	4.46e-06
4344	diHPCARP_Ic.ptpmmpd	1.140e+44	10.38	10.38	3.107e+36	4.44e-06
4345	diHPCARP_Ic.tmtppptmd	1.711e+44	10.64	10.64	3.018e+36	4.32e-06
4346	diHPCARP_Ic.mmmmtptmd	4.857e+43	9.91	9.91	2.953e+36	4.22e-06
4347	diHPCARP_Ic.tttmmpd	1.758e+44	10.69	10.69	2.880e+36	4.12e-06
4348	diHPCARP_Ic.mppmtmmd	1.957e+44	10.76	10.76	2.835e+36	4.05e-06
4349	diHPCARP_Ic.ttpmtmmd	3.405e+43	9.73	9.73	2.803e+36	4.01e-06
4350	diHPCARP_Ic.tttmpttmd	2.067e+44	10.80	10.80	2.794e+36	4e-06
4351	diHPCARP_Ic.tmtppmpd	3.091e+44	11.04	11.04	2.788e+36	3.99e-06
4352	diHPCARP_Ic.tttmmtmd	2.023e+44	10.79	10.79	2.785e+36	3.98e-06
4353	diHPCARP_Ic.pmpmpmmd	1.546e+43	9.26	9.26	2.779e+36	3.97e-06
4354	diHPCARP_Ic.ttpmpmpd	3.390e+43	9.75	9.75	2.679e+36	3.83e-06
4355	diHPCARP_Ic.tpmppppd	1.434e+44	10.62	10.62	2.641e+36	3.78e-06
4356	diHPCARP_Ic.tttppppmd	6.453e+43	10.15	10.15	2.622e+36	3.75e-06
4357	diHPCARP_Ic.pttptmmd	1.110e+44	10.47	10.47	2.598e+36	3.71e-06
4358	diHPCARP_Ic.pmpmttmd	7.090e+43	10.23	10.23	2.503e+36	3.58e-06
4359	diHPCARP_Ic.tmpmttmd	7.064e+44	11.61	11.61	2.477e+36	3.54e-06
4360	diHPCARP_Ic.ptpmmpd	1.005e+43	9.08	9.08	2.457e+36	3.51e-06
4361	diHPCARP_Ic.pmpptpmd	2.408e+43	9.60	9.60	2.440e+36	3.49e-06
4362	diHPCARP_Ic.mtptmtpmd	5.120e+44	11.45	11.45	2.315e+36	3.31e-06
4363	diHPCARP_Ic.mmtmtpmmd	5.101e+44	11.45	11.45	2.314e+36	3.31e-06
4364	diHPCARP_Ic.mmpmtmtpmd	5.296e+43	10.11	10.11	2.272e+36	3.25e-06
4365	diHPCARP_Ic.tpmmpmtpd	9.539e+43	10.48	10.48	2.203e+36	3.15e-06
4366	diHPCARP_Ic.mmpmmttmd	9.082e+43	10.46	10.46	2.173e+36	3.11e-06
4367	diHPCARP_Ic.mttmmttmd	3.191e+44	11.22	11.22	2.148e+36	3.07e-06
4368	diHPCARP_Ic.ptppmmpd	3.203e+43	9.85	9.85	2.124e+36	3.04e-06
4369	diHPCARP_Ic.tppptpmpd	2.835e+44	11.17	11.17	2.058e+36	2.94e-06

4370	diHPCARP_Ic.pmmpttpd	5.447e+43	10.21	10.21	1.996e+36	2.85e-06
4371	diHPCARP_Ic.ttpptppd	3.520e+44	11.32	11.32	1.986e+36	2.84e-06
4372	diHPCARP_Ic.mttpppppd	1.270e+44	10.73	10.73	1.934e+36	2.77e-06
4373	diHPCARP_Ic.tmppttmd	3.702e+44	11.39	11.39	1.856e+36	2.65e-06
4374	diHPCARP_Ic.mppppmpmd	1.095e+44	10.67	10.67	1.840e+36	2.63e-06
4375	diHPCARP_Ic.mtppmmtpd	2.041e+44	11.05	11.05	1.821e+36	2.6e-06
4376	diHPCARP_Ic.ptptmmtmd	1.531e+44	10.88	10.88	1.816e+36	2.6e-06
4377	diHPCARP_Ic.mmmtptpmd	6.893e+43	10.42	10.42	1.779e+36	2.54e-06
4378	diHPCARP_Ic.pmpptmpd	5.507e+43	10.29	10.29	1.764e+36	2.52e-06
4379	diHPCARP_Ic.mppmmtpd	1.643e+44	10.94	10.94	1.762e+36	2.52e-06
4380	diHPCARP_Ic.ptppmmpd	5.618e+43	10.31	10.31	1.748e+36	2.5e-06
4381	diHPCARP_Ic.mtppmtmpd	4.401e+43	10.17	10.17	1.722e+36	2.46e-06
4382	diHPCARP_Ic.mmmtmmtmd	5.650e+44	11.69	11.69	1.718e+36	2.46e-06
4383	diHPCARP_Ic.tmmmpptpd	2.556e+44	11.23	11.23	1.697e+36	2.43e-06
4384	diHPCARP_Ic.mmmtmmtmd	1.036e+45	12.06	12.06	1.693e+36	2.42e-06
4385	diHPCARP_Ic.mmmppmtmd	3.101e+44	11.35	11.35	1.679e+36	2.4e-06
4386	diHPCARP_Ic.tmpptppd	5.095e+44	11.66	11.66	1.646e+36	2.35e-06
4387	diHPCARP_Ic.tmpptpmd	1.286e+44	10.85	10.85	1.600e+36	2.29e-06
4388	diHPCARP_Ic.ttpptppd	2.426e+44	11.24	11.24	1.566e+36	2.24e-06
4389	diHPCARP_Ic.pmmpttmd	5.431e+43	10.36	10.36	1.549e+36	2.21e-06
4390	diHPCARP_Ic.pmmmmmpmd	3.292e+43	10.06	10.06	1.538e+36	2.2e-06
4391	diHPCARP_Ic.tmtppmpd	1.782e+44	11.07	11.07	1.537e+36	2.2e-06
4392	diHPCARP_Ic.pmmmmmmmd	5.080e+43	10.32	10.32	1.535e+36	2.2e-06
4393	diHPCARP_Ic.mmtmmmpmd	2.303e+44	11.23	11.23	1.512e+36	2.16e-06
4394	diHPCARP_Ic.mmmmmmpd	1.504e+44	10.99	10.99	1.481e+36	2.12e-06
4395	diHPCARP_Ic.mtmtpmpd	6.069e+43	10.45	10.45	1.479e+36	2.12e-06
4396	diHPCARP_Ic.ttttpppd	2.016e+44	11.18	11.18	1.453e+36	2.08e-06
4397	diHPCARP_Ic.mmttpppd	4.049e+44	11.60	11.60	1.446e+36	2.07e-06
4398	diHPCARP_Ic.pmmptmmd	4.649e+43	10.31	10.31	1.423e+36	2.03e-06
4399	diHPCARP_Ic.tmpptppd	2.612e+44	11.35	11.35	1.408e+36	2.01e-06
4400	diHPCARP_Ic.mtppmmtd	2.606e+44	11.35	11.35	1.397e+36	2e-06
4401	diHPCARP_Ic.mmpptmpd	2.555e+43	9.97	9.97	1.393e+36	1.99e-06
4402	diHPCARP_Ic.tmtmmppd	6.305e+43	10.51	10.51	1.385e+36	1.98e-06
4403	diHPCARP_Ic.mmmtpmmmd	1.413e+44	11.01	11.01	1.353e+36	1.93e-06
4404	diHPCARP_Ic.ptmtmpd	7.428e+43	10.63	10.63	1.346e+36	1.92e-06
4405	diHPCARP_Ic.pmpppmpd	1.162e+43	9.54	9.54	1.311e+36	1.87e-06
4406	diHPCARP_Ic.ptptmtpd	1.577e+44	11.10	11.10	1.300e+36	1.86e-06
4407	diHPCARP_Ic.ptpmmtd	6.211e+43	10.55	10.55	1.279e+36	1.83e-06
4408	diHPCARP_Ic.ptmmppmd	1.090e+44	10.89	10.89	1.261e+36	1.8e-06
4409	diHPCARP_Ic.mmmtpmtmd	2.479e+44	11.39	11.39	1.257e+36	1.8e-06
4410	diHPCARP_Ic.pppppmpd	3.751e+44	11.63	11.63	1.254e+36	1.79e-06
4411	diHPCARP_Ic.mptmtmd	4.022e+44	11.68	11.68	1.252e+36	1.79e-06
4412	diHPCARP_Ic.mptppmpd	5.780e+43	10.52	10.52	1.252e+36	1.79e-06
4413	diHPCARP_Ic.mmtppmtmd	7.420e+43	10.67	10.67	1.242e+36	1.78e-06
4414	diHPCARP_Ic.mppmmtd	1.821e+44	11.22	11.22	1.229e+36	1.76e-06
4415	diHPCARP_Ic.ttpmtppd	1.110e+44	10.93	10.93	1.219e+36	1.74e-06
4416	diHPCARP_Ic.ptpmmtpd	2.536e+43	10.06	10.06	1.196e+36	1.71e-06
4417	diHPCARP_Ic.mppmmppd	6.825e+43	10.65	10.65	1.188e+36	1.7e-06
4418	diHPCARP_Ic.ptppmtd	9.348e+43	10.85	10.85	1.168e+36	1.67e-06
4419	diHPCARP_Ic.mppmmtd	3.693e+44	11.68	11.68	1.137e+36	1.63e-06
4420	diHPCARP_Ic.mmpmtmd	8.382e+44	12.18	12.18	1.116e+36	1.6e-06
4421	diHPCARP_Ic.ptppmtmd	2.346e+43	10.08	10.08	1.073e+36	1.53e-06
4422	diHPCARP_Ic.tmmmpptmd	2.239e+44	11.44	11.44	1.037e+36	1.48e-06
4423	diHPCARP_Ic.tmpmmmpd	4.535e+43	10.49	10.49	1.031e+36	1.47e-06
4424	diHPCARP_Ic.tmpptppd	2.662e+44	11.55	11.55	1.019e+36	1.46e-06
4425	diHPCARP_Ic.mmtmtmpd	3.011e+44	11.63	11.63	1.018e+36	1.46e-06
4426	diHPCARP_Ic.mtppmmmpd	1.251e+44	11.11	11.11	1.017e+36	1.45e-06
4427	diHPCARP_Ic.mtppmpmd	1.271e+44	11.12	11.12	1.014e+36	1.45e-06
4428	diHPCARP_Ic.ptpttpd	7.754e+44	12.20	12.20	1.005e+36	1.44e-06
4429	diHPCARP_Ic.mtppmmmd	8.051e+43	10.85	10.85	9.986e+35	1.43e-06
4430	diHPCARP_Ic.ptppmtpd	7.625e+43	10.84	10.84	9.724e+35	1.39e-06
4431	diHPCARP_Ic.tmpptpmd	8.531e+43	10.91	10.91	9.554e+35	1.37e-06
4432	diHPCARP_Ic.pmmppmpd	2.014e+43	10.06	10.06	9.430e+35	1.35e-06
4433	diHPCARP_Ic.mtmmmmpd	8.375e+43	10.92	10.92	9.366e+35	1.34e-06
4434	diHPCARP_Ic.mmmmpmpd	1.797e+44	11.37	11.37	9.318e+35	1.33e-06
4435	diHPCARP_Ic.ttmmtmd	1.154e+44	11.12	11.12	9.219e+35	1.32e-06
4436	diHPCARP_Ic.mtptmpd	3.745e+44	11.83	11.83	9.072e+35	1.3e-06
4437	diHPCARP_Ic.tmmmpmmmd	1.546e+44	11.32	11.32	8.790e+35	1.26e-06
4438	diHPCARP_Ic.mpmmtmpd	7.476e+44	12.27	12.27	8.545e+35	1.22e-06
4439	diHPCARP_Ic.tppmmtpd	5.835e+43	10.77	10.77	8.388e+35	1.2e-06
4440	diHPCARP_Ic.tmpmpmpd	4.613e+44	12.02	12.02	8.083e+35	1.16e-06
4441	diHPCARP_Ic.pmmmmtpd	8.195e+43	11.02	11.02	7.720e+35	1.1e-06

4442	diHPCARP_Ic.pmppptmpd	4.236e+43	10.63	10.63	7.691e+35	1.1e-06
4443	diHPCARP_Ic.mtpppmmd	5.401e+43	10.78	10.78	7.594e+35	1.09e-06
4444	diHPCARP_Ic.mtptmtpd	2.550e+44	11.71	11.71	7.578e+35	1.08e-06
4445	diHPCARP_Ic.ptppptmd	2.794e+44	11.78	11.78	7.271e+35	1.04e-06
4446	diHPCARP_Ic.tmpmptpd	1.160e+44	11.32	11.32	6.602e+35	9.44e-07
4447	diHPCARP_Ic.tmpmptpmd	3.284e+43	10.57	10.57	6.596e+35	9.43e-07
4448	diHPCARP_Ic.ptppmpmd	2.079e+43	10.29	10.29	6.594e+35	9.43e-07
4449	diHPCARP_Ic.mmmmpmpmd	5.047e+43	10.83	10.83	6.470e+35	9.25e-07
4450	diHPCARP_Ic.mmpmttmd	2.342e+44	11.76	11.76	6.389e+35	9.14e-07
4451	diHPCARP_Ic.mttmmpmd	1.972e+44	11.68	11.68	6.158e+35	8.81e-07
4452	diHPCARP_Ic.mmmmtmtpmd	5.196e+43	10.89	10.89	6.094e+35	8.71e-07
4453	diHPCARP_Ic.pmpmtpmd	1.683e+44	11.59	11.59	6.022e+35	8.61e-07
4454	diHPCARP_Ic.mtttppmmd	2.065e+44	11.72	11.72	5.965e+35	8.53e-07
4455	diHPCARP_Ic.mtmnmmtmd	2.064e+44	11.74	11.74	5.822e+35	8.33e-07
4456	diHPCARP_Ic.mtttmmpmd	2.708e+44	11.91	11.91	5.724e+35	8.18e-07
4457	diHPCARP_Ic.mmttppmd	3.376e+44	12.05	12.05	5.646e+35	8.07e-07
4458	diHPCARP_Ic.ttttppmpd	8.200e+43	11.21	11.21	5.602e+35	8.01e-07
4459	diHPCARP_Ic.tmpmtpmd	1.999e+44	11.75	11.75	5.532e+35	7.91e-07
4460	diHPCARP_Ic.tppmmpmd	1.014e+44	11.35	11.35	5.462e+35	7.81e-07
4461	diHPCARP_Ic.mpmmtmtpmd	9.534e+43	11.32	11.32	5.420e+35	7.75e-07
4462	diHPCARP_Ic.mtppmmtmd	1.155e+44	11.43	11.43	5.413e+35	7.74e-07
4463	diHPCARP_Ic.tmpmmpmd	4.072e+43	10.82	10.82	5.343e+35	7.64e-07
4464	diHPCARP_Ic.mpmnmmpmd	9.264e+43	11.33	11.33	5.196e+35	7.43e-07
4465	diHPCARP_Ic.mtttmppmd	2.716e+44	11.97	11.97	5.150e+35	7.36e-07
4466	diHPCARP_Ic.tmpmppmd	1.160e+44	11.49	11.49	4.966e+35	7.1e-07
4467	diHPCARP_Ic.ptptmtpd	1.524e+44	11.66	11.66	4.867e+35	6.96e-07
4468	diHPCARP_Ic.mppmmpmd	7.487e+43	11.24	11.24	4.836e+35	6.92e-07
4469	diHPCARP_Ic.mmmmmmmmd	1.613e+44	11.73	11.73	4.619e+35	6.6e-07
4470	diHPCARP_Ic.mmtppmmpmd	1.651e+44	11.76	11.76	4.509e+35	6.45e-07
4471	diHPCARP_Ic.pmmtmnmmd	1.738e+44	11.79	11.79	4.488e+35	6.42e-07
4472	diHPCARP_Ic.ptppmppd	3.327e+43	10.83	10.83	4.323e+35	6.18e-07
4473	diHPCARP_Ic.mmtmtpmd	7.612e+44	12.70	12.70	4.251e+35	6.08e-07
4474	diHPCARP_Ic.mmmmmmpmd	5.402e+43	11.13	11.13	4.238e+35	6.06e-07
4475	diHPCARP_Ic.tmtptpmd	4.667e+44	12.42	12.42	4.207e+35	6.02e-07
4476	diHPCARP_Ic.mmpmtmtpd	5.094e+44	12.47	12.47	4.198e+35	6e-07
4477	diHPCARP_Ic.tmppptpd	3.759e+44	12.31	12.31	4.045e+35	5.78e-07
4478	diHPCARP_Ic.pmmtmmpmd	4.386e+43	11.03	11.03	4.019e+35	5.75e-07
4479	diHPCARP_Ic.mtttppmpd	1.575e+44	11.80	11.80	3.985e+35	5.7e-07
4480	diHPCARP_Ic.mpmmttmd	2.490e+44	12.11	12.11	3.762e+35	5.38e-07
4481	diHPCARP_Ic.pmpmtpmd	1.009e+44	11.58	11.58	3.690e+35	5.28e-07
4482	diHPCARP_Ic.tmtptpmd	2.902e+44	12.25	12.25	3.463e+35	4.95e-07
4483	diHPCARP_Ic.mtmppppd	2.382e+44	12.13	12.13	3.450e+35	4.93e-07
4484	diHPCARP_Ic.tpmppmmd	1.142e+44	11.70	11.70	3.424e+35	4.9e-07
4485	diHPCARP_Ic.mtppmtpd	1.797e+44	11.98	11.98	3.383e+35	4.84e-07
4486	diHPCARP_Ic.mtppmmpmd	6.171e+43	11.35	11.35	3.340e+35	4.78e-07
4487	diHPCARP_Ic.pmpmtpmd	8.459e+43	11.56	11.56	3.204e+35	4.58e-07
4488	diHPCARP_Ic.mmpmtpmd	2.779e+44	12.28	12.28	3.162e+35	4.52e-07
4489	diHPCARP_Ic.pmttmmtmd	2.588e+44	12.24	12.24	3.144e+35	4.5e-07
4490	diHPCARP_Ic.tpmnmmpmd	1.775e+43	10.66	10.66	3.062e+35	4.38e-07
4491	diHPCARP_Ic.ptpmmmtmd	3.273e+43	11.05	11.05	2.930e+35	4.19e-07
4492	diHPCARP_Ic.mtptmmpmd	1.347e+44	11.92	11.92	2.794e+35	4e-07
4493	diHPCARP_Ic.pmmtmmtmd	3.072e+44	12.42	12.42	2.732e+35	3.91e-07
4494	diHPCARP_Ic.tpmppmmd	1.399e+44	11.96	11.96	2.708e+35	3.87e-07
4495	diHPCARP_Ic.mmtmmtpmd	8.723e+43	11.68	11.68	2.694e+35	3.85e-07
4496	diHPCARP_Ic.mpmnmmpmd	1.217e+44	11.89	11.89	2.639e+35	3.77e-07
4497	diHPCARP_Ic.ttmppppmd	6.165e+43	11.49	11.49	2.614e+35	3.74e-07
4498	diHPCARP_Ic.mmpmmpmd	3.126e+44	12.50	12.50	2.453e+35	3.51e-07
4499	diHPCARP_Ic.mpmtmmpmd	1.512e+44	12.07	12.07	2.435e+35	3.48e-07
4500	diHPCARP_Ic.mttppmtpd	3.409e+44	12.57	12.57	2.375e+35	3.4e-07
4501	diHPCARP_Ic.pmpmtpmd	3.327e+44	12.56	12.56	2.364e+35	3.38e-07
4502	diHPCARP_Ic.mmmtpppmd	8.344e+43	11.76	11.76	2.262e+35	3.23e-07
4503	diHPCARP_Ic.mtppmtpd	1.475e+44	12.12	12.12	2.185e+35	3.12e-07
4504	diHPCARP_Ic.mpmnmmtmd	1.231e+44	12.03	12.03	2.124e+35	3.04e-07
4505	diHPCARP_Ic.ttmppmpd	5.877e+43	11.60	11.60	2.098e+35	3e-07
4506	diHPCARP_Ic.tmmtpptmd	4.351e+44	12.81	12.81	2.014e+35	2.88e-07
4507	diHPCARP_Ic.tmpmtpmd	1.896e+44	12.33	12.33	1.977e+35	2.83e-07
4508	diHPCARP_Ic.ttptpmd	7.354e+44	13.14	13.14	1.953e+35	2.79e-07
4509	diHPCARP_Ic.ptppmmpmd	1.118e+44	12.03	12.03	1.940e+35	2.77e-07
4510	diHPCARP_Ic.tppmtpd	2.562e+43	11.20	11.20	1.768e+35	2.53e-07
4511	diHPCARP_Ic.mtmmpmpmd	1.553e+44	12.28	12.28	1.750e+35	2.5e-07
4512	diHPCARP_Ic.pmmmpmpmd	1.004e+44	12.06	12.06	1.650e+35	2.36e-07
4513	diHPCARP_Ic.mpmmtmmd	2.710e+44	12.65	12.65	1.644e+35	2.35e-07

4514	diHPCARP_Ic.mmpmnmmpd	1.699e+43	11.03	11.03	1.572e+35	2.25e-07
4515	diHPCARP_Ic.mtmmpmnmmd	4.313e+43	11.59	11.59	1.547e+35	2.21e-07
4516	diHPCARP_Ic.ptptptmmd	9.153e+43	12.04	12.04	1.541e+35	2.2e-07
4517	diHPCARP_Ic.mtmmtmmtmd	1.594e+44	12.46	12.46	1.328e+35	1.9e-07
4518	diHPCARP_Ic.mpmmtmmpmd	1.726e+44	12.51	12.51	1.322e+35	1.89e-07
4519	diHPCARP_Ic.pttpmppmd	3.944e+43	11.66	11.66	1.272e+35	1.82e-07
4520	diHPCARP_Ic.tppmptmd	1.045e+44	12.27	12.27	1.209e+35	1.73e-07
4521	diHPCARP_Ic.tpmpppppd	8.206e+43	12.16	12.16	1.145e+35	1.64e-07
4522	diHPCARP_Ic.pmttmmpmd	5.948e+43	11.98	11.98	1.119e+35	1.6e-07
4523	diHPCARP_Ic.mmmtmmpd	2.958e+44	12.94	12.94	1.109e+35	1.59e-07
4524	diHPCARP_Ic.mmmtppppd	2.151e+44	12.78	12.78	1.048e+35	1.5e-07
4525	diHPCARP_Ic.mmttppmpd	3.529e+44	13.12	13.12	9.730e+34	1.39e-07
4526	diHPCARP_Ic.mtttptmpd	4.376e+44	13.30	13.30	9.031e+34	1.29e-07
4527	diHPCARP_Ic.pmpmtmmmd	7.888e+43	12.28	12.28	8.892e+34	1.27e-07
4528	diHPCARP_Ic.mtptpoptd	1.415e+44	12.65	12.65	8.679e+34	1.24e-07
4529	diHPCARP_Ic.mmmtmppmd	7.883e+43	12.30	12.30	8.669e+34	1.24e-07
4530	diHPCARP_Ic.pttpmmpmd	1.496e+44	12.68	12.68	8.610e+34	1.23e-07
4531	diHPCARP_Ic.mmtppmmpmd	9.849e+43	12.44	12.44	8.526e+34	1.22e-07
4532	diHPCARP_Ic.pmtmnmmpd	3.631e+43	11.87	11.87	8.151e+34	1.17e-07
4533	diHPCARP_Ic.tppoptmpd	3.341e+43	11.87	11.87	7.579e+34	1.08e-07
4534	diHPCARP_Ic.mtttpttpd	2.421e+44	13.08	13.08	7.124e+34	1.02e-07
4535	diHPCARP_Ic.mmmppmnmmd	8.121e+43	12.45	12.45	6.901e+34	9.87e-08
4536	diHPCARP_Ic.mmmtmnmmd	4.770e+44	13.51	13.51	6.832e+34	9.77e-08
4537	diHPCARP_Ic.ttpmpoptmd	1.401e+44	12.79	12.79	6.787e+34	9.7e-08
4538	diHPCARP_Ic.mttppmtmd	8.651e+44	13.92	13.92	6.271e+34	8.97e-08
4539	diHPCARP_Ic.mmpppppmd	1.723e+43	11.59	11.59	6.221e+34	8.9e-08
4540	diHPCARP_Ic.pmppppppd	8.846e+43	12.57	12.57	6.139e+34	8.78e-08
4541	diHPCARP_Ic.ptptmnmmd	4.577e+43	12.21	12.21	5.815e+34	8.32e-08
4542	diHPCARP_Ic.mmpmtmtpd	3.630e+44	13.50	13.50	5.315e+34	7.6e-08
4543	diHPCARP_Ic.pmpmtmmpd	6.894e+43	12.51	12.51	5.298e+34	7.58e-08
4544	diHPCARP_Ic.tttppmnmmd	2.666e+43	11.95	11.95	5.279e+34	7.55e-08
4545	diHPCARP_Ic.mtmtpmppd	1.765e+44	13.07	13.07	5.277e+34	7.55e-08
4546	diHPCARP_Ic.mtpmnmnmmd	4.034e+43	12.24	12.24	4.899e+34	7.01e-08
4547	diHPCARP_Ic.mmptpppmd	5.868e+43	12.49	12.49	4.640e+34	6.63e-08
4548	diHPCARP_Ic.pmmtmmpd	2.050e+44	13.25	13.25	4.586e+34	6.56e-08
4549	diHPCARP_Ic.ttmmpoptmd	1.451e+44	13.11	13.11	4.057e+34	5.8e-08
4550	diHPCARP_Ic.ptttmppmd	7.035e+43	12.72	12.72	3.839e+34	5.49e-08
4551	diHPCARP_Ic.mmtmppppmd	1.251e+44	13.12	13.12	3.492e+34	4.99e-08
4552	diHPCARP_Ic.mtmtpmnmmd	1.085e+44	13.05	13.05	3.372e+34	4.82e-08
4553	diHPCARP_Ic.mmpmnmnmmd	5.020e+43	12.62	12.62	3.235e+34	4.63e-08
4554	diHPCARP_Ic.pmpmnmmpd	2.513e+43	12.27	12.27	2.894e+34	4.14e-08
4555	diHPCARP_Ic.tpmppppmd	1.031e+44	13.12	13.12	2.843e+34	4.07e-08
4556	diHPCARP_Ic.mtmtpoptd	2.415e+44	13.70	13.70	2.540e+34	3.63e-08
4557	diHPCARP_Ic.tmpptpppd	8.382e+44	14.52	14.52	2.208e+34	3.16e-08
4558	diHPCARP_Ic.mmpmtmmpmd	2.054e+44	13.72	13.72	2.094e+34	2.99e-08
4559	diHPCARP_Ic.ttpppoptmd	9.539e+43	13.27	13.27	2.044e+34	2.92e-08
4560	diHPCARP_Ic.mttppmppd	6.511e+44	14.55	14.55	1.632e+34	2.33e-08
4561	diHPCARP_Ic.ptttmmpmd	2.209e+44	13.94	13.94	1.552e+34	2.22e-08
4562	diHPCARP_Ic.tmmppppmd	5.093e+43	13.08	13.08	1.515e+34	2.17e-08
4563	diHPCARP_Ic.pmpmnmppd	1.117e+44	13.63	13.63	1.318e+34	1.88e-08
4564	diHPCARP_Ic.mmttmmpmd	1.623e+44	13.89	13.89	1.242e+34	1.78e-08
4565	diHPCARP_Ic.tmpptppmd	1.237e+44	13.73	13.73	1.228e+34	1.76e-08
4566	diHPCARP_Ic.ttmtpoptmd	1.382e+44	13.80	13.80	1.228e+34	1.76e-08
4567	diHPCARP_Ic.pttmppppmd	3.663e+43	13.04	13.04	1.162e+34	1.66e-08
4568	diHPCARP_Ic.mmpmpmmpd	5.367e+43	13.28	13.28	1.143e+34	1.63e-08
4569	diHPCARP_Ic.mtmnmnmppd	5.888e+44	14.73	14.73	1.095e+34	1.57e-08
4570	diHPCARP_Ic.mtttmmpd	1.530e+45	15.35	15.35	1.009e+34	1.44e-08
4571	diHPCARP_Ic.tttppppmd	7.550e+43	13.77	13.77	6.989e+33	9.99e-09
4572	diHPCARP_Ic.mttmnmppd	1.068e+45	15.41	15.41	6.380e+33	9.12e-09
4573	diHPCARP_Ic.mmtmnmmpd	1.151e+44	14.15	14.15	5.674e+33	8.11e-09
4574	diHPCARP_Ic.mtmnmmpd	8.044e+43	14.01	14.01	5.034e+33	7.2e-09
4575	diHPCARP_Ic.tmmtpppmd	8.970e+43	14.14	14.14	4.507e+33	6.45e-09
4576	diHPCARP_Ic.tttppoptmd	4.577e+44	15.42	15.42	2.665e+33	3.81e-09
4577	diHPCARP_Ic.mtmnmmtmd	4.344e+44	15.40	15.40	2.612e+33	3.73e-09
4578	diHPCARP_Ic.mmpmtmmpmd	1.652e+44	15.00	15.00	1.951e+33	2.79e-09
4579	diHPCARP_Ic.tttppppd	5.099e+44	15.79	15.79	1.615e+33	2.31e-09
4580	diHPCARP_Ic.tttppmtpd	1.342e+44	15.01	15.01	1.554e+33	2.22e-09
4581	diHPCARP_Ic.ttttppmmd	1.295e+44	15.01	15.01	1.499e+33	2.14e-09
4582	diHPCARP_Ic.mmpmtpppd	9.639e+44	16.26	16.26	1.373e+33	1.96e-09
4583	diHPCARP_Ic.mmpmppppd	3.712e+44	15.74	15.74	1.264e+33	1.81e-09
4584	diHPCARP_Ic.mmpmnmmpd	1.526e+43	14.04	14.04	8.988e+32	1.29e-09
4585	diHPCARP_Ic.ttpmpmnmmd	4.075e+43	14.66	14.66	8.594e+32	1.23e-09

4586	diHPCARP_Ic.ttttppmpd	8.109e+44	16.77	16.77	4.895e+32	7e-10
4587	diHPCARP_Ic.mmpmpmpd	8.509e+43	15.44	15.44	4.830e+32	6.91e-10
4588	diHPCARP_Ic.ttttptmd	1.499e+44	15.78	15.78	4.787e+32	6.84e-10
4589	diHPCARP_Ic.mppmpmpd	4.276e+43	15.04	15.04	4.740e+32	6.78e-10
4590	diHPCARP_Ic.ttttppmpd	7.274e+44	16.83	16.83	4.011e+32	5.73e-10
4591	diHPCARP_Ic.ttmppmpd	1.692e+44	16.06	16.06	3.363e+32	4.81e-10
4592	diHPCARP_Ic.mmpmmtpd	1.167e+44	15.88	15.88	3.129e+32	4.47e-10
4593	diHPCARP_Ic.tttptmd	2.886e+44	17.08	17.08	1.042e+32	1.49e-10
4594	diHPCARP_Ic.mmpmmmpd	1.528e+44	18.46	18.46	5.491e+30	7.85e-12
4595	Total				6.993e+43	100

4596
4597
4598
4599 1,4-aldehyde-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
4600 =====

4601
4602 Population analysis at 300K. Vibrational scaling: 0.971.
4603 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
4604 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
4605 %: contribution to the population (with current data set assumed 100%)
4606 Compound Qtot Erel Erel2 n*Q*MB %
4607 -----

4608	TS.diHPCARP_I.14aldHshift.mmtmmpd	1.116e+43	0.00	0.00	1.116e+43	25.2
4609	TS.diHPCARP_I.14aldHshift.mmmmpd	2.025e+43	0.51	0.51	8.586e+42	19.4
4610	TS.diHPCARP_I.14aldHshift.tpmmpd	2.587e+43	1.33	1.33	2.763e+42	6.24
4611	TS.diHPCARP_I.14aldHshift.tppmpd	3.318e+42	0.40	0.40	1.705e+42	3.85
4612	TS.diHPCARP_I.14aldHshift.mmpmpd	1.128e+43	1.16	1.16	1.623e+42	3.66
4613	TS.diHPCARP_I.14aldHshift.mmtmmpd	2.174e+43	1.59	1.59	1.499e+42	3.39
4614	TS.diHPCARP_I.14aldHshift.pmpmpd	5.390e+42	0.79	0.79	1.443e+42	3.26
4615	TS.diHPCARP_I.14aldHshift.mtpmpd	3.129e+43	1.92	1.92	1.252e+42	2.83
4616	TS.diHPCARP_I.14aldHshift.tpmmpd	4.407e+43	2.19	2.19	1.127e+42	2.54
4617	TS.diHPCARP_I.14aldHshift.mppmpd	7.320e+42	1.17	1.17	1.028e+42	2.32
4618	TS.diHPCARP_I.14aldHshift.mtmmpd	3.414e+43	2.20	2.20	8.507e+41	1.92
4619	TS.diHPCARP_I.14aldHshift.mppmpd	4.388e+42	0.99	0.99	8.353e+41	1.89
4620	TS.diHPCARP_I.14aldHshift.mppmpd	2.008e+43	1.91	1.91	8.158e+41	1.84
4621	TS.diHPCARP_I.14aldHshift.pmpmpd	1.151e+43	1.67	1.67	6.952e+41	1.57
4622	TS.diHPCARP_I.14aldHshift.mtptmd	2.076e+43	2.09	2.09	6.229e+41	1.41
4623	TS.diHPCARP_I.14aldHshift.mmmmpd	1.554e+43	2.10	2.10	4.561e+41	1.03
4624	TS.diHPCARP_I.14aldHshift.mttppd	4.787e+43	2.91	2.91	3.637e+41	0.821
4625	TS.diHPCARP_I.14aldHshift.tpmppd	1.088e+43	2.04	2.04	3.582e+41	0.809
4626	TS.diHPCARP_I.14aldHshift.tmtppd	1.552e+43	2.25	2.25	3.559e+41	0.804
4627	TS.diHPCARP_I.14aldHshift.mttmmpd	5.371e+43	2.99	2.99	3.540e+41	0.799
4628	TS.diHPCARP_I.14aldHshift.mmtppd	5.939e+43	3.10	3.10	3.296e+41	0.744
4629	TS.diHPCARP_I.14aldHshift.pmtmpd	2.229e+43	2.63	2.63	2.685e+41	0.606
4630	TS.diHPCARP_I.14aldHshift.tmtptd	3.363e+43	2.90	2.90	2.581e+41	0.583
4631	TS.diHPCARP_I.14aldHshift.mppmpd	6.547e+42	1.93	1.93	2.552e+41	0.576
4632	TS.diHPCARP_I.14aldHshift.mmtmmpd	1.621e+43	2.48	2.48	2.531e+41	0.572
4633	TS.diHPCARP_I.14aldHshift.tmtppd	4.433e+43	3.08	3.08	2.519e+41	0.569
4634	TS.diHPCARP_I.14aldHshift.tmpmpd	3.655e+42	1.61	1.61	2.469e+41	0.558
4635	TS.diHPCARP_I.14aldHshift.mmtppd	6.095e+42	1.96	1.96	2.278e+41	0.514
4636	TS.diHPCARP_I.14aldHshift.pttppd	1.651e+43	2.60	2.60	2.108e+41	0.476
4637	TS.diHPCARP_I.14aldHshift.tmtmmpd	7.987e+42	2.18	2.18	2.077e+41	0.469
4638	TS.diHPCARP_I.14aldHshift.mtmmpd	8.116e+43	3.67	3.67	1.718e+41	0.388
4639	TS.diHPCARP_I.14aldHshift.ptpppd	3.526e+43	3.21	3.21	1.608e+41	0.363
4640	TS.diHPCARP_I.14aldHshift.mmtppd	2.205e+43	3.00	3.00	1.442e+41	0.326
4641	TS.diHPCARP_I.14aldHshift.ttmppd	1.595e+43	2.87	2.87	1.289e+41	0.291
4642	TS.diHPCARP_I.14aldHshift.tptppd	5.482e+42	2.36	2.36	1.051e+41	0.237
4643	TS.diHPCARP_I.14aldHshift.mmtmmpd	1.835e+43	3.09	3.09	1.031e+41	0.233
4644	TS.diHPCARP_I.14aldHshift.mmmmpd	2.303e+43	3.24	3.24	1.005e+41	0.227
4645	TS.diHPCARP_I.14aldHshift.mppmpd	1.769e+43	3.09	3.09	9.872e+40	0.223
4646	TS.diHPCARP_I.14aldHshift.tmtmmpd	9.432e+42	2.80	2.80	8.675e+40	0.196
4647	TS.diHPCARP_I.14aldHshift.tmtmmpd	7.260e+42	2.67	2.67	8.306e+40	0.188
4648	TS.diHPCARP_I.14aldHshift.mmtppd	1.040e+44	4.27	4.27	8.084e+40	0.183
4649	TS.diHPCARP_I.14aldHshift.pmtmmpd	4.331e+43	3.75	3.75	7.998e+40	0.181
4650	TS.diHPCARP_I.14aldHshift.pmpmpd	1.500e+43	3.14	3.14	7.748e+40	0.175
4651	TS.diHPCARP_I.14aldHshift.tptmmpd	2.257e+44	4.76	4.76	7.747e+40	0.175
4652	TS.diHPCARP_I.14aldHshift.mmtmmpd	2.649e+43	3.54	3.54	6.955e+40	0.157
4653	TS.diHPCARP_I.14aldHshift.mppmpd	6.307e+42	2.70	2.70	6.811e+40	0.154
4654	TS.diHPCARP_I.14aldHshift.mppmtpd	2.072e+43	3.47	3.47	6.110e+40	0.138
4655	TS.diHPCARP_I.14aldHshift.mmmmpd	3.894e+43	3.86	3.86	5.974e+40	0.135
4656	TS.diHPCARP_I.14aldHshift.pmmmpd	1.846e+44	4.79	4.79	5.944e+40	0.134
4657	TS.diHPCARP_I.14aldHshift.pmtmmpd	2.731e+43	3.66	3.66	5.847e+40	0.132

4658	TS.diHPCARP_I.14aldHshift.mpptppd	1.099e+44	4.50	4.50	5.763e+40	0.13
4659	TS.diHPCARP_I.14aldHshift.ptptpmd	2.101e+43	3.53	3.53	5.636e+40	0.127
4660	TS.diHPCARP_I.14aldHshift.mmmttppd	2.467e+44	5.01	5.01	5.546e+40	0.125
4661	TS.diHPCARP_I.14aldHshift.tmptpmd	2.347e+43	3.61	3.61	5.519e+40	0.125
4662	TS.diHPCARP_I.14aldHshift.pppppmd	2.622e+43	3.70	3.70	5.305e+40	0.12
4663	TS.diHPCARP_I.14aldHshift.ptmmmpd	5.417e+43	4.16	4.16	5.077e+40	0.115
4664	TS.diHPCARP_I.14aldHshift.mmttppd	3.127e+43	3.87	3.87	4.771e+40	0.108
4665	TS.diHPCARP_I.14aldHshift.mmttppd	6.058e+43	4.28	4.28	4.586e+40	0.104
4666	TS.diHPCARP_I.14aldHshift.ptttmmd	4.548e+43	4.12	4.12	4.518e+40	0.102
4667	TS.diHPCARP_I.14aldHshift.pmmtpmd	1.914e+43	3.63	3.63	4.333e+40	0.0979
4668	TS.diHPCARP_I.14aldHshift.ptmtppd	9.051e+43	4.56	4.56	4.318e+40	0.0975
4669	TS.diHPCARP_I.14aldHshift.mppmpmd	7.987e+42	3.14	3.14	4.153e+40	0.0938
4670	TS.diHPCARP_I.14aldHshift.tmpmpmd	2.215e+43	3.76	3.76	4.023e+40	0.0909
4671	TS.diHPCARP_I.14aldHshift.tpmtpmd	6.787e+43	4.43	4.43	3.995e+40	0.0902
4672	TS.diHPCARP_I.14aldHshift.tmpppd	1.211e+43	3.41	3.41	3.940e+40	0.089
4673	TS.diHPCARP_I.14aldHshift.tmtppmd	1.198e+43	3.42	3.42	3.874e+40	0.0875
4674	TS.diHPCARP_I.14aldHshift.ptpmpmd	1.080e+44	4.73	4.73	3.853e+40	0.087
4675	TS.diHPCARP_I.14aldHshift.ptmppmd	4.889e+43	4.27	4.27	3.804e+40	0.0859
4676	TS.diHPCARP_I.14aldHshift.mtpmtpd	3.804e+43	4.14	4.14	3.694e+40	0.0834
4677	TS.diHPCARP_I.14aldHshift.mttttmd	6.433e+43	4.46	4.46	3.636e+40	0.0821
4678	TS.diHPCARP_I.14aldHshift.mtpmpmd	3.829e+43	4.16	4.16	3.582e+40	0.0809
4679	TS.diHPCARP_I.14aldHshift.mmmttmd	9.959e+43	4.74	4.74	3.508e+40	0.0792
4680	TS.diHPCARP_I.14aldHshift.tppppd	7.418e+42	3.20	3.20	3.487e+40	0.0787
4681	TS.diHPCARP_I.14aldHshift.pmpmpmd	6.815e+42	3.17	3.17	3.368e+40	0.0761
4682	TS.diHPCARP_I.14aldHshift.ptmtppd	7.518e+43	4.60	4.60	3.353e+40	0.0757
4683	TS.diHPCARP_I.14aldHshift.ttptpmd	1.129e+43	3.47	3.47	3.323e+40	0.0751
4684	TS.diHPCARP_I.14aldHshift.pptppmd	2.352e+43	3.92	3.92	3.286e+40	0.0742
4685	TS.diHPCARP_I.14aldHshift.mmmmtppd	8.497e+43	4.71	4.71	3.137e+40	0.0709
4686	TS.diHPCARP_I.14aldHshift.ttmmtmd	7.693e+43	4.67	4.67	3.059e+40	0.0691
4687	TS.diHPCARP_I.14aldHshift.ptttppd	5.007e+43	4.41	4.41	3.044e+40	0.0688
4688	TS.diHPCARP_I.14aldHshift.tmmppmd	5.065e+42	3.07	3.07	2.937e+40	0.0663
4689	TS.diHPCARP_I.14aldHshift.mtmmpmd	2.713e+43	4.12	4.12	2.725e+40	0.0615
4690	TS.diHPCARP_I.14aldHshift.pmpmmd	1.693e+43	3.84	3.84	2.697e+40	0.0609
4691	TS.diHPCARP_I.14aldHshift.tmpmtpd	4.329e+43	4.41	4.41	2.669e+40	0.0603
4692	TS.diHPCARP_I.14aldHshift.mttppmd	2.504e+43	4.12	4.12	2.479e+40	0.056
4693	TS.diHPCARP_I.14aldHshift.tmmmtmd	1.174e+43	3.69	3.69	2.420e+40	0.0547
4694	TS.diHPCARP_I.14aldHshift.pmmtpd	3.740e+43	4.39	4.39	2.382e+40	0.0538
4695	TS.diHPCARP_I.14aldHshift.mmmppd	1.511e+43	3.86	3.86	2.343e+40	0.0529
4696	TS.diHPCARP_I.14aldHshift.mtmmtmd	3.554e+43	4.37	4.37	2.340e+40	0.0529
4697	TS.diHPCARP_I.14aldHshift.pmpmtpd	8.448e+42	3.59	3.59	2.066e+40	0.0467
4698	TS.diHPCARP_I.14aldHshift.tmpmtpd	3.540e+43	4.45	4.45	2.039e+40	0.046
4699	TS.diHPCARP_I.14aldHshift.mtpmtpd	4.182e+43	4.58	4.58	1.931e+40	0.0436
4700	TS.diHPCARP_I.14aldHshift.mppppd	1.001e+43	3.76	3.76	1.815e+40	0.041
4701	TS.diHPCARP_I.14aldHshift.ptmmpmd	3.295e+43	4.49	4.49	1.758e+40	0.0397
4702	TS.diHPCARP_I.14aldHshift.tptpmd	1.080e+43	3.83	3.83	1.746e+40	0.0394
4703	TS.diHPCARP_I.14aldHshift.mtmmpmd	4.400e+43	4.67	4.67	1.740e+40	0.0393
4704	TS.diHPCARP_I.14aldHshift.tppppd	6.595e+42	3.60	3.60	1.580e+40	0.0357
4705	TS.diHPCARP_I.14aldHshift.ttmtpmd	2.203e+43	4.34	4.34	1.507e+40	0.034
4706	TS.diHPCARP_I.14aldHshift.mtmtpmd	5.888e+43	4.98	4.98	1.384e+40	0.0313
4707	TS.diHPCARP_I.14aldHshift.tmpmtpd	2.760e+43	4.56	4.56	1.313e+40	0.0297
4708	TS.diHPCARP_I.14aldHshift.mtmtpmd	3.051e+43	4.63	4.63	1.283e+40	0.029
4709	TS.diHPCARP_I.14aldHshift.pppmpmd	1.947e+43	4.38	4.38	1.245e+40	0.0281
4710	TS.diHPCARP_I.14aldHshift.mtttppd	6.086e+43	5.11	5.11	1.154e+40	0.0261
4711	TS.diHPCARP_I.14aldHshift.tpmmpmd	2.492e+43	4.61	4.61	1.094e+40	0.0247
4712	TS.diHPCARP_I.14aldHshift.tttppmd	3.772e+43	4.92	4.92	9.907e+39	0.0224
4713	TS.diHPCARP_I.14aldHshift.tpmtpd	8.798e+43	5.43	5.43	9.682e+39	0.0219
4714	TS.diHPCARP_I.14aldHshift.tpmmtmd	1.279e+43	4.33	4.33	9.032e+39	0.0204
4715	TS.diHPCARP_I.14aldHshift.ppmtpd	7.699e+43	5.40	5.40	8.922e+39	0.0202
4716	TS.diHPCARP_I.14aldHshift.mmttppd	1.220e+44	5.70	5.70	8.550e+39	0.0193
4717	TS.diHPCARP_I.14aldHshift.ttmtpmd	3.978e+43	5.09	5.09	7.803e+39	0.0176
4718	TS.diHPCARP_I.14aldHshift.pptppd	2.107e+43	4.72	4.72	7.625e+39	0.0172
4719	TS.diHPCARP_I.14aldHshift.pppppd	3.114e+43	4.96	4.96	7.572e+39	0.0171
4720	TS.diHPCARP_I.14aldHshift.pptppd	1.242e+44	5.80	5.80	7.438e+39	0.0168
4721	TS.diHPCARP_I.14aldHshift.ptpmpmd	3.918e+43	5.15	5.15	6.976e+39	0.0158
4722	TS.diHPCARP_I.14aldHshift.ttttppd	2.970e+43	4.99	4.99	6.858e+39	0.0155
4723	TS.diHPCARP_I.14aldHshift.ppmtpmd	5.016e+43	5.31	5.31	6.764e+39	0.0153
4724	TS.diHPCARP_I.14aldHshift.pmmppd	3.754e+43	5.20	5.20	6.069e+39	0.0137
4725	TS.diHPCARP_I.14aldHshift.pptppd	6.208e+43	5.52	5.52	5.921e+39	0.0134
4726	TS.diHPCARP_I.14aldHshift.mtpppd	3.067e+43	5.13	5.13	5.643e+39	0.0127
4727	TS.diHPCARP_I.14aldHshift.tttppd	3.035e+43	5.13	5.13	5.539e+39	0.0125
4728	TS.diHPCARP_I.14aldHshift.pppppd	1.922e+43	4.86	4.86	5.515e+39	0.0125
4729	TS.diHPCARP_I.14aldHshift.mtpmtpd	1.262e+44	5.99	5.99	5.438e+39	0.0123

4730	TS.diHPCARP_I.14aldHshift.tmmtpd	2.384e+43	5.00	5.00	5.421e+39	0.0122
4731	TS.diHPCARP_I.14aldHshift.tmpttmd	3.867e+43	5.30	5.30	5.312e+39	0.012
4732	TS.diHPCARP_I.14aldHshift.pttttmd	7.718e+43	5.72	5.72	5.293e+39	0.012
4733	TS.diHPCARP_I.14aldHshift.mmtptmd	2.683e+43	5.14	5.14	4.845e+39	0.0109
4734	TS.diHPCARP_I.14aldHshift.mmttmd	1.395e+44	6.16	6.16	4.556e+39	0.0103
4735	TS.diHPCARP_I.14aldHshift.ppttmd	4.487e+43	5.48	5.48	4.546e+39	0.0103
4736	TS.diHPCARP_I.14aldHshift.mppmpmd	6.677e+43	5.73	5.73	4.497e+39	0.0102
4737	TS.diHPCARP_I.14aldHshift.tpmptmd	5.957e+43	5.66	5.66	4.456e+39	0.0101
4738	TS.diHPCARP_I.14aldHshift.pmmttmd	5.599e+43	5.64	5.64	4.384e+39	0.0099
4739	TS.diHPCARP_I.14aldHshift.pmpmtpd	2.889e+43	5.27	5.27	4.163e+39	0.0094
4740	TS.diHPCARP_I.14aldHshift.mppmtpd	2.245e+43	5.13	5.13	4.086e+39	0.00923
4741	TS.diHPCARP_I.14aldHshift.pmpptpd	2.394e+43	5.19	5.19	3.978e+39	0.00898
4742	TS.diHPCARP_I.14aldHshift.tptmpd	1.188e+43	4.79	4.79	3.847e+39	0.00869
4743	TS.diHPCARP_I.14aldHshift.mppttd	1.196e+44	6.24	6.24	3.433e+39	0.00775
4744	TS.diHPCARP_I.14aldHshift.mmttmd	1.557e+44	6.40	6.40	3.366e+39	0.0076
4745	TS.diHPCARP_I.14aldHshift.pmpmtpd	1.772e+44	6.51	6.51	3.224e+39	0.00728
4746	TS.diHPCARP_I.14aldHshift.mppmpmd	4.043e+43	5.63	5.63	3.180e+39	0.00718
4747	TS.diHPCARP_I.14aldHshift.ppmptmd	9.488e+43	6.17	6.17	3.021e+39	0.00682
4748	TS.diHPCARP_I.14aldHshift.tppmpd	9.456e+42	4.84	4.84	2.817e+39	0.00636
4749	TS.diHPCARP_I.14aldHshift.mpttmd	1.277e+44	6.42	6.42	2.669e+39	0.00603
4750	TS.diHPCARP_I.14aldHshift.ptmpppd	9.586e+43	6.26	6.26	2.651e+39	0.00599
4751	TS.diHPCARP_I.14aldHshift.mtmtpd	9.731e+43	6.28	6.28	2.583e+39	0.00583
4752	TS.diHPCARP_I.14aldHshift.mpptmpd	3.439e+43	5.66	5.66	2.570e+39	0.0058
4753	TS.diHPCARP_I.14aldHshift.mppmtpd	2.231e+43	5.43	5.43	2.487e+39	0.00562
4754	TS.diHPCARP_I.14aldHshift.ttpmtpd	3.232e+44	7.04	7.04	2.399e+39	0.00542
4755	TS.diHPCARP_I.14aldHshift.tpttmd	3.956e+43	5.79	5.79	2.394e+39	0.00541
4756	TS.diHPCARP_I.14aldHshift.ttmtpd	1.091e+44	6.41	6.41	2.352e+39	0.00531
4757	TS.diHPCARP_I.14aldHshift.tpptpd	6.673e+43	6.13	6.13	2.274e+39	0.00514
4758	TS.diHPCARP_I.14aldHshift.ppppppd	3.412e+43	5.74	5.74	2.233e+39	0.00504
4759	TS.diHPCARP_I.14aldHshift.mppmmd	6.643e+42	4.83	4.83	2.018e+39	0.00456
4760	TS.diHPCARP_I.14aldHshift.ppmmpd	3.190e+43	5.80	5.80	1.895e+39	0.00428
4761	TS.diHPCARP_I.14aldHshift.mppmtpd	8.377e+43	6.39	6.39	1.864e+39	0.00421
4762	TS.diHPCARP_I.14aldHshift.mpmtpd	9.848e+43	6.49	6.49	1.834e+39	0.00414
4763	TS.diHPCARP_I.14aldHshift.pmmtpd	1.536e+44	6.77	6.77	1.801e+39	0.00407
4764	TS.diHPCARP_I.14aldHshift.pptppd	4.483e+43	6.04	6.04	1.786e+39	0.00403
4765	TS.diHPCARP_I.14aldHshift.tppmmd	1.212e+44	6.63	6.63	1.780e+39	0.00402
4766	TS.diHPCARP_I.14aldHshift.mmmtpd	3.456e+43	5.89	5.89	1.771e+39	0.004
4767	TS.diHPCARP_I.14aldHshift.ppmtpd	1.028e+44	6.54	6.54	1.762e+39	0.00398
4768	TS.diHPCARP_I.14aldHshift.pptmtpd	1.306e+44	6.69	6.69	1.736e+39	0.00392
4769	TS.diHPCARP_I.14aldHshift.pptptd	4.386e+43	6.05	6.05	1.731e+39	0.00391
4770	TS.diHPCARP_I.14aldHshift.ptmtpd	2.003e+44	7.05	7.05	1.469e+39	0.00332
4771	TS.diHPCARP_I.14aldHshift.pttttmd	8.666e+43	6.56	6.56	1.446e+39	0.00327
4772	TS.diHPCARP_I.14aldHshift.pmpmpd	3.697e+43	6.06	6.06	1.418e+39	0.0032
4773	TS.diHPCARP_I.14aldHshift.ttmtpd	1.163e+44	6.77	6.77	1.359e+39	0.00307
4774	TS.diHPCARP_I.14aldHshift.mtmtpd	1.425e+44	6.94	6.94	1.249e+39	0.00282
4775	TS.diHPCARP_I.14aldHshift.ppmtpd	5.027e+43	6.34	6.34	1.219e+39	0.00275
4776	TS.diHPCARP_I.14aldHshift.pptmmpd	1.965e+43	5.79	5.79	1.188e+39	0.00268
4777	TS.diHPCARP_I.14aldHshift.pppmmd	6.291e+43	6.49	6.49	1.169e+39	0.00264
4778	TS.diHPCARP_I.14aldHshift.mpmtpd	2.118e+43	5.93	5.93	1.010e+39	0.00228
4779	TS.diHPCARP_I.14aldHshift.pppmpd	2.970e+43	6.15	6.15	9.880e+38	0.00223
4780	TS.diHPCARP_I.14aldHshift.pptmtpd	2.979e+43	6.15	6.15	9.808e+38	0.00222
4781	TS.diHPCARP_I.14aldHshift.ppmtpd	1.055e+44	6.91	6.91	9.801e+38	0.00221
4782	TS.diHPCARP_I.14aldHshift.pmpmtpd	1.027e+44	6.90	6.90	9.622e+38	0.00217
4783	TS.diHPCARP_I.14aldHshift.tmmtpd	4.569e+43	6.42	6.42	9.594e+38	0.00217
4784	TS.diHPCARP_I.14aldHshift.tppppd	2.142e+43	5.97	5.97	9.591e+38	0.00217
4785	TS.diHPCARP_I.14aldHshift.ptpmpd	1.292e+44	7.05	7.05	9.437e+38	0.00213
4786	TS.diHPCARP_I.14aldHshift.tpptpd	1.901e+44	7.30	7.30	9.210e+38	0.00208
4787	TS.diHPCARP_I.14aldHshift.pmpmtpd	3.434e+43	6.28	6.28	9.133e+38	0.00206
4788	TS.diHPCARP_I.14aldHshift.pptptd	1.832e+44	7.29	7.29	8.919e+38	0.00201
4789	TS.diHPCARP_I.14aldHshift.ptmtpd	1.490e+44	7.18	7.18	8.759e+38	0.00198
4790	TS.diHPCARP_I.14aldHshift.ttttmd	4.907e+43	6.53	6.53	8.627e+38	0.00195
4791	TS.diHPCARP_I.14aldHshift.mtpmtpd	4.854e+43	6.54	6.54	8.380e+38	0.00189
4792	TS.diHPCARP_I.14aldHshift.ttpmtpd	1.893e+44	7.36	7.36	8.162e+38	0.00184
4793	TS.diHPCARP_I.14aldHshift.tppmtpd	2.467e+44	7.52	7.52	8.151e+38	0.00184
4794	TS.diHPCARP_I.14aldHshift.ttmtpd	8.952e+43	6.92	6.92	8.144e+38	0.00184
4795	TS.diHPCARP_I.14aldHshift.ttpmtpd	2.177e+44	7.45	7.45	8.112e+38	0.00183
4796	TS.diHPCARP_I.14aldHshift.mmtpppd	1.084e+43	5.67	5.67	7.988e+38	0.0018
4797	TS.diHPCARP_I.14aldHshift.ptmmpd	8.170e+43	6.89	6.89	7.752e+38	0.00175
4798	TS.diHPCARP_I.14aldHshift.tppmmd	1.371e+43	5.84	5.84	7.588e+38	0.00171
4799	TS.diHPCARP_I.14aldHshift.ppmtpd	8.310e+43	6.92	6.92	7.504e+38	0.00169
4800	TS.diHPCARP_I.14aldHshift.pppmtpd	2.577e+43	6.23	6.23	7.503e+38	0.00169
4801	TS.diHPCARP_I.14aldHshift.ppmtpd	8.918e+43	6.98	6.98	7.277e+38	0.00164

4802	TS.diHPCARP_I.14aldHshift.pptptmd	6.560e+43	6.82	6.82	7.038e+38	0.00159
4803	TS.diHPCARP_I.14aldHshift.pppttpd	8.392e+43	6.97	6.97	7.025e+38	0.00159
4804	TS.diHPCARP_I.14aldHshift.pmmppmd	2.232e+43	6.19	6.19	6.920e+38	0.00156
4805	TS.diHPCARP_I.14aldHshift.pmmttptd	6.725e+43	6.86	6.86	6.744e+38	0.00152
4806	TS.diHPCARP_I.14aldHshift.mmtppmd	2.145e+43	6.24	6.24	6.149e+38	0.00139
4807	TS.diHPCARP_I.14aldHshift.pptmmmd	9.129e+43	7.12	7.12	5.956e+38	0.00135
4808	TS.diHPCARP_I.14aldHshift.pppttmd	1.133e+44	7.25	7.25	5.936e+38	0.00134
4809	TS.diHPCARP_I.14aldHshift.tpttptd	2.031e+43	6.23	6.23	5.926e+38	0.00134
4810	TS.diHPCARP_I.14aldHshift.mpppppd	1.391e+43	6.02	6.02	5.717e+38	0.00129
4811	TS.diHPCARP_I.14aldHshift.ptmmmd	3.210e+44	7.90	7.90	5.685e+38	0.00128
4812	TS.diHPCARP_I.14aldHshift.mmtptpd	1.051e+43	5.89	5.89	5.372e+38	0.00121
4813	TS.diHPCARP_I.14aldHshift.ppppmd	7.124e+43	7.18	7.18	4.196e+38	0.000948
4814	TS.diHPCARP_I.14aldHshift.ttttptd	3.920e+43	6.85	6.85	4.034e+38	0.000911
4815	TS.diHPCARP_I.14aldHshift.pppmmmd	7.487e+43	7.33	7.33	3.448e+38	0.000779
4816	TS.diHPCARP_I.14aldHshift.tmtptmd	3.798e+43	6.93	6.93	3.405e+38	0.000769
4817	TS.diHPCARP_I.14aldHshift.mmmppmd	3.580e+43	6.91	6.91	3.305e+38	0.000746
4818	TS.diHPCARP_I.14aldHshift.tptmtpd	4.555e+43	7.14	7.14	2.887e+38	0.000652
4819	TS.diHPCARP_I.14aldHshift.ptmtpd	1.280e+44	7.80	7.80	2.668e+38	0.000602
4820	TS.diHPCARP_I.14aldHshift.tmmtpd	1.149e+43	6.36	6.36	2.654e+38	0.000599
4821	TS.diHPCARP_I.14aldHshift.ttpptpd	1.342e+44	7.83	7.83	2.648e+38	0.000598
4822	TS.diHPCARP_I.14aldHshift.tmpptmd	1.148e+44	7.75	7.75	2.592e+38	0.000585
4823	TS.diHPCARP_I.14aldHshift.tmmptmd	3.195e+43	7.03	7.03	2.399e+38	0.000542
4824	TS.diHPCARP_I.14aldHshift.tpmtpd	7.305e+43	7.54	7.54	2.348e+38	0.00053
4825	TS.diHPCARP_I.14aldHshift.tptmtd	5.076e+43	7.35	7.35	2.231e+38	0.000504
4826	TS.diHPCARP_I.14aldHshift.ppmppd	3.810e+43	7.20	7.20	2.181e+38	0.000493
4827	TS.diHPCARP_I.14aldHshift.pptpmd	4.415e+43	7.32	7.32	2.055e+38	0.000464
4828	TS.diHPCARP_I.14aldHshift.mtmtpd	1.932e+44	8.20	8.20	2.052e+38	0.000463
4829	TS.diHPCARP_I.14aldHshift.pmpptmd	4.206e+43	7.30	7.30	2.036e+38	0.00046
4830	TS.diHPCARP_I.14aldHshift.tpttpmd	2.182e+43	6.93	6.93	1.940e+38	0.000438
4831	TS.diHPCARP_I.14aldHshift.mppmmmd	8.509e+42	6.57	6.57	1.403e+38	0.000317
4832	TS.diHPCARP_I.14aldHshift.ptmtpd	3.062e+44	8.71	8.71	1.390e+38	0.000314
4833	TS.diHPCARP_I.14aldHshift.tppmtpd	1.923e+44	8.57	8.57	1.104e+38	0.000249
4834	TS.diHPCARP_I.14aldHshift.mtppmmd	2.102e+43	7.28	7.28	1.047e+38	0.000236
4835	TS.diHPCARP_I.14aldHshift.tpptptd	2.363e+44	8.74	8.74	1.011e+38	0.000228
4836	TS.diHPCARP_I.14aldHshift.pmpppd	1.765e+43	7.27	7.27	8.911e+37	0.000201
4837	TS.diHPCARP_I.14aldHshift.tppmtd	2.181e+44	8.83	8.83	8.025e+37	0.000181
4838	TS.diHPCARP_I.14aldHshift.mmtppmd	1.876e+43	7.38	7.38	7.926e+37	0.000179
4839	TS.diHPCARP_I.14aldHshift.ptmtpd	5.200e+44	9.44	9.44	6.928e+37	0.000156
4840	TS.diHPCARP_I.14aldHshift.ptmmtd	2.155e+44	8.93	8.93	6.769e+37	0.000153
4841	TS.diHPCARP_I.14aldHshift.mtpptmd	1.498e+44	8.74	8.74	6.405e+37	0.000145
4842	TS.diHPCARP_I.14aldHshift.pmpptmd	2.161e+44	8.98	8.98	6.242e+37	0.000141
4843	TS.diHPCARP_I.14aldHshift.tpptmd	3.258e+44	9.28	9.28	5.643e+37	0.000127
4844	TS.diHPCARP_I.14aldHshift.tmmppmd	1.804e+43	7.59	7.59	5.339e+37	0.000121
4845	TS.diHPCARP_I.14aldHshift.tmppppd	2.226e+43	7.75	7.75	5.064e+37	0.000114
4846	TS.diHPCARP_I.14aldHshift.ptmttd	2.274e+44	9.15	9.15	4.913e+37	0.000111
4847	TS.diHPCARP_I.14aldHshift.ttmtpd	2.003e+44	9.16	9.16	4.252e+37	9.6e-05
4848	TS.diHPCARP_I.14aldHshift.ptmmpd	1.112e+44	8.88	8.88	3.777e+37	8.53e-05
4849	TS.diHPCARP_I.14aldHshift.tppmtd	3.525e+44	9.59	9.59	3.661e+37	8.27e-05
4850	TS.diHPCARP_I.14aldHshift.pmmtd	1.880e+44	9.23	9.23	3.544e+37	8.01e-05
4851	TS.diHPCARP_I.14aldHshift.pptmtpd	1.360e+44	9.10	9.10	3.204e+37	7.24e-05
4852	TS.diHPCARP_I.14aldHshift.tptttd	4.644e+43	8.56	8.56	2.691e+37	6.08e-05
4853	TS.diHPCARP_I.14aldHshift.tppmtpd	5.329e+44	10.03	10.03	2.638e+37	5.96e-05
4854	TS.diHPCARP_I.14aldHshift.pmtptd	8.611e+43	9.23	9.23	1.637e+37	3.7e-05
4855	TS.diHPCARP_I.14aldHshift.pmtppmd	3.330e+43	9.36	9.36	5.031e+36	1.14e-05
4856	TS.diHPCARP_I.14aldHshift.pmpppd	5.993e+43	9.91	9.91	3.635e+36	8.21e-06
4857	TS.diHPCARP_I.14aldHshift.pmpmmd	3.827e+43	10.26	10.26	1.293e+36	2.92e-06
4858	TS.diHPCARP_I.14aldHshift.pppppd	1.103e+44	11.03	11.03	1.026e+36	2.32e-06
4859	Total				4.428e+43	100

4860
4861
4862
4863 1,5-aldehyde-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)
4864 =====
4865
4866 Note: both enantiomers (R,R and S,S) were calculated at the M06-2X/cc-pVDZ level based
4867 on
4868 a different template, to check the robustness of the conformer space search. As can be
4869 seen,
4870 most conformers are found in both enantiomers, though some higher-energy conformers
4871 are
4872 missing in either the R,R or S,S set. The impact on the rate predictions was

4873 found to be negligible. At the M06-02X/aug-cc-pVTZ level of theory, only a single set
4874 of
4875 enantiomers was calculated.
4876 Population analysis at 300K. Vibrational scaling: 0.971.
4877 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
4878 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
4879 %: contribution to the population (with current data set assumed 100%)
4880 Compound Qtot Erel Erel2 n*Q*MB %
4881 -----
4882 TS.diHPCARP_Ib.15aldHshift.utummuud 6.449e+42 0.00 0.00 6.449e+42 22.8
4883 TS.diHPCARP_Ib.15aldHshift.dtdppdud 6.449e+42 0.00 0.00 6.449e+42 22.8
4884 TS.diHPCARP_Ib.15aldHshift.umdmuud 5.721e+42 0.30 0.30 3.470e+42 12.2
4885 TS.diHPCARP_Ib.15aldHshift.dpuppdud 5.721e+42 0.30 0.30 3.469e+42 12.2
4886 TS.diHPCARP_Ib.15aldHshift.dtdmmuud 1.241e+43 1.80 1.80 6.016e+41 2.12
4887 TS.diHPCARP_Ib.15aldHshift.utuppdu 1.241e+43 1.80 1.80 6.016e+41 2.12
4888 TS.diHPCARP_Ib.15aldHshift.dpupmuud 6.179e+42 1.46 1.46 5.348e+41 1.89
4889 TS.diHPCARP_Ib.15aldHshift.umdmpddu 6.179e+42 1.46 1.46 5.348e+41 1.89
4890 TS.diHPCARP_Ib.15aldHshift.utdmddu 1.537e+43 2.03 2.03 5.068e+41 1.79
4891 TS.diHPCARP_Ib.15aldHshift.dtdpuud 1.534e+43 2.03 2.03 5.067e+41 1.79
4892 TS.diHPCARP_Ib.15aldHshift.upummuud 1.431e+43 2.11 2.11 4.123e+41 1.46
4893 TS.diHPCARP_Ib.15aldHshift.dmdppddu 1.420e+43 2.12 2.12 4.067e+41 1.44
4894 TS.diHPCARP_Ib.15aldHshift.dtdppddu 4.576e+42 1.49 1.49 3.732e+41 1.32
4895 TS.diHPCARP_Ib.15aldHshift.utummuud 4.573e+42 1.49 1.49 3.725e+41 1.31
4896 TS.diHPCARP_Ib.15aldHshift.umdpddu 1.228e+43 2.48 2.48 1.904e+41 0.672
4897 TS.diHPCARP_Ib.15aldHshift.dpummuud 1.229e+43 2.49 2.49 1.896e+41 0.669
4898 TS.diHPCARP_Ib.15aldHshift.ututmuud 1.657e+43 2.70 2.70 1.802e+41 0.636
4899 TS.diHPCARP_Ib.15aldHshift.dtdtpdu 1.657e+43 2.70 2.70 1.802e+41 0.636
4900 TS.diHPCARP_Ib.15aldHshift.ututpddu 4.145e+43 3.38 3.38 1.422e+41 0.502
4901 TS.diHPCARP_Ib.15aldHshift.dtdtmuud 4.145e+43 3.38 3.38 1.419e+41 0.501
4902 TS.diHPCARP_Ib.15aldHshift.dputpdu 1.531e+43 2.85 2.85 1.292e+41 0.456
4903 TS.diHPCARP_Ib.15aldHshift.umdtmuud 1.531e+43 2.85 2.85 1.292e+41 0.456
4904 TS.diHPCARP_Ib.15aldHshift.dmpddu 1.122e+43 2.78 2.78 1.054e+41 0.372
4905 TS.diHPCARP_Ib.15aldHshift.umdmuud 1.122e+43 2.78 2.78 1.054e+41 0.372
4906 TS.diHPCARP_Ib.15aldHshift.dputmuud 3.453e+43 3.53 3.53 9.338e+40 0.33
4907 TS.diHPCARP_Ib.15aldHshift.umdtppdu 3.435e+43 3.53 3.53 9.242e+40 0.326
4908 TS.diHPCARP_Ib.15aldHshift.dtuupddu 8.045e+42 2.75 2.75 7.917e+40 0.279
4909 TS.diHPCARP_Ib.15aldHshift.dtdmduud 3.128e+43 3.62 3.62 7.239e+40 0.255
4910 TS.diHPCARP_Ib.15aldHshift.utuppuud 3.127e+43 3.62 3.62 7.236e+40 0.255
4911 TS.diHPCARP_Ib.15aldHshift.utuppuud 2.950e+43 3.58 3.58 7.230e+40 0.255
4912 TS.diHPCARP_Ib.15aldHshift.dtdmddu 2.949e+43 3.58 3.58 7.230e+40 0.255
4913 TS.diHPCARP_Ib.15aldHshift.upupmuud 2.868e+43 3.61 3.61 6.777e+40 0.239
4914 TS.diHPCARP_Ib.15aldHshift.dmdmpdu 2.868e+43 3.61 3.61 6.776e+40 0.239
4915 TS.diHPCARP_Ib.15aldHshift.utupmuud 1.007e+43 2.99 2.99 6.698e+40 0.236
4916 TS.diHPCARP_Ib.15aldHshift.dmuupddu 1.007e+43 2.99 2.99 6.696e+40 0.236
4917 TS.diHPCARP_Ib.15aldHshift.dtuupmuud 4.884e+42 2.74 2.74 4.921e+40 0.174
4918 TS.diHPCARP_Ib.15aldHshift.utdmpddu 4.884e+42 2.74 2.74 4.921e+40 0.174
4919 TS.diHPCARP_Ib.15aldHshift.utdtpdu 3.094e+43 3.86 3.86 4.743e+40 0.167
4920 TS.diHPCARP_Ib.15aldHshift.dtuatmuud 3.094e+43 3.86 3.86 4.742e+40 0.167
4921 TS.diHPCARP_Ib.15aldHshift.utumtuud 1.734e+43 3.53 3.53 4.649e+40 0.164
4922 TS.diHPCARP_Ib.15aldHshift.dtdptdu 1.733e+43 3.53 3.53 4.648e+40 0.164
4923 TS.diHPCARP_Ib.15aldHshift.dputmdu 3.013e+43 3.92 3.92 4.220e+40 0.149
4924 TS.diHPCARP_Ib.15aldHshift.umdtppdu 3.012e+43 3.92 3.92 4.219e+40 0.149
4925 TS.diHPCARP_Ib.15aldHshift.dtdtmdu 3.022e+43 3.99 3.99 3.746e+40 0.132
4926 TS.diHPCARP_Ib.15aldHshift.ututpdu 3.022e+43 3.99 3.99 3.746e+40 0.132
4927 TS.diHPCARP_Ib.15aldHshift.upuppuud 1.337e+44 4.97 4.97 3.190e+40 0.113
4928 TS.diHPCARP_Ib.15aldHshift.dmdmddu 1.329e+44 4.97 4.97 3.168e+40 0.112
4929 TS.diHPCARP_Ib.15aldHshift.dpdppddu 1.054e+43 3.51 3.51 2.945e+40 0.104
4930 TS.diHPCARP_Ib.15aldHshift.umummuud 1.053e+43 3.51 3.51 2.940e+40 0.104
4931 TS.diHPCARP_Ib.15aldHshift.umummuud 1.404e+43 3.73 3.73 2.685e+40 0.0948
4932 TS.diHPCARP_Ib.15aldHshift.dpdppdu 1.404e+43 3.73 3.73 2.685e+40 0.0948
4933 TS.diHPCARP_Ib.15aldHshift.utuptdu 4.602e+43 4.47 4.47 2.546e+40 0.0899
4934 TS.diHPCARP_Ib.15aldHshift.dtdmtuud 4.601e+43 4.47 4.47 2.546e+40 0.0899
4935 TS.diHPCARP_Ib.15aldHshift.dtuatmuud 2.126e+43 4.03 4.03 2.445e+40 0.0863
4936 TS.diHPCARP_Ib.15aldHshift.utdtpdu 2.126e+43 4.03 4.03 2.445e+40 0.0863
4937 TS.diHPCARP_Ib.15aldHshift.dpuptuud 4.780e+42 3.21 3.21 2.191e+40 0.0773
4938 TS.diHPCARP_Ib.15aldHshift.umdmtddu 4.780e+42 3.21 3.21 2.190e+40 0.0773
4939 TS.diHPCARP_Ib.15aldHshift.dmpptdu 4.385e+43 4.67 4.67 1.726e+40 0.0609
4940 TS.diHPCARP_Ib.15aldHshift.umdmtddu 4.385e+43 4.67 4.67 1.726e+40 0.0609
4941 TS.diHPCARP_Ib.15aldHshift.dtdtdud 4.796e+43 4.74 4.74 1.688e+40 0.0596
4942 TS.diHPCARP_Ib.15aldHshift.ututtuud 4.795e+43 4.74 4.74 1.688e+40 0.0596
4943 TS.diHPCARP_Ib.15aldHshift.dummuud 2.353e+43 4.42 4.42 1.421e+40 0.0502
4944 TS.diHPCARP_Ib.15aldHshift.dmpdu 2.353e+43 4.42 4.42 1.421e+40 0.0502

4945	TS.diHPCARP_Ib.15aldHshift.umdtmddu	5.944e+43	5.06	5.06	1.227e+40	0.0433
4946	TS.diHPCARP_Ib.15aldHshift.dputpuud	5.942e+43	5.06	5.06	1.227e+40	0.0433
4947	TS.diHPCARP_Ib.15aldHshift.umdttdudu	4.455e+43	4.93	4.93	1.148e+40	0.0405
4948	TS.diHPCARP_Ib.15aldHshift.dputtdud	4.455e+43	4.93	4.93	1.148e+40	0.0405
4949	TS.diHPCARP_Ib.15aldHshift.dtuppddu	1.093e+43	4.09	4.09	1.139e+40	0.0402
4950	TS.diHPCARP_Ib.15aldHshift.utdmuud	1.093e+43	4.09	4.09	1.138e+40	0.0402
4951	TS.diHPCARP_Ib.15aldHshift.dtdtputud	4.983e+43	5.03	5.03	1.086e+40	0.0383
4952	TS.diHPCARP_Ib.15aldHshift.ututmddu	4.981e+43	5.03	5.03	1.086e+40	0.0383
4953	TS.diHPCARP_Ib.15aldHshift.utuptdu	4.302e+43	4.95	4.95	1.062e+40	0.0375
4954	TS.diHPCARP_Ib.15aldHshift.dtdmtudu	4.300e+43	4.95	4.95	1.060e+40	0.0374
4955	TS.diHPCARP_Ib.15aldHshift.utdpmddu	6.327e+43	5.18	5.18	1.058e+40	0.0374
4956	TS.diHPCARP_Ib.15aldHshift.dtdmpuud	6.308e+43	5.18	5.18	1.054e+40	0.0372
4957	TS.diHPCARP_Ib.15aldHshift.utuptuud	9.637e+43	5.44	5.44	1.050e+40	0.037
4958	TS.diHPCARP_Ib.15aldHshift.dtdmtddu	8.893e+43	5.45	5.45	9.586e+39	0.0338
4959	TS.diHPCARP_Ib.15aldHshift.ututddu	4.377e+43	5.03	5.03	9.510e+39	0.0336
4960	TS.diHPCARP_Ib.15aldHshift.dtdttuud	4.377e+43	5.03	5.03	9.510e+39	0.0336
4961	TS.diHPCARP_Ib.15aldHshift.utuptudu	5.785e+43	5.21	5.21	9.261e+39	0.0327
4962	TS.diHPCARP_Ib.15aldHshift.dtdmtddu	5.784e+43	5.21	5.21	9.261e+39	0.0327
4963	TS.diHPCARP_Ib.15aldHshift.utdtpdu	6.327e+43	4.93	4.93	8.573e+39	0.0303
4964	TS.diHPCARP_Ib.15aldHshift.utdtmudu	3.315e+43	4.93	4.93	8.485e+39	0.0299
4965	TS.diHPCARP_Ib.15aldHshift.umdttddu	4.523e+43	5.23	5.23	6.974e+39	0.0246
4966	TS.diHPCARP_Ib.15aldHshift.dputtuud	4.520e+43	5.23	5.23	6.970e+39	0.0246
4967	TS.diHPCARP_Ib.15aldHshift.umdtmuud	4.378e+43	5.26	5.26	6.470e+39	0.0228
4968	TS.diHPCARP_Ib.15aldHshift.dpuptddu	4.378e+43	5.26	5.26	6.469e+39	0.0228
4969	TS.diHPCARP_Ib.15aldHshift.umdppuud	4.910e+43	5.36	5.36	6.100e+39	0.0215
4970	TS.diHPCARP_Ib.15aldHshift.dpummddu	4.907e+43	5.36	5.36	6.097e+39	0.0215
4971	TS.diHPCARP_Ib.15aldHshift.umdpdtdu	3.913e+43	5.23	5.23	6.084e+39	0.0215
4972	TS.diHPCARP_Ib.15aldHshift.dpumtuud	3.913e+43	5.23	5.23	6.084e+39	0.0215
4973	TS.diHPCARP_Ib.15aldHshift.dmuumddu	6.005e+43	5.51	5.51	5.799e+39	0.0205
4974	TS.diHPCARP_Ib.15aldHshift.updppuud	6.005e+43	5.51	5.51	5.799e+39	0.0205
4975	TS.diHPCARP_Ib.15aldHshift.umdpmddu	9.086e+43	5.89	5.89	4.622e+39	0.0163
4976	TS.diHPCARP_Ib.15aldHshift.dmuupdu	1.349e+43	4.78	4.78	4.407e+39	0.0156
4977	TS.diHPCARP_Ib.15aldHshift.dpdtdu	1.408e+44	6.19	6.19	4.347e+39	0.0153
4978	TS.diHPCARP_Ib.15aldHshift.umutmudu	1.404e+44	6.19	6.19	4.329e+39	0.0153
4979	TS.diHPCARP_Ib.15aldHshift.dtdppuud	2.136e+43	5.10	5.10	4.115e+39	0.0145
4980	TS.diHPCARP_Ib.15aldHshift.dpuppuud	1.681e+43	5.01	5.01	3.772e+39	0.0133
4981	TS.diHPCARP_Ib.15aldHshift.umdptudu	5.149e+43	5.73	5.73	3.467e+39	0.0122
4982	TS.diHPCARP_Ib.15aldHshift.dpumtdud	5.140e+43	5.73	5.73	3.457e+39	0.0122
4983	TS.diHPCARP_Ib.15aldHshift.ututmudu	8.650e+43	6.04	6.04	3.440e+39	0.0121
4984	TS.diHPCARP_Ib.15aldHshift.dtdtpudu	8.638e+43	6.04	6.04	3.436e+39	0.0121
4985	TS.diHPCARP_Ib.15aldHshift.umdmddu	2.354e+43	5.28	5.28	3.339e+39	0.0118
4986	TS.diHPCARP_Ib.15aldHshift.dtdtpdu	1.330e+43	4.96	4.96	3.233e+39	0.0114
4987	TS.diHPCARP_Ib.15aldHshift.ututmuud	1.330e+43	4.96	4.96	3.233e+39	0.0114
4988	TS.diHPCARP_Ib.15aldHshift.uputmudu	4.767e+43	5.76	5.76	3.026e+39	0.0107
4989	TS.diHPCARP_Ib.15aldHshift.dmdtpdu	4.755e+43	5.76	5.76	3.018e+39	0.0107
4990	TS.diHPCARP_Ib.15aldHshift.dtuupdu	4.583e+43	5.75	5.75	2.964e+39	0.0105
4991	TS.diHPCARP_Ib.15aldHshift.utdmtdu	4.583e+43	5.75	5.75	2.955e+39	0.0104
4992	TS.diHPCARP_Ib.15aldHshift.dmdtpdu	1.101e+44	6.30	6.30	2.847e+39	0.01
4993	TS.diHPCARP_Ib.15aldHshift.uputmudu	1.101e+44	6.30	6.30	2.847e+39	0.01
4994	TS.diHPCARP_Ib.15aldHshift.dtdppudu	1.937e+43	5.27	5.27	2.829e+39	0.00999
4995	TS.diHPCARP_Ib.15aldHshift.umuppdu	4.128e+43	5.72	5.72	2.789e+39	0.00984
4996	TS.diHPCARP_Ib.15aldHshift.dpdmmuud	4.111e+43	5.72	5.72	2.777e+39	0.0098
4997	TS.diHPCARP_Ib.15aldHshift.dtdpmudu	3.956e+42	4.33	4.33	2.751e+39	0.00971
4998	TS.diHPCARP_Ib.15aldHshift.utumpdu	3.956e+42	4.34	4.34	2.748e+39	0.0097
4999	TS.diHPCARP_Ib.15aldHshift.dmdppuud	1.288e+43	5.04	5.04	2.735e+39	0.00965
5000	TS.diHPCARP_Ib.15aldHshift.dmdppdu	6.730e+42	4.66	4.66	2.729e+39	0.00963
5001	TS.diHPCARP_Ib.15aldHshift.dmdtpuud	2.645e+43	5.50	5.50	2.610e+39	0.00921
5002	TS.diHPCARP_Ib.15aldHshift.uputmudu	2.637e+43	5.50	5.50	2.602e+39	0.00918
5003	TS.diHPCARP_Ib.15aldHshift.dtdptdu	4.041e+43	5.76	5.76	2.577e+39	0.0091
5004	TS.diHPCARP_Ib.15aldHshift.dpuptdu	5.904e+43	5.99	5.99	2.553e+39	0.00901
5005	TS.diHPCARP_Ib.15aldHshift.ututpdu	1.553e+43	5.24	5.24	2.381e+39	0.0084
5006	TS.diHPCARP_Ib.15aldHshift.dtdtmudu	1.553e+43	5.24	5.24	2.381e+39	0.0084
5007	TS.diHPCARP_Ib.15aldHshift.umdpdu	4.691e+42	4.52	4.52	2.381e+39	0.0084
5008	TS.diHPCARP_Ib.15aldHshift.dpupmdu	4.684e+42	4.52	4.52	2.369e+39	0.00836
5009	TS.diHPCARP_Ib.15aldHshift.upuptdu	9.309e+43	6.31	6.31	2.352e+39	0.0083
5010	TS.diHPCARP_Ib.15aldHshift.dmdtmudu	9.304e+43	6.31	6.31	2.348e+39	0.00829
5011	TS.diHPCARP_Ib.15aldHshift.utummdu	4.503e+42	4.56	4.56	2.164e+39	0.00764
5012	TS.diHPCARP_Ib.15aldHshift.dmdmtdu	2.088e+44	6.84	6.84	2.157e+39	0.00761
5013	TS.diHPCARP_Ib.15aldHshift.upuptuud	2.081e+44	6.84	6.84	2.150e+39	0.00759
5014	TS.diHPCARP_Ib.15aldHshift.utdtpdu	1.064e+43	5.09	5.09	2.084e+39	0.00735
5015	TS.diHPCARP_Ib.15aldHshift.dutmuud	1.064e+43	5.09	5.09	2.084e+39	0.00735
5016	TS.diHPCARP_Ib.15aldHshift.upumpdu	8.788e+42	4.98	4.98	2.057e+39	0.00726

5017	TS.diHPCARP_Ib.15aldHshift.dtutpudu	4.298e+43	5.94	5.94	2.008e+39	0.00709
5018	TS.diHPCARP_Ib.15aldHshift.umutpddu	1.933e+44	6.86	6.86	1.957e+39	0.00691
5019	TS.diHPCARP_Ib.15aldHshift.dpdmtmuud	1.922e+44	6.86	6.86	1.946e+39	0.00687
5020	TS.diHPCARP_Ib.15aldHshift.updppddu	2.914e+43	5.75	5.75	1.888e+39	0.00666
5021	TS.diHPCARP_Ib.15aldHshift.dmuumuud	2.914e+43	5.75	5.75	1.888e+39	0.00666
5022	TS.diHPCARP_Ib.15aldHshift.dpdmmduud	7.745e+43	6.34	6.34	1.880e+39	0.00663
5023	TS.diHPCARP_Ib.15aldHshift.umuppuud	7.745e+43	6.34	6.34	1.880e+39	0.00663
5024	TS.diHPCARP_Ib.15aldHshift.utupmudu	1.049e+43	5.15	5.15	1.851e+39	0.00653
5025	TS.diHPCARP_Ib.15aldHshift.dmuptddu	3.234e+43	5.85	5.85	1.775e+39	0.00626
5026	TS.diHPCARP_Ib.15aldHshift.utdpmduud	4.913e+43	6.10	6.10	1.770e+39	0.00625
5027	TS.diHPCARP_Ib.15aldHshift.utumtudu	4.907e+43	6.10	6.10	1.766e+39	0.00623
5028	TS.diHPCARP_Ib.15aldHshift.utumpddu	4.869e+42	4.73	4.73	1.746e+39	0.00616
5029	TS.diHPCARP_Ib.15aldHshift.dpdptddu	3.588e+43	5.94	5.94	1.675e+39	0.00591
5030	TS.diHPCARP_Ib.15aldHshift.umumtuud	3.557e+43	5.95	5.95	1.654e+39	0.00584
5031	TS.diHPCARP_Ib.15aldHshift.dtuptduud	3.012e+43	5.85	5.85	1.653e+39	0.00583
5032	TS.diHPCARP_Ib.15aldHshift.utdmtudu	3.012e+43	5.85	5.85	1.653e+39	0.00583
5033	TS.diHPCARP_Ib.15aldHshift.dmdtmuud	2.462e+43	5.79	5.79	1.494e+39	0.00527
5034	TS.diHPCARP_Ib.15aldHshift.umdmtduud	4.419e+42	4.78	4.78	1.467e+39	0.00518
5035	TS.diHPCARP_Ib.15aldHshift.udtmtudu	4.419e+42	4.78	4.78	1.467e+39	0.00518
5036	TS.diHPCARP_Ib.15aldHshift.updtmudu	3.320e+43	6.11	6.11	1.180e+39	0.00416
5037	TS.diHPCARP_Ib.15aldHshift.dmutpdud	3.317e+43	6.11	6.11	1.178e+39	0.00416
5038	TS.diHPCARP_Ib.15aldHshift.utdmpudu	1.609e+43	5.76	5.76	1.026e+39	0.00362
5039	TS.diHPCARP_Ib.15aldHshift.updmmuud	7.491e+42	5.30	5.30	1.024e+39	0.00361
5040	TS.diHPCARP_Ib.15aldHshift.dtuupmudu	1.607e+43	5.76	5.76	1.023e+39	0.00361
5041	TS.diHPCARP_Ib.15aldHshift.dmuumtudu	1.056e+44	6.89	6.89	1.016e+39	0.00359
5042	TS.diHPCARP_Ib.15aldHshift.updptduud	1.056e+44	6.89	6.89	1.016e+39	0.00359
5043	TS.diHPCARP_Ib.15aldHshift.dpumtudu	7.883e+43	6.73	6.73	9.875e+38	0.00349
5044	TS.diHPCARP_Ib.15aldHshift.umdptduud	7.783e+43	6.73	6.73	9.690e+38	0.00342
5045	TS.diHPCARP_Ib.15aldHshift.dputmduud	5.132e+42	5.16	5.16	8.897e+38	0.00314
5046	TS.diHPCARP_Ib.15aldHshift.umdtpuud	5.132e+42	5.16	5.16	8.897e+38	0.00314
5047	TS.diHPCARP_Ib.15aldHshift.utdttudu	7.782e+43	6.79	6.79	8.744e+38	0.00309
5048	TS.diHPCARP_Ib.15aldHshift.dtuuttudu	7.782e+43	6.79	6.79	8.743e+38	0.00309
5049	TS.diHPCARP_Ib.15aldHshift.dtuupddu	2.879e+43	6.21	6.21	8.686e+38	0.00307
5050	TS.diHPCARP_Ib.15aldHshift.umdpmudu	9.768e+42	5.65	5.65	7.424e+38	0.00262
5051	TS.diHPCARP_Ib.15aldHshift.uppmuud	4.123e+43	6.60	6.60	6.398e+38	0.00226
5052	TS.diHPCARP_Ib.15aldHshift.umdmtudu	4.117e+43	6.60	6.60	6.388e+38	0.00225
5053	TS.diHPCARP_Ib.15aldHshift.dtuupduud	8.804e+43	7.06	7.06	6.334e+38	0.00224
5054	TS.diHPCARP_Ib.15aldHshift.dmdptduud	3.299e+43	6.48	6.48	6.276e+38	0.00222
5055	TS.diHPCARP_Ib.15aldHshift.dputtduud	3.382e+43	6.51	6.51	6.098e+38	0.00215
5056	TS.diHPCARP_Ib.15aldHshift.umdmtmuud	3.380e+43	6.51	6.51	6.093e+38	0.00215
5057	TS.diHPCARP_Ib.15aldHshift.dtuupddu	3.487e+43	6.56	6.56	5.834e+38	0.00206
5058	TS.diHPCARP_Ib.15aldHshift.updtmuud	2.660e+43	6.50	6.50	4.927e+38	0.00174
5059	TS.diHPCARP_Ib.15aldHshift.umutpddu	2.659e+43	6.50	6.50	4.925e+38	0.00174
5060	TS.diHPCARP_Ib.15aldHshift.ututtduud	5.967e+43	7.01	7.01	4.681e+38	0.00165
5061	TS.diHPCARP_Ib.15aldHshift.dtdttudu	5.966e+43	7.01	7.01	4.680e+38	0.00165
5062	TS.diHPCARP_Ib.15aldHshift.dputmudu	2.403e+43	6.47	6.47	4.671e+38	0.00165
5063	TS.diHPCARP_Ib.15aldHshift.dtdpmdud	2.030e+43	6.37	6.37	4.670e+38	0.00165
5064	TS.diHPCARP_Ib.15aldHshift.umdtpduud	2.401e+43	6.47	6.47	4.668e+38	0.00165
5065	TS.diHPCARP_Ib.15aldHshift.dpdpmuud	1.500e+43	6.19	6.19	4.622e+38	0.00163
5066	TS.diHPCARP_Ib.15aldHshift.updmpduud	7.250e+42	5.77	5.77	4.531e+38	0.0016
5067	TS.diHPCARP_Ib.15aldHshift.umupmudu	7.249e+42	5.77	5.77	4.531e+38	0.0016
5068	TS.diHPCARP_Ib.15aldHshift.dmuptuud	7.168e+43	7.20	7.20	4.072e+38	0.00144
5069	TS.diHPCARP_Ib.15aldHshift.dpumtduud	7.168e+43	7.20	7.20	4.072e+38	0.00144
5070	TS.diHPCARP_Ib.15aldHshift.updtpduud	2.657e+43	6.62	6.62	3.983e+38	0.00141
5071	TS.diHPCARP_Ib.15aldHshift.dmutmudu	2.651e+43	6.62	6.62	3.969e+38	0.0014
5072	TS.diHPCARP_Ib.15aldHshift.umutpudu	1.470e+44	7.70	7.70	3.628e+38	0.00128
5073	TS.diHPCARP_Ib.15aldHshift.dpdmtduud	1.469e+44	7.70	7.70	3.627e+38	0.00128
5074	TS.diHPCARP_Ib.15aldHshift.uputpddu	9.696e+43	7.46	7.46	3.586e+38	0.00127
5075	TS.diHPCARP_Ib.15aldHshift.dmdppudu	3.509e+43	6.85	6.85	3.581e+38	0.00126
5076	TS.diHPCARP_Ib.15aldHshift.updptuud	1.103e+44	7.54	7.54	3.527e+38	0.00124
5077	TS.diHPCARP_Ib.15aldHshift.dmuumtduud	1.090e+44	7.55	7.55	3.467e+38	0.00122
5078	TS.diHPCARP_Ib.15aldHshift.dputpudu	7.541e+43	7.33	7.33	3.429e+38	0.00121
5079	TS.diHPCARP_Ib.15aldHshift.umdmtduud	7.540e+43	7.33	7.33	3.428e+38	0.00121
5080	TS.diHPCARP_Ib.15aldHshift.umuptduud	1.042e+44	7.55	7.55	3.305e+38	0.00117
5081	TS.diHPCARP_Ib.15aldHshift.dpdmtudu	1.042e+44	7.55	7.55	3.305e+38	0.00117
5082	TS.diHPCARP_Ib.15aldHshift.dpdppuud	3.803e+43	6.95	6.95	3.305e+38	0.00117
5083	TS.diHPCARP_Ib.15aldHshift.dupmduud	1.674e+43	6.48	6.48	3.211e+38	0.00113
5084	TS.diHPCARP_Ib.15aldHshift.umdpmuud	3.830e+43	7.02	7.02	2.933e+38	0.00104
5085	TS.diHPCARP_Ib.15aldHshift.dputpddu	3.774e+43	7.03	7.03	2.875e+38	0.00101
5086	TS.diHPCARP_Ib.15aldHshift.utdmpduud	1.047e+43	6.29	6.29	2.758e+38	0.000973
5087	TS.diHPCARP_Ib.15aldHshift.umdmduud	1.995e+43	6.69	6.69	2.670e+38	0.000942
5088	TS.diHPCARP_Ib.15aldHshift.dpuuppuud	1.981e+43	6.69	6.69	2.646e+38	0.000934

5089	TS.diHPCARP_Ib.15aldHshift.umuptuud	2.012e+44	8.19	8.19	2.167e+38	0.000765
5090	TS.diHPCARP_Ib.15aldHshift.dpdmtddu	2.010e+44	8.19	8.19	2.162e+38	0.000763
5091	TS.diHPCARP_Ib.15aldHshift.umumpdud	7.485e+42	6.26	6.26	2.053e+38	0.000724
5092	TS.diHPCARP_Ib.15aldHshift.dpdpmudu	7.484e+42	6.26	6.26	2.053e+38	0.000724
5093	TS.diHPCARP_Ib.15aldHshift.dpupmudu	7.986e+42	6.31	6.31	2.034e+38	0.000718
5094	TS.diHPCARP_Ib.15aldHshift.umutmuud	3.439e+43	7.23	7.23	1.845e+38	0.000651
5095	TS.diHPCARP_Ib.15aldHshift.dpdtpddu	3.439e+43	7.23	7.23	1.845e+38	0.000651
5096	TS.diHPCARP_Ib.15aldHshift.dtuttddu	4.190e+43	7.36	7.36	1.829e+38	0.000646
5097	TS.diHPCARP_Ib.15aldHshift.dmutmuud	3.656e+43	7.30	7.30	1.769e+38	0.000624
5098	TS.diHPCARP_Ib.15aldHshift.updtpddu	3.656e+43	7.30	7.30	1.767e+38	0.000624
5099	TS.diHPCARP_Ib.15aldHshift.dmummdud	2.482e+43	7.12	7.12	1.612e+38	0.000569
5100	TS.diHPCARP_Ib.15aldHshift.updppudu	2.481e+43	7.12	7.12	1.611e+38	0.000568
5101	TS.diHPCARP_Ib.15aldHshift.upummddu	7.661e+42	6.45	6.45	1.535e+38	0.000542
5102	TS.diHPCARP_Ib.15aldHshift.dpdmtudu	3.736e+43	7.40	7.40	1.512e+38	0.000534
5103	TS.diHPCARP_Ib.15aldHshift.umutpdud	3.736e+43	7.40	7.40	1.512e+38	0.000534
5104	TS.diHPCARP_Ib.15aldHshift.dpdmdudu	5.050e+43	7.62	7.62	1.429e+38	0.000504
5105	TS.diHPCARP_Ib.15aldHshift.umuppudu	5.050e+43	7.62	7.62	1.429e+38	0.000504
5106	TS.diHPCARP_Ib.15aldHshift.umuttudu	1.781e+44	8.38	8.38	1.394e+38	0.000492
5107	TS.diHPCARP_Ib.15aldHshift.dpdttddu	1.779e+44	8.38	8.38	1.392e+38	0.000491
5108	TS.diHPCARP_Ib.15aldHshift.updtpudu	7.025e+43	7.86	7.86	1.312e+38	0.000463
5109	TS.diHPCARP_Ib.15aldHshift.dmutmdud	7.024e+43	7.86	7.86	1.312e+38	0.000463
5110	TS.diHPCARP_Ib.15aldHshift.uputtudu	1.370e+44	8.27	8.27	1.285e+38	0.000453
5111	TS.diHPCARP_Ib.15aldHshift.dmdttudu	1.370e+44	8.28	8.28	1.284e+38	0.000453
5112	TS.diHPCARP_Ib.15aldHshift.dtdmddu	4.249e+43	7.69	7.69	1.064e+38	0.000376
5113	TS.diHPCARP_Ib.15aldHshift.ututpuud	4.246e+43	7.69	7.69	1.064e+38	0.000375
5114	TS.diHPCARP_Ib.15aldHshift.umuttudu	2.594e+44	8.78	8.78	1.044e+38	0.000368
5115	TS.diHPCARP_Ib.15aldHshift.dpdttuud	2.578e+44	8.78	8.78	1.034e+38	0.000365
5116	TS.diHPCARP_Ib.15aldHshift.umuptdu	1.082e+44	8.28	8.28	1.012e+38	0.000357
5117	TS.diHPCARP_Ib.15aldHshift.dpdmtuud	1.081e+44	8.28	8.28	1.011e+38	0.000357
5118	TS.diHPCARP_Ib.15aldHshift.dmdptuud	7.077e+43	8.03	8.03	9.997e+37	0.000353
5119	TS.diHPCARP_Ib.15aldHshift.updtpddu	9.749e+43	8.22	8.22	9.977e+37	0.000352
5120	TS.diHPCARP_Ib.15aldHshift.dmutmuud	9.746e+43	8.22	8.22	9.974e+37	0.000352
5121	TS.diHPCARP_Ib.15aldHshift.dpdptdud	6.272e+43	8.03	8.03	8.832e+37	0.000312
5122	TS.diHPCARP_Ib.15aldHshift.umdttudu	1.028e+44	8.39	8.39	7.927e+37	0.00028
5123	TS.diHPCARP_Ib.15aldHshift.dputtudu	1.028e+44	8.39	8.39	7.927e+37	0.00028
5124	TS.diHPCARP_Ib.15aldHshift.dmutpuud	2.632e+44	9.08	9.08	6.380e+37	0.000225
5125	TS.diHPCARP_Ib.15aldHshift.updtmddu	2.526e+44	9.08	9.08	6.092e+37	0.000215
5126	TS.diHPCARP_Ib.15aldHshift.dmdttudu	1.517e+44	8.81	8.81	5.840e+37	0.000206
5127	TS.diHPCARP_Ib.15aldHshift.uputtudu	1.515e+44	8.81	8.81	5.826e+37	0.000206
5128	TS.diHPCARP_Ib.15aldHshift.updttudu	1.232e+44	8.72	8.72	5.430e+37	0.000192
5129	TS.diHPCARP_Ib.15aldHshift.dmuttdud	1.231e+44	8.72	8.72	5.427e+37	0.000192
5130	TS.diHPCARP_Ib.15aldHshift.utdmtuud	3.196e+43	7.92	7.92	5.426e+37	0.000192
5131	TS.diHPCARP_Ib.15aldHshift.dpdpmudu	1.150e+43	7.33	7.33	5.298e+37	0.000187
5132	TS.diHPCARP_Ib.15aldHshift.upummdud	1.867e+43	7.69	7.69	4.632e+37	0.000163
5133	TS.diHPCARP_Ib.15aldHshift.dtutmddu	4.537e+43	8.27	8.27	4.271e+37	0.000151
5134	TS.diHPCARP_Ib.15aldHshift.updttudu	1.608e+44	9.03	9.03	4.215e+37	0.000149
5135	TS.diHPCARP_Ib.15aldHshift.dmuttdud	1.608e+44	9.03	9.03	4.213e+37	0.000149
5136	TS.diHPCARP_Ib.15aldHshift.umutmdu	1.290e+44	8.93	8.93	4.032e+37	0.000142
5137	TS.diHPCARP_Ib.15aldHshift.dpdtpuud	1.287e+44	8.93	8.93	4.019e+37	0.000142
5138	TS.diHPCARP_Ib.15aldHshift.dmuttudu	1.276e+44	8.93	8.93	3.966e+37	0.00014
5139	TS.diHPCARP_Ib.15aldHshift.dpdppudu	3.162e+43	8.11	8.11	3.935e+37	0.000139
5140	TS.diHPCARP_Ib.15aldHshift.dmuppudu	3.101e+43	8.11	8.11	3.829e+37	0.000135
5141	TS.diHPCARP_Ib.15aldHshift.updpmddu	3.113e+43	8.15	8.15	3.576e+37	0.000126
5142	TS.diHPCARP_Ib.15aldHshift.dmumpuud	3.012e+43	8.16	8.16	3.439e+37	0.000121
5143	TS.diHPCARP_Ib.15aldHshift.dpdptuud	9.551e+43	8.85	8.85	3.429e+37	0.000121
5144	TS.diHPCARP_Ib.15aldHshift.umummddu	2.776e+43	8.14	8.14	3.277e+37	0.000116
5145	TS.diHPCARP_Ib.15aldHshift.umdttuud	1.682e+44	9.22	9.22	3.225e+37	0.000114
5146	TS.diHPCARP_Ib.15aldHshift.dmdtmddu	9.085e+43	8.92	8.92	2.890e+37	0.000102
5147	TS.diHPCARP_Ib.15aldHshift.uputpuud	9.014e+43	8.92	8.92	2.854e+37	0.000101
5148	TS.diHPCARP_Ib.15aldHshift.dpdttudu	1.942e+44	9.54	9.54	2.166e+37	7.64e-05
5149	TS.diHPCARP_Ib.15aldHshift.umuttud	1.937e+44	9.54	9.54	2.158e+37	7.62e-05
5150	TS.diHPCARP_Ib.15aldHshift.updptudu	7.801e+43	9.06	9.06	1.970e+37	6.95e-05
5151	TS.diHPCARP_Ib.15aldHshift.dmutmdud	7.800e+43	9.06	9.06	1.969e+37	6.95e-05
5152	TS.diHPCARP_Ib.15aldHshift.dtdtpuud	2.739e+43	8.62	8.62	1.437e+37	5.07e-05
5153	TS.diHPCARP_Ib.15aldHshift.dpdmpuud	5.006e+43	8.98	8.98	1.427e+37	5.04e-05
5154	TS.diHPCARP_Ib.15aldHshift.umupmddu	5.002e+43	8.98	8.98	1.426e+37	5.03e-05
5155	TS.diHPCARP_Ib.15aldHshift.utdmddud	7.640e+42	8.01	8.01	1.118e+37	2.85e-05
5156	TS.diHPCARP_Ib.15aldHshift.updmdud	1.459e+43	8.44	8.44	1.031e+37	3.64e-05
5157	TS.diHPCARP_Ib.15aldHshift.umumtudu	5.737e+43	9.39	9.39	8.286e+36	2.92e-05
5158	TS.diHPCARP_Ib.15aldHshift.dmutmddu	9.545e+43	9.71	9.71	8.019e+36	2.83e-05
5159	TS.diHPCARP_Ib.15aldHshift.updtpuud	9.536e+43	9.71	9.71	8.011e+36	2.83e-05
5160	TS.diHPCARP_Ib.15aldHshift.dtuupudu	2.499e+43	8.99	8.99	7.088e+36	2.5e-05

5161	TS.diHPCARP_Ib.15aldHshift.umupmudu	2.145e+43	8.90	8.90	7.026e+36	2.48e-05
5162	TS.diHPCARP_Ib.15aldHshift.umutpuud	1.116e+44	10.53	10.53	2.363e+36	8.34e-06
5163	TS.diHPCARP_Ib.15aldHshift.dpdmtddu	1.116e+44	10.53	10.53	2.362e+36	8.34e-06
5164	TS.diHPCARP_Ib.15aldHshift.updmmddu	8.761e+43	10.43	10.43	2.203e+36	7.78e-06
5165	TS.diHPCARP_Ib.15aldHshift.umumpddu	8.038e+42	9.13	9.13	1.809e+36	6.38e-06
5166	TS.diHPCARP_Ib.15aldHshift.umumtddu	5.280e+43	10.29	10.29	1.685e+36	5.95e-06
5167	TS.diHPCARP_Ib.15aldHshift.upumtudu	3.176e+43	10.02	10.02	1.587e+36	5.6e-06
5168	TS.diHPCARP_Ib.15aldHshift.uputpudu	1.887e+43	9.86	9.86	1.233e+36	4.35e-06
5169	TS.diHPCARP_Ib.15aldHshift.umummdud	2.005e+43	10.04	10.04	9.694e+35	3.42e-06
5170	TS.diHPCARP_Ib.15aldHshift.upumtddu	2.866e+43	10.41	10.41	7.492e+35	2.64e-06
5171	TS.diHPCARP_Ib.15aldHshift.utdmtddu	3.678e+43	10.62	10.62	6.734e+35	2.38e-06
5172	TS.diHPCARP_Ib.15aldHshift.upumpudu	4.724e+43	10.78	10.78	6.620e+35	2.34e-06
5173	TS.diHPCARP_Ib.15aldHshift.utdttddu	3.397e+43	11.31	11.31	1.944e+35	6.86e-07
5174	TS.diHPCARP_Ib.15aldHshift.upummudu	5.818e+42	10.70	10.70	9.353e+34	3.3e-07
5175	Total				2.833e+43	100

1,6-aldehyde-H-shift in (2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)

Population analysis at 300K. Vibrational scaling: 0.971.
 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 %: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
5187	-----					
5188	TS.diHPCARP_Ic.16aldHshift.a.mppmuu	2.521e+42	0.00	0.00	2.521e+42	16.9
5189	TS.diHPCARP_Ic.16aldHshift.b.pmtpuu	3.939e+42	0.34	0.34	2.244e+42	15.1
5190	TS.diHPCARP_Ic.16aldHshift.b.mptpuu	5.138e+42	0.67	0.67	1.676e+42	11.3
5191	TS.diHPCARP_Ic.16aldHshift.a.pmtpuu	4.268e+42	0.72	0.72	1.282e+42	8.62
5192	TS.diHPCARP_Ic.16aldHshift.a.mptpuu	5.349e+42	0.90	0.90	1.186e+42	7.97
5193	TS.diHPCARP_Ic.16aldHshift.b.pmmuu	5.764e+42	1.05	1.05	9.938e+41	6.68
5194	TS.diHPCARP_Ic.16aldHshift.a.pmmuu	2.310e+42	0.52	0.52	9.671e+41	6.5
5195	TS.diHPCARP_Ic.16aldHshift.a.mppmuu	5.233e+42	1.40	1.40	5.035e+41	3.38
5196	TS.diHPCARP_Ic.16aldHshift.b.mppmuu	2.849e+42	1.18	1.18	3.942e+41	2.65
5197	TS.diHPCARP_Ic.16aldHshift.a.pppmuu	2.466e+42	1.16	1.16	3.507e+41	2.36
5198	TS.diHPCARP_Ic.16aldHshift.a.pmpmuu	2.220e+42	1.15	1.15	3.212e+41	2.16
5199	TS.diHPCARP_Ic.16aldHshift.a.pmpdd	1.332e+43	2.36	2.36	2.542e+41	1.71
5200	TS.diHPCARP_Ic.16aldHshift.b.mppmuu	1.200e+43	2.40	2.40	2.154e+41	1.45
5201	TS.diHPCARP_Ic.16aldHshift.b.mppmuu	2.666e+42	1.52	1.52	2.074e+41	1.39
5202	TS.diHPCARP_Ic.16aldHshift.a.mppmuu	4.229e+42	1.80	1.80	2.053e+41	1.38
5203	TS.diHPCARP_Ic.16aldHshift.a.tmmuu	6.409e+42	2.28	2.28	1.411e+41	0.948
5204	TS.diHPCARP_Ic.16aldHshift.a.tppuu	1.105e+43	2.67	2.67	1.251e+41	0.841
5205	TS.diHPCARP_Ic.16aldHshift.e.tmtpuu	7.955e+42	2.48	2.48	1.242e+41	0.835
5206	TS.diHPCARP_Ic.16aldHshift.a.pppmuu	2.748e+42	1.87	1.87	1.197e+41	0.805
5207	TS.diHPCARP_Ic.16aldHshift.a.tmtpuu	5.562e+42	2.30	2.30	1.178e+41	0.792
5208	TS.diHPCARP_Ic.16aldHshift.b.pppmuu	2.383e+42	1.85	1.85	1.066e+41	0.717
5209	TS.diHPCARP_Ic.16aldHshift.b.pppmuu	5.199e+42	2.54	2.54	7.329e+40	0.493
5210	TS.diHPCARP_Ic.16aldHshift.b.mppuu	8.737e+42	2.93	2.93	6.377e+40	0.429
5211	TS.diHPCARP_Ic.16aldHshift.c.mppmuu	5.332e+42	2.65	2.65	6.207e+40	0.417
5212	TS.diHPCARP_Ic.16aldHshift.b.pmpuu	2.452e+42	2.25	2.25	5.664e+40	0.381
5213	TS.diHPCARP_Ic.16aldHshift.a.pmpdd	3.249e+43	3.90	3.90	4.704e+40	0.316
5214	TS.diHPCARP_Ic.16aldHshift.a.pmpdd	4.949e+43	4.23	4.23	4.115e+40	0.277
5215	TS.diHPCARP_Ic.16aldHshift.b.pmpuu	3.013e+42	2.67	2.67	3.439e+40	0.231
5216	TS.diHPCARP_Ic.16aldHshift.a.tmmuu	5.011e+42	3.06	3.06	2.967e+40	0.199
5217	TS.diHPCARP_Ic.16aldHshift.b.mptuu	1.332e+43	3.68	3.68	2.790e+40	0.188
5218	TS.diHPCARP_Ic.16aldHshift.e.pppuu	4.415e+42	3.03	3.03	2.718e+40	0.183
5219	TS.diHPCARP_Ic.16aldHshift.e.mppdd	4.214e+42	3.11	3.11	2.284e+40	0.154
5220	TS.diHPCARP_Ic.16aldHshift.a.pmmdd	3.589e+43	4.41	4.41	2.189e+40	0.147
5221	TS.diHPCARP_Ic.16aldHshift.a.pmpuu	4.345e+42	3.16	3.16	2.173e+40	0.146
5222	TS.diHPCARP_Ic.16aldHshift.b.tmpuu	5.146e+42	3.29	3.29	2.069e+40	0.139
5223	TS.diHPCARP_Ic.16aldHshift.e.tmpuu	5.142e+42	3.29	3.29	2.063e+40	0.139
5224	TS.diHPCARP_Ic.16aldHshift.a.pppdd	1.747e+43	4.04	4.04	1.976e+40	0.133
5225	TS.diHPCARP_Ic.16aldHshift.c.tmmuu	4.119e+42	3.30	3.30	1.636e+40	0.11
5226	TS.diHPCARP_Ic.16aldHshift.e.tptuu	1.141e+43	3.96	3.96	1.490e+40	0.1
5227	TS.diHPCARP_Ic.16aldHshift.a.pppuu	3.320e+43	4.60	4.60	1.474e+40	0.0991
5228	TS.diHPCARP_Ic.16aldHshift.a.pppuu	1.432e+43	4.19	4.19	1.279e+40	0.086
5229	TS.diHPCARP_Ic.16aldHshift.a.pppuu	6.956e+42	3.77	3.77	1.255e+40	0.0844
5230	TS.diHPCARP_Ic.16aldHshift.b.pppuu	1.179e+43	4.09	4.09	1.226e+40	0.0824
5231	TS.diHPCARP_Ic.16aldHshift.e.pmpdd	6.579e+42	3.84	3.84	1.055e+40	0.0709
5232	TS.diHPCARP_Ic.16aldHshift.a.mptuu	1.519e+43	4.38	4.38	9.761e+39	0.0656

5233	TS.diHPCARP_Ic.16aldHshift.a.pmtmdd	3.790e+43	4.93	4.93	9.639e+39	0.0648
5234	TS.diHPCARP_Ic.16aldHshift.a.pmtpdd	3.340e+43	4.88	4.88	9.334e+39	0.0627
5235	TS.diHPCARP_Ic.16aldHshift.e.pptmuu	7.638e+42	4.03	4.03	8.868e+39	0.0596
5236	TS.diHPCARP_Ic.16aldHshift.a.tppmuu	6.102e+42	4.00	4.00	7.399e+39	0.0497
5237	TS.diHPCARP_Ic.16aldHshift.a.tptpuu	9.873e+42	4.33	4.33	6.864e+39	0.0461
5238	TS.diHPCARP_Ic.16aldHshift.e.tmtmuu	9.590e+42	4.33	4.33	6.775e+39	0.0455
5239	TS.diHPCARP_Ic.16aldHshift.a.pppmdd	3.786e+43	5.16	5.16	6.649e+39	0.0447
5240	TS.diHPCARP_Ic.16aldHshift.a.mmtpuu	9.182e+42	4.38	4.38	5.958e+39	0.04
5241	TS.diHPCARP_Ic.16aldHshift.a.pppmdd	3.920e+43	5.35	5.35	4.989e+39	0.0335
5242	TS.diHPCARP_Ic.16aldHshift.a.tppmuu	1.036e+43	4.57	4.57	4.820e+39	0.0324
5243	TS.diHPCARP_Ic.16aldHshift.b.mmtpuu	1.003e+43	4.64	4.64	4.198e+39	0.0282
5244	TS.diHPCARP_Ic.16aldHshift.a.tppmdd	2.334e+43	5.20	5.20	3.818e+39	0.0257
5245	TS.diHPCARP_Ic.16aldHshift.e.tppmuu	9.244e+42	4.81	4.81	2.907e+39	0.0195
5246	TS.diHPCARP_Ic.16aldHshift.a.tmtmuu	8.626e+42	4.80	4.80	2.741e+39	0.0184
5247	TS.diHPCARP_Ic.16aldHshift.a.tppmuu	1.558e+43	5.16	5.16	2.704e+39	0.0182
5248	TS.diHPCARP_Ic.16aldHshift.b.pmpmdd	4.177e+43	5.77	5.77	2.632e+39	0.0177
5249	TS.diHPCARP_Ic.16aldHshift.a.pptpdd	3.163e+43	5.67	5.67	2.339e+39	0.0157
5250	TS.diHPCARP_Ic.16aldHshift.a.mmpmuu	5.201e+42	4.71	4.71	1.930e+39	0.013
5251	TS.diHPCARP_Ic.16aldHshift.b.tppmuu	1.64e+42	4.97	4.97	1.728e+39	0.0116
5252	TS.diHPCARP_Ic.16aldHshift.a.mmmmuu	7.856e+42	5.11	5.11	1.495e+39	0.01
5253	TS.diHPCARP_Ic.16aldHshift.a.mpppdd	6.876e+42	5.13	5.13	1.262e+39	0.00849
5254	TS.diHPCARP_Ic.16aldHshift.e.pmpmdd	2.288e+43	5.86	5.86	1.239e+39	0.00833
5255	TS.diHPCARP_Ic.16aldHshift.a.mpppdd	1.278e+43	5.56	5.56	1.141e+39	0.00767
5256	TS.diHPCARP_Ic.16aldHshift.b.mmmmdd	1.505e+43	5.66	5.66	1.135e+39	0.00763
5257	TS.diHPCARP_Ic.16aldHshift.e.tppmuu	1.496e+43	5.66	5.66	1.119e+39	0.00752
5258	TS.diHPCARP_Ic.16aldHshift.b.pmtpdd	2.470e+43	6.00	6.00	1.050e+39	0.00706
5259	TS.diHPCARP_Ic.16aldHshift.b.mmpmdd	1.470e+43	5.70	5.70	1.033e+39	0.00695
5260	TS.diHPCARP_Ic.16aldHshift.e.mpppdd	4.938e+42	5.08	5.08	9.775e+38	0.00657
5261	TS.diHPCARP_Ic.16aldHshift.b.pppmdd	2.578e+43	6.11	6.11	9.077e+38	0.0061
5262	TS.diHPCARP_Ic.16aldHshift.b.mmtpdd	8.762e+42	5.50	5.50	8.573e+38	0.00576
5263	TS.diHPCARP_Ic.16aldHshift.a.pptmuu	8.616e+42	5.49	5.49	8.565e+38	0.00576
5264	TS.diHPCARP_Ic.16aldHshift.b.mmtmdd	8.317e+42	5.50	5.50	8.250e+38	0.00555
5265	TS.diHPCARP_Ic.16aldHshift.e.pmtmdd	3.982e+43	6.43	6.43	8.242e+38	0.00554
5266	TS.diHPCARP_Ic.16aldHshift.c.mmtmdd	3.912e+42	5.09	5.09	7.653e+38	0.00514
5267	TS.diHPCARP_Ic.16aldHshift.c.tppmuu	7.597e+42	5.51	5.51	7.320e+38	0.00492
5268	TS.diHPCARP_Ic.16aldHshift.e.tppmdd	1.542e+43	6.00	6.00	6.617e+38	0.00445
5269	TS.diHPCARP_Ic.16aldHshift.a.tppmdd	2.304e+43	6.25	6.25	6.450e+38	0.00434
5270	TS.diHPCARP_Ic.16aldHshift.e.tppmuu	7.374e+42	5.57	5.57	6.429e+38	0.00432
5271	TS.diHPCARP_Ic.16aldHshift.c.pmppdd	9.622e+42	5.76	5.76	6.136e+38	0.00412
5272	TS.diHPCARP_Ic.16aldHshift.e.pmpmdd	3.584e+43	6.58	6.58	5.776e+38	0.00388
5273	TS.diHPCARP_Ic.16aldHshift.e.tpppdd	2.119e+43	6.31	6.31	5.382e+38	0.00362
5274	TS.diHPCARP_Ic.16aldHshift.c.mpppdd	3.936e+42	5.31	5.31	5.311e+38	0.00357
5275	TS.diHPCARP_Ic.16aldHshift.b.ppppdd	4.077e+43	6.79	6.79	4.616e+38	0.0031
5276	TS.diHPCARP_Ic.16aldHshift.e.mppmdd	2.620e+43	6.54	6.54	4.519e+38	0.00304
5277	TS.diHPCARP_Ic.16aldHshift.e.pmtpdd	1.865e+43	6.38	6.38	4.179e+38	0.00281
5278	TS.diHPCARP_Ic.16aldHshift.c.mmmmuu	6.297e+42	5.74	5.74	4.153e+38	0.00279
5279	TS.diHPCARP_Ic.16aldHshift.e.ppppuu	1.601e+43	6.31	6.31	4.080e+38	0.00274
5280	TS.diHPCARP_Ic.16aldHshift.b.pmtmuu	1.096e+43	6.08	6.08	4.078e+38	0.00274
5281	TS.diHPCARP_Ic.16aldHshift.a.tmpmdd	3.213e+43	6.76	6.76	3.814e+38	0.00256
5282	TS.diHPCARP_Ic.16aldHshift.a.tppmuu	1.025e+43	6.09	6.09	3.760e+38	0.00253
5283	TS.diHPCARP_Ic.16aldHshift.b.mmpmuu	5.313e+42	5.74	5.74	3.499e+38	0.00235
5284	TS.diHPCARP_Ic.16aldHshift.e.mtpmdd	1.663e+43	6.48	6.48	3.188e+38	0.00214
5285	TS.diHPCARP_Ic.16aldHshift.b.mmpmuu	5.760e+42	5.85	5.85	3.134e+38	0.00211
5286	TS.diHPCARP_Ic.16aldHshift.a.mmpmuu	7.627e+42	6.05	6.05	3.004e+38	0.00202
5287	TS.diHPCARP_Ic.16aldHshift.e.pmmdd	3.448e+43	6.99	6.99	2.800e+38	0.00188
5288	TS.diHPCARP_Ic.16aldHshift.e.mppmdd	1.204e+43	6.36	6.36	2.793e+38	0.00188
5289	TS.diHPCARP_Ic.16aldHshift.a.tpppuu	2.558e+43	6.82	6.82	2.759e+38	0.00185
5290	TS.diHPCARP_Ic.16aldHshift.e.tpppuu	2.068e+43	6.79	6.79	2.340e+38	0.00157
5291	TS.diHPCARP_Ic.16aldHshift.a.tmmdd	3.847e+43	7.16	7.16	2.325e+38	0.00156
5292	TS.diHPCARP_Ic.16aldHshift.e.mppmdd	3.368e+43	7.09	7.09	2.313e+38	0.00155
5293	TS.diHPCARP_Ic.16aldHshift.b.pptpdd	3.380e+43	7.21	7.21	1.894e+38	0.00127
5294	TS.diHPCARP_Ic.16aldHshift.a.mmpmdd	8.391e+42	6.39	6.39	1.860e+38	0.00125
5295	TS.diHPCARP_Ic.16aldHshift.a.ppppuu	1.405e+43	6.70	6.70	1.853e+38	0.00125
5296	TS.diHPCARP_Ic.16aldHshift.e.mppmdd	7.326e+42	6.33	6.33	1.787e+38	0.0012
5297	TS.diHPCARP_Ic.16aldHshift.a.mppmdd	1.566e+44	8.19	8.19	1.706e+38	0.00115
5298	TS.diHPCARP_Ic.16aldHshift.a.mpppuu	1.922e+43	7.03	7.03	1.451e+38	0.000976
5299	TS.diHPCARP_Ic.16aldHshift.b.pppmdd	5.615e+43	7.79	7.79	1.195e+38	0.000804
5300	TS.diHPCARP_Ic.16aldHshift.b.pptmdd	4.083e+43	7.66	7.66	1.074e+38	0.000722
5301	TS.diHPCARP_Ic.16aldHshift.a.tptpdd	2.078e+43	7.28	7.28	1.031e+38	0.000693
5302	TS.diHPCARP_Ic.16aldHshift.e.tmpmdd	4.202e+43	7.80	7.80	8.736e+37	0.000587
5303	TS.diHPCARP_Ic.16aldHshift.b.pppmdd	5.205e+43	8.01	8.01	7.323e+37	0.000492
5304	TS.diHPCARP_Ic.16aldHshift.a.tptmdd	3.890e+43	7.87	7.87	7.152e+37	0.000481

5305	TS.diHPCARP_Ic.16aldHshift.b.tmtppdd	3.145e+43	7.78	7.78	6.738e+37	0.000453
5306	TS.diHPCARP_Ic.16aldHshift.a.tmtppdd	2.845e+43	7.73	7.73	6.624e+37	0.000445
5307	TS.diHPCARP_Ic.16aldHshift.e.tptmuu	2.384e+43	7.63	7.63	6.608e+37	0.000444
5308	TS.diHPCARP_Ic.16aldHshift.b.mmpuu	1.981e+43	7.53	7.53	6.460e+37	0.000434
5309	TS.diHPCARP_Ic.16aldHshift.a.tmtmdd	4.598e+43	8.08	8.08	5.947e+37	0.0004
5310	TS.diHPCARP_Ic.16aldHshift.b.tmtmdd	4.311e+43	8.14	8.14	5.106e+37	0.000343
5311	TS.diHPCARP_Ic.16aldHshift.a.mppmdd	9.885e+43	8.64	8.64	4.995e+37	0.000336
5312	TS.diHPCARP_Ic.16aldHshift.b.tpppdd	9.191e+42	7.28	7.28	4.604e+37	0.000309
5313	TS.diHPCARP_Ic.16aldHshift.c.ppppdd	9.823e+42	7.34	7.34	4.408e+37	0.000296
5314	TS.diHPCARP_Ic.16aldHshift.e.tmmdd	4.179e+43	8.29	8.29	3.832e+37	0.000258
5315	TS.diHPCARP_Ic.16aldHshift.a.mptmdd	3.865e+43	8.30	8.30	3.451e+37	0.000232
5316	TS.diHPCARP_Ic.16aldHshift.e.tppmdd	2.491e+43	8.12	8.12	3.005e+37	0.000202
5317	TS.diHPCARP_Ic.16aldHshift.e.tptpdd	1.825e+43	8.21	8.21	1.892e+37	0.000127
5318	TS.diHPCARP_Ic.16aldHshift.e.tptmdd	4.889e+43	8.80	8.80	1.887e+37	0.000127
5319	TS.diHPCARP_Ic.16aldHshift.a.tptmuu	2.945e+43	8.54	8.54	1.760e+37	0.000118
5320	TS.diHPCARP_Ic.16aldHshift.b.tmpmdd	3.404e+43	8.70	8.70	1.555e+37	0.000105
5321	TS.diHPCARP_Ic.16aldHshift.c.mppmdd	5.857e+42	7.84	7.84	1.132e+37	7.61e-05
5322	TS.diHPCARP_Ic.16aldHshift.c.pmtmdd	8.964e+42	8.31	8.31	7.927e+36	5.33e-05
5323	TS.diHPCARP_Ic.16aldHshift.a.mpppdd	3.549e+42	7.90	7.90	6.288e+36	4.23e-05
5324	TS.diHPCARP_Ic.16aldHshift.b.tpppdd	2.962e+43	9.18	9.18	6.047e+36	4.06e-05
5325	TS.diHPCARP_Ic.16aldHshift.c.pmpmdd	3.186e+43	9.23	9.23	6.008e+36	4.04e-05
5326	TS.diHPCARP_Ic.16aldHshift.e.mmmdd	2.165e+43	9.28	9.28	3.758e+36	2.53e-05
5327	TS.diHPCARP_Ic.16aldHshift.b.tppmdd	2.846e+43	9.47	9.47	3.597e+36	2.42e-05
5328	TS.diHPCARP_Ic.16aldHshift.c.mtppdd	7.489e+42	8.71	8.71	3.359e+36	2.26e-05
5329	TS.diHPCARP_Ic.16aldHshift.c.tptmdd	9.677e+42	8.95	8.95	2.936e+36	1.97e-05
5330	TS.diHPCARP_Ic.16aldHshift.c.tpppdd	8.288e+42	8.94	8.94	2.545e+36	1.71e-05
5331	TS.diHPCARP_Ic.16aldHshift.c.mmmdd	1.338e+43	9.48	9.48	1.657e+36	1.11e-05
5332	TS.diHPCARP_Ic.16aldHshift.c.tppmdd	8.253e+42	9.29	9.29	1.399e+36	9.41e-06
5333	TS.diHPCARP_Ic.16aldHshift.c.ppppdd	3.880e+43	10.41	10.41	1.018e+36	6.85e-06
5334	TS.diHPCARP_Ic.16aldHshift.c.mpppdd	1.510e+43	10.27	10.27	5.010e+35	3.37e-06
5335	TS.diHPCARP_Ic.16aldHshift.c.pppmdd	5.993e+43	11.09	11.09	4.984e+35	3.35e-06
5336	TS.diHPCARP_Ic.16aldHshift.c.tppmdd	1.917e+43	10.44	10.44	4.783e+35	3.22e-06
5337	TS.diHPCARP_Ic.16aldHshift.c.pptmdd	1.171e+43	10.31	10.31	3.609e+35	2.43e-06
5338	TS.diHPCARP_Ic.16aldHshift.c.tptpdd	1.657e+43	10.59	10.59	3.198e+35	2.15e-06
5339	TS.diHPCARP_Ic.16aldHshift.c.tpppdd	1.922e+43	10.71	10.71	3.016e+35	2.03e-06
5340	TS.diHPCARP_Ic.16aldHshift.c.mptmdd	8.341e+42	10.36	10.36	2.376e+35	1.6e-06
5341	TS.diHPCARP_Ic.16aldHshift.c.tmtmdd	7.668e+42	10.89	10.89	8.966e+34	6.03e-07
5342	TS.diHPCARP_Ic.16aldHshift.c.mtppdd	3.249e+43	14.25	14.25	1.352e+33	9.09e-09
5343	TS.diHPCARP_Ic.16aldHshift.c.tppmdd	4.859e+43	15.67	15.67	1.879e+32	1.26e-09
5344	TS.diHPCARP_Ic.16aldHshift.c.mppmdd	2.576e+43	15.31	15.31	1.800e+32	1.21e-09
5345	Total				1.488e+43	100

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5349 1,6-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
5350 HPCARP-Ia), forming B (di-HPCARP-Ib)
5351 =====
5352 =====
5353 =====

5354 Population analysis at 300K. Vibrational scaling: 0.971.
5355 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
5356 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
5357 %: contribution to the population (with current data set assumed 100%)

5358 Compound	Qtot	Erel	Erel2	n*Q*MB	%
5359					
5360	TS.diHPCARP_I.1600HHshift.a.tppmdd	3.203e+42	0.00	0.00	3.203e+42 72.1
5361	TS.diHPCARP_I.1600HHshift.a.tmmuu	3.425e+43	2.81	2.81	3.068e+41 6.9
5362	TS.diHPCARP_I.1600HHshift.a.ttptuu	4.834e+43	3.50	3.50	1.354e+41 3.05
5363	TS.diHPCARP_I.1600HHshift.b.ttptuu	5.725e+43	3.73	3.73	1.100e+41 2.48
5364	TS.diHPCARP_I.1600HHshift.a.htppuu	6.014e+43	3.86	3.86	9.277e+40 2.09
5365	TS.diHPCARP_I.1600HHshift.b.htppuu	6.621e+43	4.02	4.02	7.798e+40 1.75
5366	TS.diHPCARP_I.1600HHshift.b.lptuu	3.959e+42	2.58	2.58	5.266e+40 1.18
5367	TS.diHPCARP_I.1600HHshift.b.tptpdd	3.177e+42	2.51	2.51	4.683e+40 1.05
5368	TS.diHPCARP_I.1600HHshift.b.lmmtuu	4.688e+43	4.14	4.14	4.533e+40 1.02
5369	TS.diHPCARP_I.1600HHshift.b.tmmuu	4.388e+43	4.13	4.13	4.313e+40 0.97
5370	TS.diHPCARP_I.1600HHshift.b.tptuu	6.553e+42	3.00	3.00	4.299e+40 0.967
5371	TS.diHPCARP_I.1600HHshift.b.ttmpuu	4.559e+43	4.21	4.21	3.884e+40 0.874
5372	TS.diHPCARP_I.1600HHshift.a.lppuu	7.206e+42	3.21	3.21	3.301e+40 0.743
5373	TS.diHPCARP_I.1600HHshift.a.ttmpuu	1.795e+43	3.87	3.87	2.741e+40 0.617
5374	TS.diHPCARP_I.1600HHshift.b.tptpdd	5.330e+42	3.20	3.20	2.503e+40 0.563
5375	TS.diHPCARP_I.1600HHshift.b.lppuu	1.220e+43	3.69	3.69	2.500e+40 0.563
5376	TS.diHPCARP_I.1600HHshift.b.tmtuu	7.281e+42	3.46	3.46	2.186e+40 0.492

5377	TS.diHPCARP_I.1600HHshift.b.tttpuu	6.356e+43	5.16	5.16	1.115e+40	0.251
5378	TS.diHPCARP_I.1600HHshift.a.tmtpuu	4.306e+43	5.11	5.11	8.145e+39	0.183
5379	TS.diHPCARP_I.1600HHshift.a.tttpuu	5.875e+43	5.31	5.31	7.995e+39	0.18
5380	TS.diHPCARP_I.1600HHshift.a.ltmpdd	1.007e+43	4.26	4.26	7.991e+39	0.18
5381	TS.diHPCARP_I.1600HHshift.b.tmtmdd	2.680e+42	3.55	3.55	6.979e+39	0.157
5382	TS.diHPCARP_I.1600HHshift.b.tttmuu	8.501e+43	5.62	5.62	6.798e+39	0.153
5383	TS.diHPCARP_I.1600HHshift.a.tttmuu	3.499e+43	5.17	5.17	6.041e+39	0.136
5384	TS.diHPCARP_I.1600HHshift.b.lpptuu	1.540e+43	4.79	4.79	4.991e+39	0.112
5385	TS.diHPCARP_I.1600HHshift.a.tmtmuu	1.081e+43	4.62	4.62	4.675e+39	0.105
5386	TS.diHPCARP_I.1600HHshift.b.tpmdd	4.735e+42	4.13	4.13	4.667e+39	0.105
5387	TS.diHPCARP_I.1600HHshift.b.lpptuu	5.085e+43	5.63	5.63	4.052e+39	0.0912
5388	TS.diHPCARP_I.1600HHshift.a.cpptdd	1.591e+43	4.99	4.99	3.715e+39	0.0836
5389	TS.diHPCARP_I.1600HHshift.a.lmptuu	3.310e+43	5.42	5.42	3.711e+39	0.0835
5390	TS.diHPCARP_I.1600HHshift.a.hmppuu	3.310e+43	5.42	5.42	3.711e+39	0.0835
5391	TS.diHPCARP_I.1600HHshift.b.tmtppdd	1.315e+43	4.91	4.91	3.458e+39	0.0778
5392	TS.diHPCARP_I.1600HHshift.a.tpttdd	4.372e+43	5.66	5.66	3.307e+39	0.0744
5393	TS.diHPCARP_I.1600HHshift.a.tppmuu	2.716e+42	4.03	4.03	3.127e+39	0.0703
5394	TS.diHPCARP_I.1600HHshift.a.lpptuu	5.644e+42	4.50	4.50	2.993e+39	0.0673
5395	TS.diHPCARP_I.1600HHshift.a.tmtmdd	1.200e+43	5.08	5.08	2.409e+39	0.0542
5396	TS.diHPCARP_I.1600HHshift.a.ttttuu	6.383e+43	6.14	6.14	2.162e+39	0.0487
5397	TS.diHPCARP_I.1600HHshift.a.ttpmdd	1.054e+43	5.07	5.07	2.144e+39	0.0482
5398	TS.diHPCARP_I.1600HHshift.b.pppmuu	3.544e+42	4.59	4.59	1.608e+39	0.0362
5399	TS.diHPCARP_I.1600HHshift.b.lmtpuu	6.430e+43	6.46	6.46	1.268e+39	0.0285
5400	TS.diHPCARP_I.1600HHshift.b.tmpuu	8.886e+42	5.36	5.36	1.101e+39	0.0248
5401	TS.diHPCARP_I.1600HHshift.a.mptmuu	3.973e+43	6.32	6.32	9.813e+38	0.0221
5402	TS.diHPCARP_I.1600HHshift.b.lmppuu	2.574e+43	6.08	6.08	9.651e+38	0.0217
5403	TS.diHPCARP_I.1600HHshift.b.ttpmdd	1.383e+43	5.74	5.74	9.050e+38	0.0204
5404	TS.diHPCARP_I.1600HHshift.a.lppmuu	1.895e+43	6.03	6.03	7.647e+38	0.0172
5405	TS.diHPCARP_I.1600HHshift.a.cptpdd	5.214e+42	5.28	5.28	7.391e+38	0.0166
5406	TS.diHPCARP_I.1600HHshift.a.tmtppdd	1.594e+43	6.04	6.04	6.333e+38	0.0142
5407	TS.diHPCARP_I.1600HHshift.a.mptmuu	1.031e+43	5.86	5.86	5.563e+38	0.0125
5408	TS.diHPCARP_I.1600HHshift.a.tmpppdd	4.184e+42	5.45	5.45	4.446e+38	0.01
5409	TS.diHPCARP_I.1600HHshift.b.tttmdd	3.290e+43	6.71	6.71	4.289e+38	0.00965
5410	TS.diHPCARP_I.1600HHshift.b.cmmuu	1.549e+43	6.28	6.28	4.093e+38	0.00921
5411	TS.diHPCARP_I.1600HHshift.b.hpttdd	3.654e+43	6.82	6.82	3.915e+38	0.00881
5412	TS.diHPCARP_I.1600HHshift.b.cpptdd	1.590e+43	6.47	6.47	3.085e+38	0.00694
5413	TS.diHPCARP_I.1600HHshift.b.tptmdd	2.623e+43	6.81	6.81	2.875e+38	0.00647
5414	TS.diHPCARP_I.1600HHshift.b.tpttdd	1.081e+43	6.34	6.34	2.621e+38	0.0059
5415	TS.diHPCARP_I.1600HHshift.a.tmtmdd	2.099e+43	6.82	6.82	2.258e+38	0.00508
5416	TS.diHPCARP_I.1600HHshift.a.ctmtdd	1.143e+44	7.97	7.97	1.790e+38	0.00403
5417	TS.diHPCARP_I.1600HHshift.a.ctmpdd	1.317e+43	7.36	7.36	5.703e+37	0.00128
5418	TS.diHPCARP_I.1600HHshift.b.tmpppdd	2.949e+42	6.53	6.53	5.120e+37	0.00115
5419	TS.diHPCARP_I.1600HHshift.b.pmtpuu	2.813e+43	7.89	7.89	5.051e+37	0.00114
5420	TS.diHPCARP_I.1600HHshift.a.cptmdd	3.534e+43	8.03	8.03	5.002e+37	0.00113
5421	TS.diHPCARP_I.1600HHshift.b.ctptuu	4.670e+43	8.39	8.39	3.623e+37	0.000815
5422	TS.diHPCARP_I.1600HHshift.b.cmtpuu	3.406e+43	8.25	8.25	3.344e+37	0.000752
5423	TS.diHPCARP_I.1600HHshift.b.lmpuu	5.902e+42	7.29	7.29	2.893e+37	0.000651
5424	TS.diHPCARP_I.1600HHshift.a.pmpppdd	6.240e+42	7.32	7.32	2.889e+37	0.00065
5425	TS.diHPCARP_I.1600HHshift.b.tpmuu	7.256e+42	7.48	7.48	2.560e+37	0.000576
5426	TS.diHPCARP_I.1600HHshift.b.mptpdd	3.052e+42	6.99	6.99	2.465e+37	0.000555
5427	TS.diHPCARP_I.1600HHshift.b.cmpuu	3.147e+43	8.43	8.43	2.281e+37	0.000513
5428	TS.diHPCARP_I.1600HHshift.a.ctptuu	6.851e+43	9.05	9.05	1.762e+37	0.000396
5429	TS.diHPCARP_I.1600HHshift.a.cmmuu	1.891e+43	8.40	8.40	1.448e+37	0.000326
5430	TS.diHPCARP_I.1600HHshift.b.cmtuu	3.151e+43	8.70	8.70	1.447e+37	0.000326
5431	TS.diHPCARP_I.1600HHshift.b.cmpmdd	2.116e+42	7.20	7.20	1.207e+37	0.000271
5432	TS.diHPCARP_I.1600HHshift.b.cpttuu	5.059e+43	9.10	9.10	1.184e+37	0.000266
5433	TS.diHPCARP_I.1600HHshift.b.ctmtdd	2.731e+43	8.76	8.76	1.127e+37	0.000254
5434	TS.diHPCARP_I.1600HHshift.b.cmttdd	5.437e+43	9.25	9.25	9.882e+36	0.000222
5435	TS.diHPCARP_I.1600HHshift.b.ctmpuu	2.193e+43	8.73	8.73	9.601e+36	0.000216
5436	TS.diHPCARP_I.1600HHshift.b.cptmdd	2.564e+43	8.87	8.87	8.927e+36	0.000201
5437	TS.diHPCARP_I.1600HHshift.b.mppmdd	9.715e+42	8.31	8.31	8.623e+36	0.000194
5438	TS.diHPCARP_I.1600HHshift.a.ctppdd	7.990e+43	9.79	9.79	5.892e+36	0.000133
5439	TS.diHPCARP_I.1600HHshift.a.cttmd	4.993e+43	9.57	9.57	5.341e+36	0.00012
5440	TS.diHPCARP_I.1600HHshift.b.cmtmdd	3.069e+43	9.28	9.28	5.293e+36	0.000119
5441	TS.diHPCARP_I.1600HHshift.b.ctmdd	2.776e+43	9.28	9.28	4.789e+36	0.000108
5442	TS.diHPCARP_I.1600HHshift.b.cttptuu	4.589e+43	9.93	9.93	2.695e+36	6.06e-05
5443	TS.diHPCARP_I.1600HHshift.b.cppuu	1.260e+43	9.29	9.29	2.149e+36	4.84e-05
5444	TS.diHPCARP_I.1600HHshift.a.ctttd	7.456e+43	10.37	10.37	2.086e+36	4.69e-05
5445	TS.diHPCARP_I.1600HHshift.a.cmpuu	1.486e+43	9.57	9.57	1.596e+36	3.59e-05
5446	TS.diHPCARP_I.1600HHshift.a.cmpmdd	5.427e+42	9.12	9.12	1.236e+36	2.78e-05
5447	TS.diHPCARP_I.1600HHshift.a.cttptuu	6.887e+43	10.63	10.63	1.233e+36	2.77e-05
5448	TS.diHPCARP_I.1600HHshift.b.ctmuu	4.387e+43	10.37	10.37	1.224e+36	2.75e-05

5449	TS.diHPCARP_I.1600HHshift.b.ctpmd	9.530e+42	9.58	9.58	9.992e+35	2.25e-05
5450	TS.diHPCARP_I.1600HHshift.b.cttmdd	2.820e+43	10.40	10.40	7.424e+35	1.67e-05
5451	TS.diHPCARP_I.1600HHshift.a.cmtpuu	3.696e+43	10.58	10.58	7.286e+35	1.64e-05
5452	TS.diHPCARP_I.1600HHshift.b.cmpuu	6.146e+42	9.56	9.56	6.648e+35	1.5e-05
5453	TS.diHPCARP_I.1600HHshift.a.cmtmuu	4.041e+43	10.88	10.88	4.824e+35	1.09e-05
5454	TS.diHPCARP_I.1600HHshift.b.ctppdd	1.317e+43	10.68	10.68	2.202e+35	4.95e-06
5455	TS.diHPCARP_I.1600HHshift.a.pmttdd	4.292e+43	11.43	11.43	2.032e+35	4.57e-06
5456	TS.diHPCARP_I.1600HHshift.b.cpppdd	9.840e+43	12.13	12.13	1.425e+35	3.21e-06
5457	TS.diHPCARP_I.1600HHshift.b.pptmuu	4.797e+43	14.21	14.21	2.130e+33	4.79e-08
5458	TS.diHPCARP_I.1600HHshift.a.tpppuu	2.644e+42	13.85	13.85	2.144e+32	4.82e-09
5459	TS.diHPCARP_I.1600HHshift.b.hpttuu	3.811e+42	14.96	14.96	4.830e+31	1.09e-09
5460	Total				4.445e+42	100

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5464 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
5465 HPCARP-Ia), forming C (di-HPCARP-Ic)
5466 =====
5467 =====
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5469 Population analysis at 300K. Vibrational scaling: 0.971.
5470 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
5471 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
5472 %: contribution to the population (with current data set assumed 100%)
5473 Compound Qtot Erel Erel2 n*Q*MB %

5474	Compound	Qtot	Erel	Erel2	n*Q*MB	%
5475	TS.diHPCARP_I.1700HHshift.BB.hpddd	5.194e+42	0.00	0.00	5.194e+42	91.1
5476	TS.diHPCARP_I.1700HHshift.BB.tmudd	3.080e+42	1.32	1.32	3.374e+41	5.92
5477	TS.diHPCARP_I.1700HHshift.BB.ltddd	3.217e+43	3.61	3.61	7.482e+40	1.31
5478	TS.diHPCARP_I.1700HHshift.BB.ltduu	2.880e+42	2.50	2.50	4.368e+40	0.766
5479	TS.diHPCARP_I.1700HHshift.BB.lpudd	1.308e+43	4.05	4.05	1.454e+40	0.255
5480	TS.diHPCARP_I.1700HHshift.CR.hmddd	3.816e+42	3.57	3.57	9.491e+39	0.166
5481	TS.diHPCARP_I.1700HHshift.BB.lmduu	1.117e+43	4.56	4.56	5.311e+39	0.0932
5482	TS.diHPCARP_I.1700HHshift.BB.hmddd	9.960e+42	4.54	4.54	4.884e+39	0.0857
5483	TS.diHPCARP_I.1700HHshift.BB.lmuu	1.117e+43	4.67	4.67	4.393e+39	0.0771
5484	TS.diHPCARP_I.1700HHshift.BB.hpudd	4.287e+42	4.14	4.14	4.101e+39	0.0719
5485	TS.diHPCARP_I.1700HHshift.BB.lpuu	2.788e+42	4.08	4.08	2.997e+39	0.0526
5486	TS.diHPCARP_I.1700HHshift.BB.tpuu	4.959e+42	4.62	4.62	2.121e+39	0.0372
5487	TS.diHPCARP_I.1700HHshift.BC.tmuu	1.125e+43	5.61	5.61	9.235e+38	0.0162
5488	TS.diHPCARP_I.1700HHshift.BB.ctddd	2.224e+43	6.33	6.33	5.446e+38	0.00955
5489	TS.diHPCARP_I.1700HHshift.BB.cmddd	1.495e+43	6.13	6.13	5.157e+38	0.00905
5490	TS.diHPCARP_I.1700HHshift.CR.hmudd	8.572e+42	5.81	5.81	5.050e+38	0.00886
5491	TS.diHPCARP_I.1700HHshift.BB.cpuu	1.268e+43	6.39	6.39	2.812e+38	0.00493
5492	TS.diHPCARP_I.1700HHshift.BC.ttuu	1.962e+43	7.34	7.34	8.886e+37	0.00156
5493	TS.diHPCARP_I.1700HHshift.BB.tmuu	3.297e+42	6.69	6.69	4.384e+37	0.000769
5494	TS.diHPCARP_I.1700HHshift.BC.hmduu	1.489e+43	7.88	7.88	2.713e+37	0.000476
5495	TS.diHPCARP_I.1700HHshift.BC.lmuu	5.321e+42	7.32	7.32	2.471e+37	0.000433
5496	TS.diHPCARP_I.1700HHshift.BC.lpuu	1.420e+43	8.34	8.34	1.186e+37	0.000208
5497	TS.diHPCARP_I.1700HHshift.BC.tpuu	4.037e+42	7.87	7.87	7.507e+36	0.000132
5498	TS.diHPCARP_I.1700HHshift.CR.ltudd	2.165e+43	9.57	9.57	2.295e+36	4.03e-05
5499	TS.diHPCARP_I.1700HHshift.BC.ctduu	2.369e+43	10.12	10.12	1.001e+36	1.76e-05
5500	TS.diHPCARP_I.1700HHshift.BB.cpuu	7.709e+42	9.52	9.52	8.959e+35	1.57e-05
5501	TS.diHPCARP_I.1700HHshift.BC.cpuu	9.667e+42	10.39	10.39	2.605e+35	4.57e-06
5502	TS.diHPCARP_I.1700HHshift.BC.tmuu	3.452e+42	10.93	10.93	3.789e+34	6.65e-07
5503	TS.diHPCARP_I.1700HHshift.BB.cmuu	4.666e+42	11.20	11.20	3.262e+34	5.72e-07
5504	TS.diHPCARP_I.1700HHshift.BC.ttuu	9.870e+42	12.24	12.24	1.206e+34	2.12e-07
5505	TS.diHPCARP_I.1700HHshift.BC.tpuu	4.665e+42	12.59	12.59	3.165e+33	5.55e-08
5506	TS.diHPCARP_I.1700HHshift.BC.ppuu	3.165e+43	14.33	14.33	1.155e+33	2.03e-08
5507	TS.diHPCARP_I.1700HHshift.BC.cmuu	5.451e+42	15.30	15.30	3.880e+31	6.81e-10
5508	TS.diHPCARP_I.1700HHshift.BC.ctuu	1.713e+43	16.70	16.70	1.168e+31	2.05e-10
5509	TS.diHPCARP_I.1700HHshift.BC.cpuu	3.960e+42	16.98	16.98	1.694e+30	2.97e-11
5510	Total				5.701e+42	100

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5514 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-
5515 HPCARP-Ib), forming C (di-HPCARP-Ic)
5516 =====
5517 =====
5518

5519 Population analysis at 300K. Vibrational scaling: 0.971.
5520 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

5521	n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.					
5522	%: contribution to the population (with current data set assumed 100%)					
5523	Compound	Qtot	Erel	Erel2	n*Q*MB	%
5524	-----					
5525	TS.diHPCARP_Ib.1600HHshift.b.htpmuu	5.868e+42	0.23	0.23	4.009e+42	25.6
5526	TS.diHPCARP_Ib.1600HHshift.a.ctpmdd	3.629e+42	0.00	0.00	3.629e+42	23.2
5527	TS.diHPCARP_Ib.1600HHshift.b.ctmpuu	6.442e+42	0.56	0.56	2.503e+42	16
5528	TS.diHPCARP_Ib.1600HHshift.b.hpmmuu	1.449e+43	1.32	1.32	1.577e+42	10.1
5529	TS.diHPCARP_Ib.1600HHshift.a.hpmmuu	9.669e+42	1.24	1.24	1.203e+42	7.69
5530	TS.diHPCARP_Ib.1600HHshift.a.lmppdd	5.387e+42	1.38	1.38	5.350e+41	3.42
5531	TS.diHPCARP_Ib.1600HHshift.b.ctpmuu	2.587e+43	2.32	2.32	5.264e+41	3.37
5532	TS.diHPCARP_Ib.1600HHshift.b.cptpuu	9.959e+42	2.05	2.05	3.210e+41	2.05
5533	TS.diHPCARP_Ib.1600HHshift.a.ctmpdd	3.986e+42	1.77	1.77	2.049e+41	1.31
5534	TS.diHPCARP_Ib.1600HHshift.a.ctmpuu	2.515e+43	3.17	3.17	1.229e+41	0.786
5535	TS.diHPCARP_Ib.1600HHshift.a.hptpuu	1.282e+43	2.95	2.95	9.051e+40	0.579
5536	TS.diHPCARP_Ib.1600HHshift.a.ctmmuu	1.782e+43	3.16	3.16	8.829e+40	0.565
5537	TS.diHPCARP_Ib.1600HHshift.b.cpmuu	4.083e+43	3.71	3.71	8.157e+40	0.522
5538	TS.diHPCARP_Ib.1600HHshift.b.hptpuu	1.737e+43	3.24	3.24	7.533e+40	0.482
5539	TS.diHPCARP_Ib.1600HHshift.a.ctmmuu	1.303e+43	3.09	3.09	7.354e+40	0.47
5540	TS.diHPCARP_Ib.1600HHshift.b.lmppdd	9.194e+42	3.00	3.00	5.975e+40	0.382
5541	TS.diHPCARP_Ib.1600HHshift.a.cpmuu	2.350e+43	3.79	3.79	4.058e+40	0.26
5542	TS.diHPCARP_Ib.1600HHshift.a.cmmpuu	1.360e+43	3.49	3.49	3.892e+40	0.249
5543	TS.diHPCARP_Ib.1600HHshift.b.ctmmuu	3.022e+43	4.08	4.08	3.236e+40	0.207
5544	TS.diHPCARP_Ib.1600HHshift.b.pttpdd	3.288e+43	4.17	4.17	3.028e+40	0.194
5545	TS.diHPCARP_Ib.1600HHshift.a.httpuu	9.968e+42	3.48	3.48	2.891e+40	0.185
5546	TS.diHPCARP_Ib.1600HHshift.b.mmpuu	2.766e+43	4.12	4.12	2.757e+40	0.176
5547	TS.diHPCARP_Ib.1600HHshift.a.lmtmdd	7.153e+42	3.32	3.32	2.707e+40	0.173
5548	TS.diHPCARP_Ib.1600HHshift.a.ctpuu	1.865e+43	3.93	3.93	2.554e+40	0.163
5549	TS.diHPCARP_Ib.1600HHshift.b.cttmuu	4.004e+43	4.42	4.42	2.404e+40	0.154
5550	TS.diHPCARP_Ib.1600HHshift.b.pptpdd	9.797e+42	3.64	3.64	2.194e+40	0.14
5551	TS.diHPCARP_Ib.1600HHshift.a.mttmdd	2.659e+43	4.24	4.24	2.150e+40	0.138
5552	TS.diHPCARP_Ib.1600HHshift.a.mmpuu	2.371e+43	4.22	4.22	2.009e+40	0.128
5553	TS.diHPCARP_Ib.1600HHshift.b.ctppuu	2.834e+43	4.35	4.35	1.912e+40	0.122
5554	TS.diHPCARP_Ib.1600HHshift.a.mtppuu	1.070e+43	3.78	3.78	1.886e+40	0.121
5555	TS.diHPCARP_Ib.1600HHshift.b.lpmuu	8.037e+43	4.99	4.99	1.852e+40	0.118
5556	TS.diHPCARP_Ib.1600HHshift.b.mmpuu	1.678e+43	4.09	4.09	1.748e+40	0.112
5557	TS.diHPCARP_Ib.1600HHshift.a.htmmuu	8.347e+42	3.74	3.74	1.564e+40	0.1
5558	TS.diHPCARP_Ib.1600HHshift.b.httpuu	1.742e+43	4.19	4.19	1.539e+40	0.0984
5559	TS.diHPCARP_Ib.1600HHshift.a.lptpuu	5.464e+43	5.07	5.07	1.101e+40	0.0704
5560	TS.diHPCARP_Ib.1600HHshift.b.mmtpuu	1.441e+43	4.29	4.29	1.072e+40	0.0686
5561	TS.diHPCARP_Ib.1600HHshift.a.lptmuu	3.437e+43	4.85	4.85	1.014e+40	0.0648
5562	TS.diHPCARP_Ib.1600HHshift.a.mmtpuu	1.519e+43	4.63	4.63	6.489e+39	0.0415
5563	TS.diHPCARP_Ib.1600HHshift.b.mmtmuu	1.316e+43	4.63	4.63	5.560e+39	0.0356
5564	TS.diHPCARP_Ib.1600HHshift.a.cmppdd	1.996e+43	4.90	4.90	5.351e+39	0.0342
5565	TS.diHPCARP_Ib.1600HHshift.b.lptmuu	3.842e+43	5.38	5.38	4.643e+39	0.0297
5566	TS.diHPCARP_Ib.1600HHshift.b.hmtmuu	1.059e+43	4.72	4.72	3.843e+39	0.0246
5567	TS.diHPCARP_Ib.1600HHshift.a.mmtmuu	1.390e+43	4.96	4.96	3.383e+39	0.0216
5568	TS.diHPCARP_Ib.1600HHshift.b.lmtmdd	8.045e+42	4.65	4.65	3.289e+39	0.021
5569	TS.diHPCARP_Ib.1600HHshift.b.mmpuu	1.982e+43	5.23	5.23	3.050e+39	0.0195
5570	TS.diHPCARP_Ib.1600HHshift.a.lptmdd	3.896e+42	4.29	4.29	2.939e+39	0.0188
5571	TS.diHPCARP_Ib.1600HHshift.b.lptpuu	4.170e+43	5.74	5.74	2.752e+39	0.0176
5572	TS.diHPCARP_Ib.1600HHshift.a.lpppdd	5.804e+42	4.60	4.60	2.598e+39	0.0166
5573	TS.diHPCARP_Ib.1600HHshift.b.lptmdd	6.216e+42	4.79	4.79	2.031e+39	0.013
5574	TS.diHPCARP_Ib.1600HHshift.a.mppuu	1.739e+43	5.41	5.41	1.985e+39	0.0127
5575	TS.diHPCARP_Ib.1600HHshift.a.hmtppdd	2.801e+43	5.80	5.80	1.679e+39	0.0107
5576	TS.diHPCARP_Ib.1600HHshift.b.hmtmdd	2.794e+43	5.96	5.96	1.270e+39	0.00812
5577	TS.diHPCARP_Ib.1600HHshift.b.mmmuu	4.421e+43	6.26	6.26	1.208e+39	0.00772
5578	TS.diHPCARP_Ib.1600HHshift.b.lppuu	3.240e+43	6.13	6.13	1.111e+39	0.00711
5579	TS.diHPCARP_Ib.1600HHshift.a.lppuu	3.268e+43	6.19	6.19	1.015e+39	0.00649
5580	TS.diHPCARP_Ib.1600HHshift.b.lpppdd	7.043e+42	5.32	5.32	9.326e+38	0.00596
5581	TS.diHPCARP_Ib.1600HHshift.a.hmtmdd	3.799e+43	6.36	6.36	8.883e+38	0.00568
5582	TS.diHPCARP_Ib.1600HHshift.b.hptmuu	3.841e+43	6.48	6.48	7.252e+38	0.00464
5583	TS.diHPCARP_Ib.1600HHshift.a.htppuu	2.580e+43	6.55	6.55	4.370e+38	0.00279
5584	TS.diHPCARP_Ib.1600HHshift.a.hmtpuu	8.208e+42	5.89	5.89	4.231e+38	0.00271
5585	TS.diHPCARP_Ib.1600HHshift.b.hmtpuu	9.724e+42	6.01	6.01	4.068e+38	0.0026
5586	TS.diHPCARP_Ib.1600HHshift.a.cppuu	2.007e+43	6.56	6.56	3.312e+38	0.00212
5587	TS.diHPCARP_Ib.1600HHshift.a.pttmuu	2.073e+43	6.59	6.59	3.269e+38	0.00209
5588	TS.diHPCARP_Ib.1600HHshift.a.hmmuu	8.189e+42	6.14	6.14	2.745e+38	0.00176
5589	TS.diHPCARP_Ib.1600HHshift.b.hmmuu	9.304e+42	6.25	6.25	2.621e+38	0.00168
5590	TS.diHPCARP_Ib.1600HHshift.a.hmmdd	1.575e+43	6.61	6.61	2.407e+38	0.00154
5591	TS.diHPCARP_Ib.1600HHshift.b.cppuu	2.255e+43	7.00	7.00	1.791e+38	0.00115
5592	TS.diHPCARP_Ib.1600HHshift.b.cppuu	3.816e+43	7.34	7.34	1.713e+38	0.0011

5593	TS.diHPCARP_Ib.1600HHshift.a.mmmuu	2.469e+43	7.10	7.10	1.651e+38	0.00106
5594	TS.diHPCARP_Ib.1600HHshift.b.htmpuu	1.323e+43	6.79	6.79	1.504e+38	0.000962
5595	TS.diHPCARP_Ib.1600HHshift.b.cptmuu	3.200e+43	7.32	7.32	1.492e+38	0.000954
5596	TS.diHPCARP_Ib.1600HHshift.a.cptmuu	2.819e+43	7.29	7.29	1.379e+38	0.000882
5597	TS.diHPCARP_Ib.1600HHshift.b.lmtpdd	2.538e+43	7.30	7.30	1.223e+38	0.000782
5598	TS.diHPCARP_Ib.1600HHshift.b.htppuu	2.756e+43	7.46	7.46	1.011e+38	0.000647
5599	TS.diHPCARP_Ib.1600HHshift.a.htmpuu	6.202e+43	8.28	8.28	5.728e+37	0.000366
5600	TS.diHPCARP_Ib.1600HHshift.a.cmmdd	1.251e+43	7.37	7.37	5.367e+37	0.000343
5601	TS.diHPCARP_Ib.1600HHshift.a.mmtppdd	2.512e+43	7.86	7.86	4.730e+37	0.000303
5602	TS.diHPCARP_Ib.1600HHshift.a.lmtpdd	2.554e+43	8.10	8.10	3.206e+37	0.000205
5603	TS.diHPCARP_Ib.1600HHshift.a.lmmdd	1.504e+43	8.01	8.01	2.204e+37	0.000141
5604	TS.diHPCARP_Ib.1600HHshift.a.ltpmdd	5.092e+42	7.50	7.50	1.754e+37	0.000112
5605	TS.diHPCARP_Ib.1600HHshift.b.cmpdd	1.653e+43	8.22	8.22	1.700e+37	0.000109
5606	TS.diHPCARP_Ib.1600HHshift.a.lppmdd	8.618e+42	7.90	7.90	1.526e+37	9.76e-05
5607	TS.diHPCARP_Ib.1600HHshift.b.lppmdd	1.928e+43	8.58	8.58	1.078e+37	6.9e-05
5608	TS.diHPCARP_Ib.1600HHshift.b.lmpmdd	2.166e+43	8.76	8.76	8.954e+36	5.73e-05
5609	TS.diHPCARP_Ib.1600HHshift.b.tppmdd	2.232e+43	9.00	9.00	6.230e+36	3.98e-05
5610	TS.diHPCARP_Ib.1600HHshift.b.mppmdd	5.383e+42	8.30	8.30	4.834e+36	3.09e-05
5611	TS.diHPCARP_Ib.1600HHshift.a.hmpuu	3.320e+43	9.48	9.48	4.105e+36	2.63e-05
5612	TS.diHPCARP_Ib.1600HHshift.b.hmpuu	4.292e+43	9.65	9.65	4.008e+36	2.56e-05
5613	TS.diHPCARP_Ib.1600HHshift.a.lppmdd	5.012e+42	8.69	8.69	2.346e+36	1.5e-05
5614	TS.diHPCARP_Ib.1600HHshift.a.hmpuu	1.973e+43	9.59	9.59	2.024e+36	1.29e-05
5615	TS.diHPCARP_Ib.1600HHshift.b.ltpmdd	1.066e+43	10.95	10.95	1.129e+35	7.22e-07
5616	TS.diHPCARP_Ib.1600HHshift.b.hmtmdd	2.227e+43	11.67	11.67	7.006e+34	4.48e-07
5617	TS.diHPCARP_Ib.1600HHshift.a.hmtmdd	2.121e+43	11.65	11.65	6.916e+34	4.42e-07
5618	TS.diHPCARP_Ib.1600HHshift.a.ltpmdd	8.857e+42	11.19	11.19	6.235e+34	3.99e-07
5619	TS.diHPCARP_Ib.1600HHshift.b.cmtppdd	2.005e+43	11.91	11.91	4.233e+34	2.71e-07
5620	Total				1.564e+43	100

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5623
5624 1,4-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-
5625 di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde
5626 =====
5627 =====

5628
5629 Population analysis at 300K. Vibrational scaling: 0.971.
5630 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
5631 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
5632 %: contribution to the population (with current data set assumed 100%)
5633 Compound Qtot Erel Erel2 n*Q*MB %
5634 -----

5635	TS.diHPCARP_I.14HPHshift.mtmmttu	3.231e+42	0.00	0.00	3.231e+42	43.8
5636	TS.diHPCARP_I.14HPHshift.mmmmttu	5.248e+42	0.36	0.36	2.854e+42	38.7
5637	TS.diHPCARP_I.14HPHshift.mmtmttu	4.996e+42	1.18	1.18	6.941e+41	9.41
5638	TS.diHPCARP_I.14HPHshift.mmmmttu	5.757e+42	1.95	1.95	2.192e+41	2.97
5639	TS.diHPCARP_I.14HPHshift.mtmmttu	5.893e+42	2.15	2.15	1.612e+41	2.19
5640	TS.diHPCARP_I.14HPHshift.mmtmttu	5.845e+42	2.56	2.56	7.925e+40	1.07
5641	TS.diHPCARP_I.14HPHshift.mtpmttu	1.649e+43	3.67	3.67	3.476e+40	0.471
5642	TS.diHPCARP_I.14HPHshift.mtpmttu	2.583e+43	4.32	4.32	1.846e+40	0.25
5643	TS.diHPCARP_I.14HPHshift.pmpmttu	8.977e+42	3.78	3.78	1.595e+40	0.216
5644	TS.diHPCARP_I.14HPHshift.mmmmttu	2.257e+43	4.37	4.37	1.474e+40	0.2
5645	TS.diHPCARP_I.14HPHshift.mmmpppu	7.145e+43	5.18	5.18	1.198e+40	0.162
5646	TS.diHPCARP_I.14HPHshift.mmtpppu	2.228e+43	4.52	4.52	1.127e+40	0.153
5647	TS.diHPCARP_I.14HPHshift.pmpmttu	7.454e+42	4.17	4.17	6.782e+39	0.0919
5648	TS.diHPCARP_I.14HPHshift.pmpmttu	7.278e+42	4.28	4.28	5.549e+39	0.0752
5649	TS.diHPCARP_I.14HPHshift.pmpmttu	2.615e+43	5.14	5.14	4.687e+39	0.0635
5650	TS.diHPCARP_I.14HPHshift.mmmmttu	3.976e+43	6.28	6.28	1.065e+39	0.0144
5651	TS.diHPCARP_I.14HPHshift.mmmppmu	1.434e+44	7.09	7.09	9.777e+38	0.0133
5652	TS.diHPCARP_I.14HPHshift.pmpmttu	7.507e+42	5.39	5.39	8.844e+38	0.012
5653	TS.diHPCARP_I.14HPHshift.mmmmttu	1.158e+44	7.05	7.05	8.497e+38	0.0115
5654	TS.diHPCARP_I.14HPHshift.mmmmttu	9.667e+43	7.03	7.03	7.284e+38	0.00987
5655	TS.diHPCARP_I.14HPHshift.mmmmttu	3.544e+43	6.44	6.44	7.229e+38	0.0098
5656	TS.diHPCARP_I.14HPHshift.mmpmttu	1.258e+43	5.83	5.83	7.163e+38	0.00971
5657	TS.diHPCARP_I.14HPHshift.mtpmttu	7.414e+43	6.95	6.95	6.428e+38	0.00871
5658	TS.diHPCARP_I.14HPHshift.pmpmttu	3.280e+43	6.55	6.55	5.548e+38	0.00752
5659	TS.diHPCARP_I.14HPHshift.mmtpppu	7.164e+43	7.06	7.06	5.186e+38	0.00703
5660	TS.diHPCARP_I.14HPHshift.mtmmttu	2.638e+43	6.49	6.49	4.902e+38	0.00665
5661	TS.diHPCARP_I.14HPHshift.pmpmttu	1.738e+43	6.27	6.27	4.682e+38	0.00635
5662	TS.diHPCARP_I.14HPHshift.mtmmttu	1.395e+43	6.16	6.16	4.510e+38	0.00611
5663	TS.diHPCARP_I.14HPHshift.mtpmttu	1.604e+44	7.62	7.62	4.504e+38	0.00611
5664	TS.diHPCARP_I.14HPHshift.mtmmttu	5.178e+43	7.08	7.08	3.585e+38	0.00486

5665	TS.diHPCARP_I.14HPHshift.mmmptmu	1.769e+43	6.45	6.45	3.550e+38	0.00481
5666	TS.diHPCARP_I.14HPHshift.mmmptpu	8.063e+43	7.36	7.36	3.515e+38	0.00477
5667	TS.diHPCARP_I.14HPHshift.mmtptmtu	8.804e+42	6.28	6.28	2.338e+38	0.00317
5668	TS.diHPCARP_I.14HPHshift.pmpmtmtu	1.310e+43	6.59	6.59	2.082e+38	0.00282
5669	TS.diHPCARP_I.14HPHshift.tmpmmmu	3.796e+43	7.29	7.29	1.871e+38	0.00254
5670	TS.diHPCARP_I.14HPHshift.pmpptpu	1.100e+43	6.55	6.55	1.862e+38	0.00252
5671	TS.diHPCARP_I.14HPHshift.mmmmttu	6.870e+43	7.87	7.87	1.267e+38	0.00172
5672	TS.diHPCARP_I.14HPHshift.mpppppu	2.574e+43	7.30	7.30	1.248e+38	0.00169
5673	TS.diHPCARP_I.14HPHshift.mmtmmmu	7.303e+43	7.93	7.93	1.214e+38	0.00165
5674	TS.diHPCARP_I.14HPHshift.pmpmmmu	1.557e+43	7.05	7.05	1.130e+38	0.00153
5675	TS.diHPCARP_I.14HPHshift.mmtmtpu	9.259e+43	8.13	8.13	1.102e+38	0.00149
5676	TS.diHPCARP_I.14HPHshift.mmtptmu	1.217e+44	8.31	8.31	1.071e+38	0.00145
5677	TS.diHPCARP_I.14HPHshift.mtmmtpu	8.660e+43	8.19	8.19	9.321e+37	0.00126
5678	TS.diHPCARP_I.14HPHshift.mmttptmu	3.453e+43	7.68	7.68	8.801e+37	0.00119
5679	TS.diHPCARP_I.14HPHshift.mtptmpu	4.605e+43	7.94	7.94	7.596e+37	0.00103
5680	TS.diHPCARP_I.14HPHshift.mmttmmu	8.400e+43	8.33	8.33	7.223e+37	0.000979
5681	TS.diHPCARP_I.14HPHshift.mmtptpu	1.365e+44	8.65	8.65	6.781e+37	0.000919
5682	TS.diHPCARP_I.14HPHshift.ttpmpu	7.813e+43	8.34	8.34	6.576e+37	0.000891
5683	TS.diHPCARP_I.14HPHshift.mmmmttu	9.202e+43	8.44	8.44	6.507e+37	0.000882
5684	TS.diHPCARP_I.14HPHshift.mppmtmu	6.472e+43	8.24	8.24	6.421e+37	0.00087
5685	TS.diHPCARP_I.14HPHshift.pmpptmu	2.842e+43	7.76	7.76	6.337e+37	0.000859
5686	TS.diHPCARP_I.14HPHshift.tmmmmmu	3.038e+43	7.82	7.82	6.150e+37	0.000834
5687	TS.diHPCARP_I.14HPHshift.mptpptu	8.026e+43	8.44	8.44	5.660e+37	0.000767
5688	TS.diHPCARP_I.14HPHshift.mmpmmmu	1.473e+44	8.82	8.82	5.525e+37	0.000749
5689	TS.diHPCARP_I.14HPHshift.mmmmttu	1.589e+44	8.92	8.92	5.057e+37	0.000685
5690	TS.diHPCARP_I.14HPHshift.tmmmmmu	4.186e+43	8.23	8.23	4.254e+37	0.000577
5691	TS.diHPCARP_I.14HPHshift.tmmmttu	4.535e+43	8.28	8.28	4.193e+37	0.000568
5692	TS.diHPCARP_I.14HPHshift.tmmpptu	2.372e+43	7.91	7.91	4.103e+37	0.000556
5693	TS.diHPCARP_I.14HPHshift.mmpmttu	6.609e+43	8.63	8.63	3.397e+37	0.00046
5694	TS.diHPCARP_I.14HPHshift.mtpptmu	2.491e+44	9.44	9.44	3.335e+37	0.000452
5695	TS.diHPCARP_I.14HPHshift.mppmtmu	2.439e+43	8.05	8.05	3.309e+37	0.000449
5696	TS.diHPCARP_I.14HPHshift.mtptmmu	1.367e+44	9.12	9.12	3.092e+37	0.000419
5697	TS.diHPCARP_I.14HPHshift.mtptptu	8.450e+43	8.95	8.95	2.564e+37	0.000348
5698	TS.diHPCARP_I.14HPHshift.mtmmtmu	5.465e+43	8.76	8.76	2.252e+37	0.000305
5699	TS.diHPCARP_I.14HPHshift.mtmpttu	2.104e+44	9.64	9.64	1.997e+37	0.000271
5700	TS.diHPCARP_I.14HPHshift.mtpmtmu	1.854e+44	9.61	9.61	1.858e+37	0.000252
5701	TS.diHPCARP_I.14HPHshift.mtmtpu	4.129e+43	8.75	8.75	1.750e+37	0.000237
5702	TS.diHPCARP_I.14HPHshift.mpmmttu	2.164e+43	8.39	8.39	1.678e+37	0.000227
5703	TS.diHPCARP_I.14HPHshift.mppmttu	3.995e+43	8.80	8.80	1.564e+37	0.000212
5704	TS.diHPCARP_I.14HPHshift.tmmpppu	9.489e+43	9.36	9.36	1.440e+37	0.000195
5705	TS.diHPCARP_I.14HPHshift.mtppmtu	3.700e+43	8.81	8.81	1.405e+37	0.00019
5706	TS.diHPCARP_I.14HPHshift.mmttttu	1.211e+44	9.53	9.53	1.377e+37	0.000187
5707	TS.diHPCARP_I.14HPHshift.mtppmmu	2.112e+44	9.99	9.99	1.121e+37	0.000152
5708	TS.diHPCARP_I.14HPHshift.mmtttmu	1.274e+44	9.71	9.71	1.080e+37	0.000146
5709	TS.diHPCARP_I.14HPHshift.tmtpptu	3.349e+43	8.98	8.98	9.697e+36	0.000131
5710	TS.diHPCARP_I.14HPHshift.mmpmpu	3.026e+43	8.98	8.98	8.748e+36	0.000119
5711	TS.diHPCARP_I.14HPHshift.tmmmttu	1.094e+44	9.75	9.75	8.681e+36	0.000118
5712	TS.diHPCARP_I.14HPHshift.mmttptu	9.638e+43	9.74	9.74	7.773e+36	0.000105
5713	TS.diHPCARP_I.14HPHshift.pmppttu	8.225e+43	9.74	9.74	6.642e+36	9e-05
5714	TS.diHPCARP_I.14HPHshift.mppmmmu	1.086e+43	8.63	8.63	5.595e+36	7.58e-05
5715	TS.diHPCARP_I.14HPHshift.tppmmu	7.549e+43	9.81	9.81	5.386e+36	7.3e-05
5716	TS.diHPCARP_I.14HPHshift.ptpmmu	3.602e+43	9.40	9.40	5.106e+36	6.92e-05
5717	TS.diHPCARP_I.14HPHshift.mtptmtu	2.335e+44	10.56	10.56	4.776e+36	6.47e-05
5718	TS.diHPCARP_I.14HPHshift.tmmptu	1.903e+43	9.19	9.19	3.825e+36	5.18e-05
5719	TS.diHPCARP_I.14HPHshift.mpmmttu	1.405e+43	9.06	9.06	3.507e+36	4.75e-05
5720	TS.diHPCARP_I.14HPHshift.mtmmttu	9.650e+43	10.21	10.21	3.501e+36	4.75e-05
5721	TS.diHPCARP_I.14HPHshift.mtpttu	2.064e+44	10.74	10.74	3.085e+36	4.18e-05
5722	TS.diHPCARP_I.14HPHshift.pmpptpu	1.316e+44	10.50	10.50	2.949e+36	4e-05
5723	TS.diHPCARP_I.14HPHshift.ptppptu	5.641e+43	10.02	10.02	2.813e+36	3.81e-05
5724	TS.diHPCARP_I.14HPHshift.tmmmtu	5.986e+43	10.10	10.10	2.619e+36	3.55e-05
5725	TS.diHPCARP_I.14HPHshift.ttpmptu	7.251e+43	10.23	10.23	2.580e+36	3.5e-05
5726	TS.diHPCARP_I.14HPHshift.tmmptu	5.845e+43	10.13	10.13	2.436e+36	3.3e-05
5727	TS.diHPCARP_I.14HPHshift.mpmmtmu	5.965e+43	10.23	10.23	2.109e+36	2.86e-05
5728	TS.diHPCARP_I.14HPHshift.mtptttu	1.330e+44	10.74	10.74	2.009e+36	2.72e-05
5729	TS.diHPCARP_I.14HPHshift.ttttptu	9.085e+43	10.59	10.59	1.743e+36	2.36e-05
5730	TS.diHPCARP_I.14HPHshift.mpmptmu	2.265e+43	9.78	9.78	1.693e+36	2.29e-05
5731	TS.diHPCARP_I.14HPHshift.ttpmtmu	1.501e+44	10.91	10.91	1.693e+36	2.29e-05
5732	TS.diHPCARP_I.14HPHshift.tmmptmu	1.062e+44	10.79	10.79	1.455e+36	1.97e-05
5733	TS.diHPCARP_I.14HPHshift.tmmptu	1.733e+43	9.73	9.73	1.405e+36	1.9e-05
5734	TS.diHPCARP_I.14HPHshift.tmtmptu	6.978e+43	10.58	10.58	1.364e+36	1.85e-05
5735	TS.diHPCARP_I.14HPHshift.mtmtpu	9.094e+43	10.93	10.93	9.878e+35	1.34e-05
5736	TS.diHPCARP_I.14HPHshift.tmmppmu	1.014e+44	11.21	11.21	6.936e+35	9.4e-06

5737	TS.diHPCARP_I.14HPHshift.ttpmtpu	2.445e+44	11.74	11.74	6.816e+35	9.24e-06
5738	TS.diHPCARP_I.14HPHshift.ptmpppu	1.325e+44	11.41	11.41	6.452e+35	8.75e-06
5739	TS.diHPCARP_I.14HPHshift.ttmmtpu	8.189e+43	11.26	11.26	5.103e+35	6.92e-06
5740	TS.diHPCARP_I.14HPHshift.ttmmtu	2.145e+43	10.95	10.95	2.266e+35	3.07e-06
5741	TS.diHPCARP_I.14HPHshift.ttmmttu	1.739e+44	12.27	12.27	2.013e+35	2.73e-06
5742	TS.diHPCARP_I.14HPHshift.ttptmtu	4.729e+43	11.50	11.50	1.986e+35	2.69e-06
5743	TS.diHPCARP_I.14HPHshift.tmmmtmu	2.639e+44	12.53	12.53	1.975e+35	2.68e-06
5744	TS.diHPCARP_I.14HPHshift.ptppmtu	3.897e+43	11.68	11.68	1.203e+35	1.63e-06
5745	TS.diHPCARP_I.14HPHshift.tmttmu	1.709e+44	12.78	12.78	8.360e+34	1.13e-06
5746	TS.diHPCARP_I.14HPHshift.ttpptmu	1.785e+44	12.84	12.84	7.883e+34	1.07e-06
5747	TS.diHPCARP_I.14HPHshift.ttpttu	7.279e+43	12.50	12.50	5.750e+34	7.79e-07
5748	TS.diHPCARP_I.14HPHshift.ttppppu	1.067e+44	12.99	12.99	3.702e+34	5.02e-07
5749	TS.diHPCARP_I.14HPHshift.mpmtppu	2.890e+43	12.24	12.24	3.478e+34	4.71e-07
5750	TS.diHPCARP_I.14HPHshift.ttptmmu	1.007e+44	13.04	13.04	3.190e+34	4.32e-07
5751	TS.diHPCARP_I.14HPHshift.tmtmttu	2.700e+44	13.89	13.89	2.087e+34	2.68e-07
5752	TS.diHPCARP_I.14HPHshift.tmttttu	2.555e+44	13.97	13.97	1.695e+34	2.3e-07
5753	TS.diHPCARP_I.14HPHshift.ttmmtmu	6.570e+43	13.37	13.37	1.199e+34	1.63e-07
5754	TS.diHPCARP_I.14HPHshift.ttpttu	2.057e+44	14.31	14.31	7.698e+33	1.04e-07
5755	TS.diHPCARP_I.14HPHshift.ttppttu	1.784e+44	14.28	14.28	7.084e+33	9.6e-08
5756	TS.diHPCARP_I.14HPHshift.tmtppu	1.275e+44	14.22	14.22	5.569e+33	7.55e-08
5757	TS.diHPCARP_I.14HPHshift.ttmtpu	1.373e+44	14.57	14.57	3.348e+33	4.54e-08
5758	TS.diHPCARP_I.14HPHshift.tmtttu	9.332e+43	14.63	14.63	2.059e+33	2.79e-08
5759	TS.diHPCARP_I.14HPHshift.tmtttu	1.124e+44	15.55	15.55	5.251e+32	7.12e-09
5760	Total				7.377e+42	100

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1,5-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxy (A, R, R-di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde

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Population analysis at 300K. Vibrational scaling: 0.971.

5770 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
5771 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
5772 %: contribution to the population (with current data set assumed 100%)

5773	Compound	Qtot	Erel	Erel2	n*Q*MB	%
5774	TS.diHPCARP_I.15HPHshift.dmtdmuud	7.796e+42	0.00	0.00	7.796e+42	46.7
5775	TS.diHPCARP_I.15HPHshift.dmtdpdud	2.528e+43	1.27	1.27	2.981e+42	17.8
5776	TS.diHPCARP_I.15HPHshift.dmtmdud	1.790e+43	1.86	1.86	7.914e+41	4.74
5777	TS.diHPCARP_I.15HPHshift.dcpdpddd	5.229e+43	2.64	2.64	6.290e+41	3.76
5778	TS.diHPCARP_I.15HPHshift.dmpupuud	4.559e+43	2.62	2.62	5.582e+41	3.34
5779	TS.diHPCARP_I.15HPHshift.dmpumdud	3.761e+43	2.65	2.65	4.389e+41	2.63
5780	TS.diHPCARP_I.15HPHshift.dcmupudd	3.057e+43	2.56	2.56	4.189e+41	2.51
5781	TS.diHPCARP_I.15HPHshift.dcmupddd	3.358e+43	2.72	2.72	3.528e+41	2.11
5782	TS.diHPCARP_I.15HPHshift.dmpumuud	9.573e+42	2.04	2.04	3.125e+41	1.87
5783	TS.diHPCARP_I.15HPHshift.dcmutudd	8.689e+42	2.07	2.07	2.720e+41	1.63
5784	TS.diHPCARP_I.15HPHshift.dppdmudd	1.268e+43	2.32	2.32	2.574e+41	1.54
5785	TS.diHPCARP_I.15HPHshift.dlpdtddd	3.142e+43	2.94	2.94	2.253e+41	1.35
5786	TS.diHPCARP_I.15HPHshift.dcmumddd	6.665e+42	2.13	2.13	1.867e+41	1.12
5787	TS.diHPCARP_I.15HPHshift.dtpdmud	7.391e+42	2.27	2.27	1.641e+41	0.982
5788	TS.diHPCARP_I.15HPHshift.dcpdmudd	1.557e+43	2.81	2.81	1.389e+41	0.831
5789	TS.diHPCARP_I.15HPHshift.dcmumudd	1.420e+43	2.84	2.84	1.212e+41	0.726
5790	TS.diHPCARP_I.15HPHshift.dcmdpddd	2.732e+43	3.24	3.24	1.186e+41	0.71
5791	TS.diHPCARP_I.15HPHshift.umtumdud	8.617e+42	2.71	2.71	9.133e+40	0.546
5792	TS.diHPCARP_I.15HPHshift.dcpdpudd	3.821e+43	3.71	3.71	7.517e+40	0.45
5793	TS.diHPCARP_I.15HPHshift.uppupuud	8.904e+43	4.36	4.36	5.972e+40	0.357
5794	TS.diHPCARP_I.15HPHshift.umpupuud	4.390e+43	4.03	4.03	5.090e+40	0.305
5795	TS.diHPCARP_I.15HPHshift.umpupud	3.500e+43	3.94	3.94	4.716e+40	0.282
5796	TS.diHPCARP_I.15HPHshift.dcpumddd	1.330e+43	3.44	3.44	4.157e+40	0.249
5797	TS.diHPCARP_I.15HPHshift.dcmupudd	1.027e+44	4.68	4.68	3.995e+40	0.239
5798	TS.diHPCARP_I.15HPHshift.dmmumuud	1.085e+44	4.74	4.74	3.854e+40	0.231
5799	TS.diHPCARP_I.15HPHshift.dctdmdud	3.189e+43	4.03	4.03	3.684e+40	0.22
5800	TS.diHPCARP_I.15HPHshift.dlmdmuud	2.044e+43	3.79	3.79	3.564e+40	0.213
5801	TS.diHPCARP_I.15HPHshift.uctdmuud	6.297e+43	4.67	4.67	2.492e+40	0.149
5802	TS.diHPCARP_I.15HPHshift.uppumud	2.260e+43	4.07	4.07	2.435e+40	0.146
5803	TS.diHPCARP_I.15HPHshift.dcmumdud	1.110e+43	3.66	3.66	2.379e+40	0.142
5804	TS.diHPCARP_I.15HPHshift.uppupud	2.226e+43	4.21	4.21	1.897e+40	0.113
5805	TS.diHPCARP_I.15HPHshift.dctumudd	2.780e+43	4.40	4.40	1.730e+40	0.104
5806	TS.diHPCARP_I.15HPHshift.dcpupddd	2.700e+44	5.78	5.78	1.662e+40	0.0995
5807	TS.diHPCARP_I.15HPHshift.dcpdtdud	1.246e+43	4.00	4.00	1.517e+40	0.0908

5809	TS.diHPCARP_I.15HPHshift.ummdpdud	9.782e+43	5.24	5.24	1.493e+40	0.0894
5810	TS.diHPCARP_I.15HPHshift.ummdpuud	1.387e+44	5.47	5.47	1.445e+40	0.0865
5811	TS.diHPCARP_I.15HPHshift.ulmumuud	2.107e+44	5.74	5.74	1.389e+40	0.0831
5812	TS.diHPCARP_I.15HPHshift.uctdpuud	6.089e+43	5.05	5.05	1.278e+40	0.0765
5813	TS.diHPCARP_I.15HPHshift.ummupdud	1.304e+44	5.51	5.51	1.262e+40	0.0755
5814	TS.diHPCARP_I.15HPHshift.ummdmdud	9.271e+43	5.37	5.37	1.144e+40	0.0685
5815	TS.diHPCARP_I.15HPHshift.ummdmuud	7.216e+43	5.24	5.24	1.091e+40	0.0653
5816	TS.diHPCARP_I.15HPHshift.uctdpdud	4.347e+43	4.96	4.96	1.060e+40	0.0635
5817	TS.diHPCARP_I.15HPHshift.ummupuud	1.526e+44	5.75	5.75	9.883e+39	0.0591
5818	TS.diHPCARP_I.15HPHshift.dcpuuud	7.507e+42	4.03	4.03	8.683e+39	0.052
5819	TS.diHPCARP_I.15HPHshift.dcmumuud	2.936e+43	4.91	4.91	7.756e+39	0.0464
5820	TS.diHPCARP_I.15HPHshift.dtpupddd	1.434e+44	5.86	5.86	7.676e+39	0.0459
5821	TS.diHPCARP_I.15HPHshift.umtutudd	1.312e+43	4.49	4.49	7.074e+39	0.0423
5822	TS.diHPCARP_I.15HPHshift.dctdpuud	7.640e+43	5.54	5.54	6.984e+39	0.0418
5823	TS.diHPCARP_I.15HPHshift.dmmduud	9.795e+42	4.38	4.38	6.302e+39	0.0377
5824	TS.diHPCARP_I.15HPHshift.uctdmdud	5.771e+42	4.08	4.08	6.125e+39	0.0367
5825	TS.diHPCARP_I.15HPHshift.dmtddud	3.447e+43	5.16	5.16	5.985e+39	0.0358
5826	TS.diHPCARP_I.15HPHshift.dcpuudd	3.332e+43	5.15	5.15	5.914e+39	0.0354
5827	TS.diHPCARP_I.15HPHshift.dcpumuud	8.814e+43	5.80	5.80	5.263e+39	0.0315
5828	TS.diHPCARP_I.15HPHshift.dcpumuud	1.821e+43	4.87	4.87	5.132e+39	0.0307
5829	TS.diHPCARP_I.15HPHshift.dltumuud	3.165e+43	5.23	5.23	4.883e+39	0.0292
5830	TS.diHPCARP_I.15HPHshift.umpumuud	5.698e+43	5.63	5.63	4.537e+39	0.0272
5831	TS.diHPCARP_I.15HPHshift.dctupud	6.587e+43	5.75	5.75	4.301e+39	0.0257
5832	TS.diHPCARP_I.15HPHshift.dttduud	2.953e+43	5.27	5.27	4.259e+39	0.0255
5833	TS.diHPCARP_I.15HPHshift.umtupudd	4.195e+43	5.51	5.51	4.041e+39	0.0242
5834	TS.diHPCARP_I.15HPHshift.dptumudd	2.776e+43	5.28	5.28	3.941e+39	0.0236
5835	TS.diHPCARP_I.15HPHshift.ucpdmuud	6.432e+43	5.79	5.79	3.918e+39	0.0234
5836	TS.diHPCARP_I.15HPHshift.ucpdmddd	6.927e+42	4.49	4.49	3.735e+39	0.0223
5837	TS.diHPCARP_I.15HPHshift.ulpdpdud	7.028e+43	5.92	5.92	3.403e+39	0.0204
5838	TS.diHPCARP_I.15HPHshift.ultdpuud	2.158e+44	6.60	6.60	3.374e+39	0.0202
5839	TS.diHPCARP_I.15HPHshift.umpdmuud	2.394e+43	5.35	5.35	3.052e+39	0.0183
5840	TS.diHPCARP_I.15HPHshift.dcmdpuud	1.008e+44	6.24	6.24	2.860e+39	0.0171
5841	TS.diHPCARP_I.15HPHshift.ultupdud	1.721e+44	6.57	6.57	2.807e+39	0.0168
5842	TS.diHPCARP_I.15HPHshift.umpudud	5.262e+43	5.87	5.87	2.791e+39	0.0167
5843	TS.diHPCARP_I.15HPHshift.dcmdmuud	2.662e+43	5.46	5.46	2.782e+39	0.0166
5844	TS.diHPCARP_I.15HPHshift.dcmdpdud	9.200e+43	6.22	6.22	2.723e+39	0.0163
5845	TS.diHPCARP_I.15HPHshift.umtupdud	1.244e+44	6.43	6.43	2.577e+39	0.0154
5846	TS.diHPCARP_I.15HPHshift.ulpdpuud	4.371e+43	5.82	5.82	2.524e+39	0.0151
5847	TS.diHPCARP_I.15HPHshift.dlmdpdud	4.405e+44	7.21	7.21	2.480e+39	0.0148
5848	TS.diHPCARP_I.15HPHshift.dctumuud	2.677e+43	5.54	5.54	2.476e+39	0.0148
5849	TS.diHPCARP_I.15HPHshift.dctdmuud	1.407e+43	5.19	5.19	2.336e+39	0.014
5850	TS.diHPCARP_I.15HPHshift.upputudd	2.550e+43	5.58	5.58	2.186e+39	0.0131
5851	TS.diHPCARP_I.15HPHshift.ulpumddd	2.709e+43	5.62	5.62	2.168e+39	0.013
5852	TS.diHPCARP_I.15HPHshift.ulpdmdud	9.136e+42	5.00	5.00	2.074e+39	0.0124
5853	TS.diHPCARP_I.15HPHshift.dcpupddd	1.098e+44	6.49	6.49	2.042e+39	0.0122
5854	TS.diHPCARP_I.15HPHshift.ultdpud	9.071e+43	6.47	6.47	1.751e+39	0.0105
5855	TS.diHPCARP_I.15HPHshift.ucpdpddd	3.910e+43	6.08	6.08	1.452e+39	0.00869
5856	TS.diHPCARP_I.15HPHshift.ummdtdud	1.250e+44	6.84	6.84	1.293e+39	0.00774
5857	TS.diHPCARP_I.15HPHshift.dcmutuud	3.259e+43	6.05	6.05	1.268e+39	0.00759
5858	TS.diHPCARP_I.15HPHshift.ucputudd	3.106e+43	6.05	6.05	1.210e+39	0.00724
5859	TS.diHPCARP_I.15HPHshift.uctdtdud	4.813e+43	6.42	6.42	1.012e+39	0.00606
5860	TS.diHPCARP_I.15HPHshift.dcpdpdud	3.056e+43	6.17	6.17	9.844e+38	0.00589
5861	TS.diHPCARP_I.15HPHshift.ultumuud	5.322e+43	6.51	6.51	9.641e+38	0.00577
5862	TS.diHPCARP_I.15HPHshift.ulpdtdud	4.241e+43	6.38	6.38	9.624e+38	0.00576
5863	TS.diHPCARP_I.15HPHshift.ultdmuud	6.698e+43	6.65	6.65	9.591e+38	0.00574
5864	TS.diHPCARP_I.15HPHshift.dlpdpdud	1.234e+44	7.02	7.02	9.531e+38	0.0057
5865	TS.diHPCARP_I.15HPHshift.dcpdmuud	3.423e+43	6.26	6.26	9.457e+38	0.00566
5866	TS.diHPCARP_I.15HPHshift.dctutudd	3.382e+43	6.32	6.32	8.469e+38	0.00507
5867	TS.diHPCARP_I.15HPHshift.ucpdmuud	2.386e+43	6.19	6.19	7.344e+38	0.00439
5868	TS.diHPCARP_I.15HPHshift.ucpupudd	1.360e+44	7.25	7.25	7.149e+38	0.00428
5869	TS.diHPCARP_I.15HPHshift.ummudud	1.855e+44	7.44	7.44	7.015e+38	0.0042
5870	TS.diHPCARP_I.15HPHshift.dcmdtuud	1.797e+43	6.05	6.05	7.006e+38	0.00419
5871	TS.diHPCARP_I.15HPHshift.ultdpuud	3.091e+43	6.41	6.41	6.599e+38	0.00395
5872	TS.diHPCARP_I.15HPHshift.dcpdmud	3.509e+43	6.53	6.53	6.155e+38	0.00368
5873	TS.diHPCARP_I.15HPHshift.umtdpdud	2.546e+43	6.35	6.35	6.014e+38	0.0036
5874	TS.diHPCARP_I.15HPHshift.ultdmud	4.966e+43	6.75	6.75	5.997e+38	0.00359
5875	TS.diHPCARP_I.15HPHshift.ulpdmuud	3.533e+43	6.56	6.56	5.851e+38	0.0035
5876	TS.diHPCARP_I.15HPHshift.ultdmdud	1.441e+43	6.14	6.14	4.874e+38	0.00292
5877	TS.diHPCARP_I.15HPHshift.ulputudd	3.235e+43	6.66	6.66	4.561e+38	0.00273
5878	TS.diHPCARP_I.15HPHshift.uhtdpuud	1.948e+44	7.74	7.74	4.483e+38	0.00268
5879	TS.diHPCARP_I.15HPHshift.ultudud	2.125e+44	7.82	7.82	4.291e+38	0.00257
5880	TS.diHPCARP_I.15HPHshift.ulpupddd	2.709e+44	8.07	8.07	3.594e+38	0.00215

5881	TS.diHPCARP_I.15HPHshift.uhtdpdud	1.045e+44	7.52	7.52	3.453e+38	0.00207
5882	TS.diHPCARP_I.15HPHshift.ucmutudd	7.070e+42	5.93	5.93	3.383e+38	0.00202
5883	TS.diHPCARP_I.15HPHshift.ucpdtddd	3.327e+43	6.95	6.95	2.887e+38	0.00173
5884	TS.diHPCARP_I.15HPHshift.uldpdud	1.525e+44	7.91	7.91	2.616e+38	0.00157
5885	TS.diHPCARP_I.15HPHshift.ulpupudd	1.600e+44	7.98	7.98	2.453e+38	0.00147
5886	TS.diHPCARP_I.15HPHshift.uhpdpddd	4.913e+43	7.30	7.30	2.366e+38	0.00142
5887	TS.diHPCARP_I.15HPHshift.ulpdtudd	1.791e+43	6.72	6.72	2.294e+38	0.00137
5888	TS.diHPCARP_I.15HPHshift.ulpdtud	8.965e+43	7.71	7.71	2.155e+38	0.00129
5889	TS.diHPCARP_I.15HPHshift.dctdtudd	3.864e+43	7.25	7.25	2.015e+38	0.00121
5890	TS.diHPCARP_I.15HPHshift.ultdtud	1.346e+44	8.01	8.01	1.953e+38	0.00117
5891	TS.diHPCARP_I.15HPHshift.uctdtudd	1.095e+43	6.65	6.65	1.562e+38	0.000935
5892	TS.diHPCARP_I.15HPHshift.dhpumuud	9.120e+42	6.61	6.61	1.406e+38	0.000841
5893	TS.diHPCARP_I.15HPHshift.umtumudd	1.637e+43	6.97	6.97	1.359e+38	0.000813
5894	TS.diHPCARP_I.15HPHshift.uctdpudd	5.155e+43	7.66	7.66	1.355e+38	0.000811
5895	TS.diHPCARP_I.15HPHshift.uhmupudd	1.434e+44	8.27	8.27	1.353e+38	0.00081
5896	TS.diHPCARP_I.15HPHshift.uhpdmddd	8.910e+42	6.67	6.67	1.235e+38	0.000739
5897	TS.diHPCARP_I.15HPHshift.ultdpudd	1.067e+44	8.15	8.15	1.230e+38	0.000736
5898	TS.diHPCARP_I.15HPHshift.uhmumuud	1.010e+44	8.18	8.18	1.105e+38	0.000661
5899	TS.diHPCARP_I.15HPHshift.ucpumudd	9.923e+43	8.20	8.20	1.054e+38	0.00063
5900	TS.diHPCARP_I.15HPHshift.uhmupuud	1.791e+44	8.60	8.60	9.765e+37	0.000584
5901	TS.diHPCARP_I.15HPHshift.uhtdmuud	5.823e+43	7.94	7.94	9.546e+37	0.000571
5902	TS.diHPCARP_I.15HPHshift.ummdmddd	3.539e+42	6.30	6.30	9.148e+37	0.000547
5903	TS.diHPCARP_I.15HPHshift.uhpdtdud	7.285e+42	6.74	6.74	8.892e+37	0.000532
5904	TS.diHPCARP_I.15HPHshift.uhpdtddd	3.466e+43	7.71	7.71	8.445e+37	0.000505
5905	TS.diHPCARP_I.15HPHshift.uhmumdud	8.683e+43	8.29	8.29	7.928e+37	0.000474
5906	TS.diHPCARP_I.15HPHshift.dhmupudd	1.184e+44	8.48	8.48	7.842e+37	0.000469
5907	TS.diHPCARP_I.15HPHshift.dhtumuud	1.541e+43	7.29	7.29	7.487e+37	0.000448
5908	TS.diHPCARP_I.15HPHshift.uhpdmuud	2.962e+43	7.73	7.73	6.958e+37	0.000416
5909	TS.diHPCARP_I.15HPHshift.dhpumuud	1.045e+43	7.16	7.16	6.382e+37	0.000382
5910	TS.diHPCARP_I.15HPHshift.ucpdtudd	1.300e+43	7.35	7.35	5.730e+37	0.000343
5911	TS.diHPCARP_I.15HPHshift.uhmdpudd	2.541e+43	7.77	7.77	5.550e+37	0.000332
5912	TS.diHPCARP_I.15HPHshift.uhtdtud	1.418e+44	8.83	8.83	5.194e+37	0.000311
5913	TS.diHPCARP_I.15HPHshift.uhtdmud	3.501e+43	8.05	8.05	4.760e+37	0.000285
5914	TS.diHPCARP_I.15HPHshift.uhmdmuud	7.250e+43	8.50	8.50	4.625e+37	0.000277
5915	TS.diHPCARP_I.15HPHshift.ulpupddd	3.453e+43	8.08	8.08	4.498e+37	0.000269
5916	TS.diHPCARP_I.15HPHshift.dhpupdud	3.000e+43	8.00	8.00	4.442e+37	0.000266
5917	TS.diHPCARP_I.15HPHshift.uhmutdud	5.089e+44	9.79	9.79	3.748e+37	0.000224
5918	TS.diHPCARP_I.15HPHshift.uptupddd	8.040e+43	8.69	8.69	3.742e+37	0.000224
5919	TS.diHPCARP_I.15HPHshift.dhmumuud	8.559e+43	8.73	8.73	3.742e+37	0.000224
5920	TS.diHPCARP_I.15HPHshift.dhpdpud	1.430e+44	9.09	9.09	3.421e+37	0.000205
5921	TS.diHPCARP_I.15HPHshift.dhmumdud	2.050e+43	7.97	7.97	3.229e+37	0.000193
5922	TS.diHPCARP_I.15HPHshift.uhtupdud	4.090e+44	9.80	9.80	2.948e+37	0.000176
5923	TS.diHPCARP_I.15HPHshift.uhputudd	5.771e+43	8.69	8.69	2.691e+37	0.000161
5924	TS.diHPCARP_I.15HPHshift.dhputdud	1.117e+43	7.72	7.72	2.655e+37	0.000159
5925	TS.diHPCARP_I.15HPHshift.ultdtudd	2.316e+43	8.16	8.16	2.650e+37	0.000159
5926	TS.diHPCARP_I.15HPHshift.uhpmddd	2.112e+43	8.11	8.11	2.596e+37	0.000155
5927	TS.diHPCARP_I.15HPHshift.ucpumddd	3.123e+43	8.37	8.37	2.486e+37	0.000149
5928	TS.diHPCARP_I.15HPHshift.uhpdtdud	1.776e+43	8.28	8.28	1.653e+37	9.89e-05
5929	TS.diHPCARP_I.15HPHshift.ulpumuud	1.118e+44	9.40	9.40	1.599e+37	9.57e-05
5930	TS.diHPCARP_I.15HPHshift.dhpdpddd	6.401e+43	9.19	9.19	1.294e+37	7.74e-05
5931	TS.diHPCARP_I.15HPHshift.uhtdmud	1.397e+43	8.39	8.39	1.086e+37	6.5e-05
5932	TS.diHPCARP_I.15HPHshift.dhmdmud	3.618e+43	9.00	9.00	1.006e+37	6.02e-05
5933	TS.diHPCARP_I.15HPHshift.umtdmuud	1.654e+43	8.55	8.55	9.848e+36	5.89e-05
5934	TS.diHPCARP_I.15HPHshift.uctdmud	1.488e+43	8.50	8.50	9.503e+36	5.69e-05
5935	TS.diHPCARP_I.15HPHshift.uhpupudd	1.859e+44	10.01	10.01	9.500e+36	5.68e-05
5936	TS.diHPCARP_I.15HPHshift.uptumuud	7.585e+43	9.55	9.55	8.337e+36	4.99e-05
5937	TS.diHPCARP_I.15HPHshift.dhmutdud	5.510e+43	9.37	9.37	8.233e+36	4.93e-05
5938	TS.diHPCARP_I.15HPHshift.ucmumddd	7.153e+42	8.23	8.23	7.278e+36	4.36e-05
5939	TS.diHPCARP_I.15HPHshift.uhmupddd	4.835e+43	9.39	9.39	7.026e+36	4.2e-05
5940	TS.diHPCARP_I.15HPHshift.dhmutuud	1.017e+44	9.85	9.85	6.837e+36	4.09e-05
5941	TS.diHPCARP_I.15HPHshift.ulmumddd	1.064e+43	8.52	8.52	6.621e+36	3.96e-05
5942	TS.diHPCARP_I.15HPHshift.uhpuddd	1.762e+44	10.21	10.21	6.395e+36	3.83e-05
5943	TS.diHPCARP_I.15HPHshift.ultdmud	5.615e+43	9.55	9.55	6.242e+36	3.74e-05
5944	TS.diHPCARP_I.15HPHshift.dhmdpddd	2.489e+43	9.07	9.07	6.176e+36	3.7e-05
5945	TS.diHPCARP_I.15HPHshift.uptutudd	3.053e+43	9.21	9.21	5.986e+36	3.58e-05
5946	TS.diHPCARP_I.15HPHshift.uhtumuud	2.521e+43	9.11	9.11	5.866e+36	3.51e-05
5947	TS.diHPCARP_I.15HPHshift.dhpdmuud	2.694e+43	9.22	9.22	5.210e+36	3.12e-05
5948	TS.diHPCARP_I.15HPHshift.dhmupudd	3.554e+43	9.40	9.40	5.077e+36	3.04e-05
5949	TS.diHPCARP_I.15HPHshift.ucmmdddd	1.951e+43	9.07	9.07	4.828e+36	2.89e-05
5950	TS.diHPCARP_I.15HPHshift.dhmutuud	8.453e+42	8.58	8.58	4.787e+36	2.86e-05
5951	TS.diHPCARP_I.15HPHshift.ultmupddd	3.096e+43	9.43	9.43	4.208e+36	2.52e-05
5952	TS.diHPCARP_I.15HPHshift.uhmutddd	1.747e+43	9.25	9.25	3.209e+36	1.92e-05

5953	TS.diHPCARP_I.15HPHshift.dhmumddd	7.995e+42	8.86	8.86	2.790e+36	1.67e-05
5954	TS.diHPCARP_I.15HPHshift.dhpdtdddd	5.689e+43	10.06	10.06	2.676e+36	1.6e-05
5955	TS.diHPCARP_I.15HPHshift.dhpdpudd	5.792e+43	10.20	10.20	2.140e+36	1.28e-05
5956	TS.diHPCARP_I.15HPHshift.ucmutddd	1.760e+43	9.51	9.51	2.079e+36	1.24e-05
5957	TS.diHPCARP_I.15HPHshift.dcpdtuud	2.555e+43	9.79	9.79	1.893e+36	1.13e-05
5958	TS.diHPCARP_I.15HPHshift.dhmumudd	1.336e+43	9.48	9.48	1.673e+36	1e-05
5959	TS.diHPCARP_I.15HPHshift.dhmutddd	3.999e+43	10.15	10.15	1.621e+36	9.7e-06
5960	TS.diHPCARP_I.15HPHshift.ucmdudd	1.830e+43	9.76	9.76	1.429e+36	8.55e-06
5961	TS.diHPCARP_I.15HPHshift.dlpdtuud	2.540e+43	10.05	10.05	1.216e+36	7.28e-06
5962	TS.diHPCARP_I.15HPHshift.ucmumudd	1.424e+43	9.85	9.85	9.469e+35	5.67e-06
5963	TS.diHPCARP_I.15HPHshift.uhtutdud	1.255e+44	11.16	11.16	9.264e+35	5.54e-06
5964	TS.diHPCARP_I.15HPHshift.uhmutddd	2.385e+43	10.20	10.20	8.783e+35	5.26e-06
5965	TS.diHPCARP_I.15HPHshift.dhpumddd	2.326e+43	10.29	10.29	7.484e+35	4.48e-06
5966	TS.diHPCARP_I.15HPHshift.dhpdtdudd	1.729e+43	10.11	10.11	7.420e+35	4.44e-06
5967	TS.diHPCARP_I.15HPHshift.dhmdpudd	9.442e+42	9.82	9.82	6.613e+35	3.96e-06
5968	TS.diHPCARP_I.15HPHshift.uhpmuudd	9.578e+43	11.24	11.24	6.217e+35	3.72e-06
5969	TS.diHPCARP_I.15HPHshift.dhpdtdud	4.284e+43	10.84	10.84	5.475e+35	3.28e-06
5970	TS.diHPCARP_I.15HPHshift.dhtdmddd	4.841e+43	11.06	11.06	4.253e+35	2.54e-06
5971	TS.diHPCARP_I.15HPHshift.uhmumudd	1.295e+43	10.29	10.29	4.117e+35	2.46e-06
5972	TS.diHPCARP_I.15HPHshift.ulmuudd	1.500e+43	10.40	10.40	4.006e+35	2.4e-06
5973	TS.diHPCARP_I.15HPHshift.dhpdtduud	2.755e+43	10.83	10.83	3.549e+35	2.12e-06
5974	TS.diHPCARP_I.15HPHshift.dhmdmddd	1.396e+43	10.43	10.43	3.523e+35	2.11e-06
5975	TS.diHPCARP_I.15HPHshift.uhmpuudd	9.188e+44	13.01	13.01	3.039e+35	1.82e-06
5976	TS.diHPCARP_I.15HPHshift.dhtumddd	3.403e+43	11.05	11.05	3.018e+35	1.81e-06
5977	TS.diHPCARP_I.15HPHshift.dhtutdud	1.640e+44	12.10	12.10	2.524e+35	1.51e-06
5978	TS.diHPCARP_I.15HPHshift.dhtdpddd	7.026e+43	11.89	11.89	1.534e+35	9.18e-07
5979	TS.diHPCARP_I.15HPHshift.uhmduudd	1.678e+43	11.38	11.38	8.594e+34	5.14e-07
5980	TS.diHPCARP_I.15HPHshift.uhmdmddd	2.713e+43	11.67	11.67	8.589e+34	5.14e-07
5981	TS.diHPCARP_I.15HPHshift.uhmdtudd	2.899e+43	11.79	11.79	7.450e+34	4.46e-07
5982	TS.diHPCARP_I.15HPHshift.dhtutudd	4.683e+43	12.14	12.14	6.727e+34	4.03e-07
5983	TS.diHPCARP_I.15HPHshift.dhpuudd	1.443e+44	12.96	12.96	5.201e+34	3.11e-07
5984	TS.diHPCARP_I.15HPHshift.dhtdmudd	1.108e+44	13.65	13.65	1.271e+34	7.6e-08
5985	TS.diHPCARP_I.15HPHshift.uhmutudd	3.341e+43	13.31	13.31	6.704e+33	4.01e-08
5986	TS.diHPCARP_I.15HPHshift.uhmdmudd	2.695e+43	15.58	15.58	1.204e+32	7.21e-10
5987	Total				1.671e+43	100

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(2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia)

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Population analysis at 300K. Vibrational scaling: 0.971.

5995 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)

5996 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

5997 %: contribution to the population (with current data set assumed 100%)

5998	Compound	Qtot	Erel	Erel2	n*Q*MB	%
6000	diHPCARP_I.tmmmppttmu	6.155e+42	0.00	0.00	6.155e+42	30.3
6001	diHPCARP_I.mmmmppttmu	8.995e+42	0.51	0.51	3.797e+42	18.7
6002	diHPCARP_I.pmmmppttmu	8.053e+42	0.93	0.93	1.679e+42	8.27
6003	diHPCARP_I.tmmmpptpmu	1.772e+43	1.69	1.69	1.044e+42	5.14
6004	diHPCARP_I.tmmmpptpmu	1.596e+43	1.66	1.66	9.791e+41	4.82
6005	diHPCARP_I.tmmmpptmpu	9.830e+42	1.50	1.50	7.936e+41	3.91
6006	diHPCARP_I.tpmmppttmu	3.062e+43	2.27	2.27	6.788e+41	3.34
6007	diHPCARP_I.mmmmpptmpu	9.428e+42	1.85	1.85	4.262e+41	2.1
6008	diHPCARP_I.ppmmpptmpu	1.145e+43	2.13	2.13	3.190e+41	1.57
6009	diHPCARP_I.ptppmtpmu	9.557e+42	2.33	2.33	1.925e+41	0.949
6010	diHPCARP_I.tptpmtpmu	2.348e+43	2.98	2.98	1.592e+41	0.785
6011	diHPCARP_I.tmpptpmu	1.692e+43	2.84	2.84	1.442e+41	0.711
6012	diHPCARP_I.mmpptpmu	3.153e+43	3.28	3.28	1.291e+41	0.636
6013	diHPCARP_I.mmtppppu	2.342e+43	3.14	3.14	1.204e+41	0.594
6014	diHPCARP_I.tpmmpmttu	2.836e+43	3.27	3.27	1.173e+41	0.578
6015	diHPCARP_I.ptmmpmtpu	1.253e+45	5.54	5.54	1.145e+41	0.564
6016	diHPCARP_I.tmtppppu	2.817e+43	3.31	3.31	1.090e+41	0.537
6017	diHPCARP_I.tpmmpmtmu	1.684e+43	3.08	3.08	9.643e+40	0.475
6018	diHPCARP_I.pmmmpptpmu	1.189e+43	2.87	2.87	9.613e+40	0.474
6019	diHPCARP_I.tptpmttmu	4.421e+43	3.80	3.80	7.596e+40	0.374
6020	diHPCARP_I.tptpmtppu	4.956e+43	3.91	3.91	6.994e+40	0.345
6021	diHPCARP_I.mmmmtpppu	1.538e+43	3.27	3.27	6.371e+40	0.314
6022	diHPCARP_I.tmmmppttmu	2.455e+43	3.57	3.57	6.199e+40	0.305
6023	diHPCARP_I.tmmmpmttu	1.851e+43	3.40	3.40	6.192e+40	0.305
6024	diHPCARP_I.ptmmppttmu	5.057e+43	4.01	4.01	6.072e+40	0.299

6025	diHPCARP_I.tmmmtpppu	1.303e+43	3.20	3.20	6.036e+40	0.297
6026	diHPCARP_I.tmmmtpppu	6.495e+42	2.85	2.85	5.455e+40	0.269
6027	diHPCARP_I.ppppmtmpu	4.365e+43	4.02	4.02	5.153e+40	0.254
6028	diHPCARP_I.mmmmtmtu	2.101e+43	3.62	3.62	4.878e+40	0.24
6029	diHPCARP_I.tptmptppu	3.645e+43	3.95	3.95	4.864e+40	0.24
6030	diHPCARP_I.pmmmtpppu	6.421e+42	2.92	2.92	4.797e+40	0.236
6031	diHPCARP_I.tpppmtppu	6.064e+44	5.66	5.66	4.598e+40	0.227
6032	diHPCARP_I.mmtpppppu	3.466e+43	3.96	3.96	4.517e+40	0.223
6033	diHPCARP_I.tmtpppppu	4.246e+43	4.12	4.12	4.216e+40	0.208
6034	diHPCARP_I.mptpmtppu	3.063e+43	3.94	3.94	4.157e+40	0.205
6035	diHPCARP_I.tmmmtmpu	2.595e+43	3.85	3.85	4.087e+40	0.201
6036	diHPCARP_I.mmmmtppu	2.951e+43	3.94	3.94	3.973e+40	0.196
6037	diHPCARP_I.mtppmtppu	9.071e+42	3.25	3.25	3.923e+40	0.193
6038	diHPCARP_I.mmmmtppu	8.251e+42	3.22	3.22	3.735e+40	0.184
6039	diHPCARP_I.ptppmtmpu	2.029e+43	3.82	3.82	3.364e+40	0.166
6040	diHPCARP_I.pppmpttmu	1.225e+43	3.53	3.53	3.292e+40	0.162
6041	diHPCARP_I.mmmmtppmu	5.472e+43	4.43	4.43	3.248e+40	0.16
6042	diHPCARP_I.tppppmpu	1.190e+44	4.96	4.96	2.902e+40	0.143
6043	diHPCARP_I.pttmtppu	4.036e+43	4.32	4.32	2.861e+40	0.141
6044	diHPCARP_I.tmmtppmu	5.308e+43	4.50	4.50	2.776e+40	0.137
6045	diHPCARP_I.mmmmtttmu	8.862e+43	4.81	4.81	2.772e+40	0.137
6046	diHPCARP_I.tppmptppu	1.682e+43	3.83	3.83	2.736e+40	0.135
6047	diHPCARP_I.tmmmtmpu	8.952e+43	4.83	4.83	2.691e+40	0.133
6048	diHPCARP_I.tpppmtppu	2.420e+44	5.43	5.43	2.686e+40	0.132
6049	diHPCARP_I.ptmmmttmu	7.926e+43	4.77	4.77	2.655e+40	0.131
6050	diHPCARP_I.tpppmtttu	7.626e+44	6.14	6.14	2.571e+40	0.127
6051	diHPCARP_I.tpppmtptu	1.981e+44	5.34	5.34	2.559e+40	0.126
6052	diHPCARP_I.tmtmptppu	3.644e+43	4.37	4.37	2.383e+40	0.117
6053	diHPCARP_I.mmmmtpppu	2.652e+43	4.20	4.20	2.321e+40	0.114
6054	diHPCARP_I.tppmptptu	4.142e+43	4.47	4.47	2.305e+40	0.114
6055	diHPCARP_I.tptptttmu	1.328e+44	5.20	5.20	2.148e+40	0.106
6056	diHPCARP_I.mmmmpmpu	9.100e+42	3.63	3.63	2.057e+40	0.101
6057	diHPCARP_I.tmmmtpppu	2.639e+43	4.27	4.27	2.051e+40	0.101
6058	diHPCARP_I.tppmptppu	9.567e+42	3.68	3.68	2.003e+40	0.0987
6059	diHPCARP_I.tptmmttmu	1.067e+44	5.12	5.12	1.973e+40	0.0972
6060	diHPCARP_I.pppmptppu	8.752e+42	3.64	3.64	1.964e+40	0.0968
6061	diHPCARP_I.tptpmtppu	3.257e+43	4.43	4.43	1.940e+40	0.0956
6062	diHPCARP_I.mmmmttmu	2.711e+43	4.34	4.34	1.872e+40	0.0923
6063	diHPCARP_I.mptmpttmu	7.428e+43	4.94	4.94	1.862e+40	0.0918
6064	diHPCARP_I.tppppppu	3.960e+43	4.58	4.58	1.810e+40	0.0892
6065	diHPCARP_I.mmmmtmpu	6.694e+43	4.91	4.91	1.782e+40	0.0878
6066	diHPCARP_I.mmtppppu	2.051e+43	4.24	4.24	1.669e+40	0.0822
6067	diHPCARP_I.tmmtppmu	3.308e+43	4.53	4.53	1.662e+40	0.0819
6068	diHPCARP_I.tmmppmpu	2.657e+43	4.41	4.41	1.639e+40	0.0808
6069	diHPCARP_I.tptmptppu	4.405e+44	6.08	6.08	1.634e+40	0.0805
6070	diHPCARP_I.ptmpttmu	5.607e+43	4.85	4.85	1.631e+40	0.0804
6071	diHPCARP_I.tmpmptppu	1.406e+43	4.05	4.05	1.573e+40	0.0775
6072	diHPCARP_I.tppmptppu	6.754e+43	5.00	5.00	1.537e+40	0.0757
6073	diHPCARP_I.mppmptppu	5.966e+43	4.95	4.95	1.472e+40	0.0725
6074	diHPCARP_I.pppmpmpu	5.596e+43	4.92	4.92	1.463e+40	0.0721
6075	diHPCARP_I.tmmmtppu	2.341e+43	4.40	4.40	1.458e+40	0.0718
6076	diHPCARP_I.pmtppppu	2.064e+43	4.34	4.34	1.420e+40	0.07
6077	diHPCARP_I.mtppmtppu	1.156e+43	4.02	4.02	1.352e+40	0.0666
6078	diHPCARP_I.tmtppppu	2.492e+43	4.51	4.51	1.285e+40	0.0633
6079	diHPCARP_I.pppmptppu	9.670e+42	3.95	3.95	1.279e+40	0.063
6080	diHPCARP_I.tptmptppu	9.521e+43	5.32	5.32	1.267e+40	0.0624
6081	diHPCARP_I.mmmptppu	3.135e+43	4.67	4.67	1.248e+40	0.0615
6082	diHPCARP_I.ptmptppu	5.595e+43	5.01	5.01	1.244e+40	0.0613
6083	diHPCARP_I.tmmpttmu	3.704e+43	4.77	4.77	1.234e+40	0.0608
6084	diHPCARP_I.tppmpmpu	3.195e+43	4.69	4.69	1.223e+40	0.0602
6085	diHPCARP_I.tmmtpttu	1.778e+44	5.71	5.71	1.222e+40	0.0602
6086	diHPCARP_I.tppmtppu	2.371e+43	4.52	4.52	1.216e+40	0.0599
6087	diHPCARP_I.pmtmptppu	1.876e+43	4.38	4.38	1.205e+40	0.0594
6088	diHPCARP_I.pppppmpu	3.708e+43	4.79	4.79	1.200e+40	0.0591
6089	diHPCARP_I.tmtmptppu	2.358e+43	4.52	4.52	1.197e+40	0.059
6090	diHPCARP_I.ppppmtppu	1.019e+44	5.41	5.41	1.177e+40	0.058
6091	diHPCARP_I.tmmmpmpu	1.269e+43	4.18	4.18	1.146e+40	0.0565
6092	diHPCARP_I.tppmpttmu	1.714e+44	5.74	5.74	1.127e+40	0.0555
6093	diHPCARP_I.pmmptmtu	1.675e+43	4.36	4.36	1.115e+40	0.0549
6094	diHPCARP_I.mmtmptppu	2.686e+43	4.64	4.64	1.112e+40	0.0548
6095	diHPCARP_I.mmmmttmu	4.701e+43	4.98	4.98	1.104e+40	0.0544
6096	diHPCARP_I.tppmptppu	1.737e+43	4.41	4.41	1.058e+40	0.0521

6097	diHPCARP_I.tpppttttu	6.897e+44	6.61	6.61	1.052e+40	0.0518
6098	diHPCARP_I.pptpmtmpu	1.573e+43	4.36	4.36	1.052e+40	0.0518
6099	diHPCARP_I.ptppmtmmu	1.624e+43	4.38	4.38	1.043e+40	0.0514
6100	diHPCARP_I.ttmmpptmu	5.057e+43	5.06	5.06	1.037e+40	0.0511
6101	diHPCARP_I.tmtptmpmu	4.824e+43	5.05	5.05	1.009e+40	0.0497
6102	diHPCARP_I.mmmtpmtmu	3.217e+43	4.81	4.81	1.008e+40	0.0497
6103	diHPCARP_I.ptmmppttu	1.030e+44	5.52	5.52	9.842e+39	0.0485
6104	diHPCARP_I.tptmpttptu	3.655e+43	4.90	4.90	9.810e+39	0.0483
6105	diHPCARP_I.mmmmtmtmu	4.940e+43	5.08	5.08	9.775e+39	0.0482
6106	diHPCARP_I.ptppmtptu	1.576e+43	4.42	4.42	9.563e+39	0.0471
6107	diHPCARP_I.mmmmpmtmu	6.298e+43	5.24	5.24	9.562e+39	0.0471
6108	diHPCARP_I.pttppttptu	7.995e+43	5.39	5.39	9.533e+39	0.047
6109	diHPCARP_I.tptpmtttu	2.945e+44	6.18	6.18	9.343e+39	0.046
6110	diHPCARP_I.tttmpttptu	6.592e+43	5.31	5.31	8.946e+39	0.0441
6111	diHPCARP_I.pptmpttmu	2.572e+43	4.76	4.76	8.804e+39	0.0434
6112	diHPCARP_I.pmtptttmu	2.140e+44	6.02	6.02	8.774e+39	0.0432
6113	diHPCARP_I.mmmmtmtmu	7.264e+43	5.40	5.40	8.417e+39	0.0415
6114	diHPCARP_I.pttmmttmu	1.560e+44	5.87	5.87	8.246e+39	0.0406
6115	diHPCARP_I.tpmmpmtmu	8.640e+43	5.53	5.53	8.125e+39	0.04
6116	diHPCARP_I.ptmmpptmu	1.926e+43	4.63	4.63	8.120e+39	0.04
6117	diHPCARP_I.tttpttptu	3.693e+43	5.02	5.02	8.116e+39	0.04
6118	diHPCARP_I.tttptmtmu	4.804e+43	5.18	5.18	8.074e+39	0.0398
6119	diHPCARP_I.pttmtpttu	1.445e+44	5.84	5.84	7.996e+39	0.0394
6120	diHPCARP_I.tpmmpmtptu	4.304e+43	5.13	5.13	7.912e+39	0.039
6121	diHPCARP_I.ptppmttptu	7.368e+43	5.48	5.48	7.503e+39	0.037
6122	diHPCARP_I.tmpptmtmu	5.721e+43	5.33	5.33	7.469e+39	0.0368
6123	diHPCARP_I.pmmmttptu	4.451e+43	5.19	5.19	7.360e+39	0.0363
6124	diHPCARP_I.mmpmttptu	1.260e+43	4.46	4.46	7.104e+39	0.035
6125	diHPCARP_I.tptmmtptu	9.562e+43	5.68	5.68	6.950e+39	0.0342
6126	diHPCARP_I.mtmmppttu	1.522e+43	4.59	4.59	6.916e+39	0.0341
6127	diHPCARP_I.ptppptptu	3.846e+44	6.51	6.51	6.909e+39	0.034
6128	diHPCARP_I.ptpmttptu	7.598e+43	5.57	5.57	6.622e+39	0.0326
6129	diHPCARP_I.tmmpttptu	1.257e+43	4.50	4.50	6.593e+39	0.0325
6130	diHPCARP_I.ppptmtptu	4.518e+43	5.31	5.31	6.103e+39	0.0301
6131	diHPCARP_I.mmmpttptu	1.287e+43	4.57	4.57	6.058e+39	0.0299
6132	diHPCARP_I.pmmmtpppu	1.234e+43	4.55	4.55	6.025e+39	0.0297
6133	diHPCARP_I.pttptttmu	1.353e+44	5.98	5.98	5.985e+39	0.0295
6134	diHPCARP_I.mmtptmtmu	7.279e+43	5.61	5.61	5.936e+39	0.0292
6135	diHPCARP_I.mtmmpptmu	1.448e+43	4.65	4.65	5.916e+39	0.0292
6136	diHPCARP_I.tttmptttmu	4.191e+43	5.29	5.29	5.859e+39	0.0289
6137	diHPCARP_I.ptpmtptmu	2.248e+43	4.92	4.92	5.811e+39	0.0286
6138	diHPCARP_I.tptmmtmmu	2.859e+44	6.44	6.44	5.772e+39	0.0284
6139	diHPCARP_I.tmmpttptu	1.653e+43	4.75	4.75	5.761e+39	0.0284
6140	diHPCARP_I.tmmmtmtmu	6.168e+43	5.53	5.53	5.733e+39	0.0282
6141	diHPCARP_I.tmpptmtu	6.564e+43	5.57	5.57	5.705e+39	0.0281
6142	diHPCARP_I.mppptptmu	1.691e+44	6.15	6.15	5.594e+39	0.0276
6143	diHPCARP_I.pmmmtpppu	3.253e+43	5.17	5.17	5.588e+39	0.0275
6144	diHPCARP_I.mptmpttptu	4.214e+43	5.32	5.32	5.586e+39	0.0275
6145	diHPCARP_I.pttmttptu	6.943e+43	5.63	5.63	5.538e+39	0.0273
6146	diHPCARP_I.pmmmtptmu	1.152e+43	4.56	4.56	5.495e+39	0.0271
6147	diHPCARP_I.mmpptptmu	3.035e+43	5.14	5.14	5.426e+39	0.0267
6148	diHPCARP_I.tmmpttptu	2.261e+43	4.98	4.98	5.303e+39	0.0261
6149	diHPCARP_I.pmmpttptu	2.041e+43	4.93	4.93	5.262e+39	0.0259
6150	diHPCARP_I.mmmmttptu	3.191e+43	5.19	5.19	5.261e+39	0.0259
6151	diHPCARP_I.tmmmtmtmu	3.745e+43	5.29	5.29	5.239e+39	0.0258
6152	diHPCARP_I.mmtmmpppu	4.027e+43	5.34	5.34	5.219e+39	0.0257
6153	diHPCARP_I.tpppttmmu	1.105e+44	5.95	5.95	5.107e+39	0.0252
6154	diHPCARP_I.tmtpttptu	6.457e+43	5.65	5.65	4.967e+39	0.0245
6155	diHPCARP_I.pppmptmmu	1.999e+43	4.95	4.95	4.963e+39	0.0245
6156	diHPCARP_I.pmmmpmpmu	9.864e+42	4.53	4.53	4.952e+39	0.0244
6157	diHPCARP_I.mptmmttmu	1.366e+44	6.10	6.10	4.935e+39	0.0243
6158	diHPCARP_I.mptpttptu	3.635e+43	5.31	5.31	4.915e+39	0.0242
6159	diHPCARP_I.tmmmttptu	7.951e+43	5.78	5.78	4.894e+39	0.0241
6160	diHPCARP_I.ptpmttptu	6.400e+43	5.65	5.65	4.875e+39	0.024
6161	diHPCARP_I.tmpptptmu	3.038e+43	5.22	5.22	4.817e+39	0.0237
6162	diHPCARP_I.mttmttptu	1.942e+44	6.32	6.32	4.799e+39	0.0236
6163	diHPCARP_I.tmtmpttmu	6.761e+43	5.70	5.70	4.763e+39	0.0235
6164	diHPCARP_I.pttpttmmu	1.983e+43	4.98	4.98	4.635e+39	0.0228
6165	diHPCARP_I.mmtmmpmu	1.575e+44	6.22	6.22	4.606e+39	0.0227
6166	diHPCARP_I.mtppmpmu	2.655e+43	5.17	5.17	4.576e+39	0.0225
6167	diHPCARP_I.ttpppttptu	4.375e+44	6.84	6.84	4.568e+39	0.0225
6168	diHPCARP_I.ppppttptu	2.116e+44	6.42	6.42	4.427e+39	0.0218

6169	diHPCARP_I.ttmmptmpu	4.050e+43	5.44	5.44	4.397e+39	0.0217
6170	diHPCARP_I.pmtpppppu	3.201e+43	5.31	5.31	4.302e+39	0.0212
6171	diHPCARP_I.tptmmpptu	1.813e+44	6.35	6.35	4.264e+39	0.021
6172	diHPCARP_I.tpmptmtu	3.297e+43	5.34	5.34	4.254e+39	0.021
6173	diHPCARP_I.pptmptmpu	1.460e+43	4.85	4.85	4.252e+39	0.021
6174	diHPCARP_I.mtptmptmpu	9.840e+42	4.62	4.62	4.249e+39	0.0209
6175	diHPCARP_I.pttpmtttu	1.103e+44	6.06	6.06	4.210e+39	0.0207
6176	diHPCARP_I.ttmmmtttu	4.585e+43	5.55	5.55	4.182e+39	0.0206
6177	diHPCARP_I.tmtmmpppu	1.460e+44	6.24	6.24	4.170e+39	0.0206
6178	diHPCARP_I.tptptmpu	1.023e+44	6.04	6.04	4.040e+39	0.0199
6179	diHPCARP_I.mmmptttu	2.845e+43	5.28	5.28	4.027e+39	0.0198
6180	diHPCARP_I.pptmptmpu	3.750e+43	5.45	5.45	4.004e+39	0.0197
6181	diHPCARP_I.mttmptmpu	1.911e+43	5.05	5.05	3.993e+39	0.0197
6182	diHPCARP_I.tppptmpu	8.285e+43	5.93	5.93	3.934e+39	0.0194
6183	diHPCARP_I.pmmmtttu	5.023e+43	5.64	5.64	3.929e+39	0.0194
6184	diHPCARP_I.ptptptmpu	4.729e+43	5.60	5.60	3.929e+39	0.0194
6185	diHPCARP_I.tptmtpmpu	1.233e+44	6.18	6.18	3.903e+39	0.0192
6186	diHPCARP_I.pmtmmpu	3.598e+43	5.45	5.45	3.854e+39	0.019
6187	diHPCARP_I.tmmmtttu	2.383e+43	5.21	5.21	3.826e+39	0.0189
6188	diHPCARP_I.mpmptmpu	1.221e+43	4.82	4.82	3.771e+39	0.0186
6189	diHPCARP_I.mppppppmu	5.473e+43	5.71	5.71	3.768e+39	0.0186
6190	diHPCARP_I.tttmtttu	1.237e+44	6.20	6.20	3.754e+39	0.0185
6191	diHPCARP_I.mmpptmmtu	6.034e+43	5.78	5.78	3.742e+39	0.0184
6192	diHPCARP_I.tmtmmmpu	5.070e+43	5.68	5.68	3.713e+39	0.0183
6193	diHPCARP_I.mpppppttu	9.251e+43	6.05	6.05	3.628e+39	0.0179
6194	diHPCARP_I.tptptttu	6.824e+43	5.87	5.87	3.605e+39	0.0178
6195	diHPCARP_I.pmtptttu	9.393e+43	6.06	6.06	3.601e+39	0.0177
6196	diHPCARP_I.tmmmpmttu	3.334e+43	5.45	5.45	3.595e+39	0.0177
6197	diHPCARP_I.pmtptmpu	6.650e+43	5.87	5.87	3.547e+39	0.0175
6198	diHPCARP_I.mmtmptttu	1.458e+44	6.35	6.35	3.475e+39	0.0171
6199	diHPCARP_I.tmtptptu	1.771e+44	6.47	6.47	3.409e+39	0.0168
6200	diHPCARP_I.pppppppmu	6.019e+43	5.83	5.83	3.400e+39	0.0168
6201	diHPCARP_I.mmmptmmtu	3.311e+43	5.48	5.48	3.398e+39	0.0167
6202	diHPCARP_I.mpppppttu	4.181e+44	6.99	6.99	3.383e+39	0.0167
6203	diHPCARP_I.pttpmtmpu	3.644e+43	5.54	5.54	3.381e+39	0.0167
6204	diHPCARP_I.pmtmppppu	1.897e+43	5.15	5.15	3.379e+39	0.0167
6205	diHPCARP_I.mmtmptmpu	2.380e+43	5.28	5.28	3.373e+39	0.0166
6206	diHPCARP_I.tmtmptmpu	1.634e+44	6.47	6.47	3.186e+39	0.0157
6207	diHPCARP_I.tmtmptppu	3.780e+43	5.59	5.59	3.176e+39	0.0156
6208	diHPCARP_I.mptptttu	1.268e+44	6.33	6.33	3.096e+39	0.0153
6209	diHPCARP_I.tpptmptmpu	3.203e+44	6.89	6.89	3.068e+39	0.0151
6210	diHPCARP_I.tmtmptmpu	6.149e+43	5.91	5.91	3.061e+39	0.0151
6211	diHPCARP_I.pmmptptmpu	4.150e+43	5.68	5.68	3.033e+39	0.0149
6212	diHPCARP_I.tppptttu	1.170e+44	6.30	6.30	3.024e+39	0.0149
6213	diHPCARP_I.ppppppttu	2.288e+44	6.70	6.70	3.006e+39	0.0148
6214	diHPCARP_I.tmtptttu	1.425e+44	6.43	6.43	2.958e+39	0.0146
6215	diHPCARP_I.ptpmtttu	2.803e+43	5.46	5.46	2.948e+39	0.0145
6216	diHPCARP_I.ptmmtmptu	6.177e+43	5.94	5.94	2.888e+39	0.0142
6217	diHPCARP_I.mppptttu	1.828e+45	7.98	7.98	2.832e+39	0.014
6218	diHPCARP_I.ptmmtmpu	1.521e+44	6.49	6.49	2.830e+39	0.0139
6219	diHPCARP_I.mmpptmtu	1.275e+44	6.39	6.39	2.824e+39	0.0139
6220	diHPCARP_I.pptmptttu	3.889e+43	5.68	5.68	2.820e+39	0.0139
6221	diHPCARP_I.ptptptttu	4.482e+43	5.78	5.78	2.776e+39	0.0137
6222	diHPCARP_I.pmtmptppu	3.336e+43	5.62	5.62	2.699e+39	0.0133
6223	diHPCARP_I.pppptttu	5.889e+43	5.96	5.96	2.667e+39	0.0131
6224	diHPCARP_I.mmtmptmpu	1.044e+44	6.31	6.31	2.655e+39	0.0131
6225	diHPCARP_I.tptmptptu	9.956e+43	6.29	6.29	2.624e+39	0.0129
6226	diHPCARP_I.pmtmmtttu	7.877e+43	6.15	6.15	2.605e+39	0.0128
6227	diHPCARP_I.pptmmtttu	6.092e+43	6.00	6.00	2.603e+39	0.0128
6228	diHPCARP_I.tptptttu	2.832e+43	5.54	5.54	2.591e+39	0.0128
6229	diHPCARP_I.mpppppttu	8.437e+44	7.57	7.57	2.590e+39	0.0128
6230	diHPCARP_I.pmtmptttu	2.982e+43	5.58	5.58	2.574e+39	0.0127
6231	diHPCARP_I.mppppptmpu	6.695e+43	6.07	6.07	2.553e+39	0.0126
6232	diHPCARP_I.tttmmtppu	1.247e+44	6.44	6.44	2.552e+39	0.0126
6233	diHPCARP_I.tttmmtttu	8.653e+43	6.22	6.22	2.549e+39	0.0126
6234	diHPCARP_I.tmmptmptu	9.078e+42	4.88	4.88	2.530e+39	0.0125
6235	diHPCARP_I.tttptttu	8.704e+43	6.23	6.23	2.518e+39	0.0124
6236	diHPCARP_I.tmtmmtttu	1.874e+44	6.70	6.70	2.449e+39	0.0121
6237	diHPCARP_I.ptmmtppu	4.642e+43	5.87	5.87	2.447e+39	0.0121
6238	diHPCARP_I.tmpmmtttu	7.306e+43	6.15	6.15	2.401e+39	0.0118
6239	diHPCARP_I.tmtmptmpu	2.680e+43	5.57	5.57	2.356e+39	0.0116
6240	diHPCARP_I.pmtmptmpu	1.601e+43	5.26	5.26	2.347e+39	0.0116

6241	diHPCARP_I.pmtpptppu	2.661e+43	5.57	5.57	2.344e+39	0.0115
6242	diHPCARP_I.ttptptmmu	2.204e+43	5.46	5.46	2.340e+39	0.0115
6243	diHPCARP_I.mmtptptmu	1.092e+44	6.41	6.41	2.332e+39	0.0115
6244	diHPCARP_I.mmtpptppu	3.617e+43	5.76	5.76	2.302e+39	0.0113
6245	diHPCARP_I.tpmpmttptu	7.162e+43	6.18	6.18	2.263e+39	0.0111
6246	diHPCARP_I.mmtmmtpmu	2.702e+44	6.98	6.98	2.240e+39	0.011
6247	diHPCARP_I.ptmtmtmpu	6.130e+43	6.09	6.09	2.226e+39	0.011
6248	diHPCARP_I.pmmmtmpu	1.625e+43	5.31	5.31	2.202e+39	0.0108
6249	diHPCARP_I.tpttpttmmu	1.772e+44	6.73	6.73	2.201e+39	0.0108
6250	diHPCARP_I.ttptpttptu	4.358e+43	5.91	5.91	2.175e+39	0.0107
6251	diHPCARP_I.pmmmtmmpu	4.582e+43	5.95	5.95	2.119e+39	0.0104
6252	diHPCARP_I.pttmtptmu	1.441e+44	6.65	6.65	2.071e+39	0.0102
6253	diHPCARP_I.mpppttmtu	8.027e+43	6.30	6.30	2.049e+39	0.0101
6254	diHPCARP_I.tttmtptmu	1.067e+44	6.48	6.48	2.022e+39	0.00996
6255	diHPCARP_I.mmpmpmpu	3.451e+43	5.81	5.81	2.018e+39	0.00994
6256	diHPCARP_I.ttppmtptu	5.819e+43	6.12	6.12	2.014e+39	0.00992
6257	diHPCARP_I.tmtmmtptu	1.453e+44	6.67	6.67	2.010e+39	0.00991
6258	diHPCARP_I.mpppttmmu	9.899e+43	6.44	6.44	2.008e+39	0.0099
6259	diHPCARP_I.mmmmtmmpu	1.291e+44	6.60	6.60	2.007e+39	0.00989
6260	diHPCARP_I.ptmmtptmu	8.163e+43	6.33	6.33	1.986e+39	0.00979
6261	diHPCARP_I.mptmpttptu	2.985e+43	5.73	5.73	1.985e+39	0.00978
6262	diHPCARP_I.tpppttmtu	7.550e+43	6.29	6.29	1.980e+39	0.00976
6263	diHPCARP_I.tpmpmtmmu	2.592e+43	5.66	5.66	1.957e+39	0.00964
6264	diHPCARP_I.tpmmpmpu	2.280e+43	5.59	5.59	1.943e+39	0.00957
6265	diHPCARP_I.tttmpttptu	7.399e+43	6.29	6.29	1.942e+39	0.00957
6266	diHPCARP_I.tmpmpttptu	8.737e+43	6.39	6.39	1.940e+39	0.00956
6267	diHPCARP_I.mtppppppu	4.614e+43	6.01	6.01	1.938e+39	0.00955
6268	diHPCARP_I.ptppptmmu	9.533e+43	6.44	6.44	1.935e+39	0.00953
6269	diHPCARP_I.mmtmptppu	2.407e+43	5.62	5.62	1.926e+39	0.00949
6270	diHPCARP_I.tpttttptu	5.085e+44	7.44	7.44	1.924e+39	0.00948
6271	diHPCARP_I.tmtmptppu	7.418e+43	6.30	6.30	1.901e+39	0.00937
6272	diHPCARP_I.ttptmpttptu	5.107e+43	6.08	6.08	1.894e+39	0.00933
6273	diHPCARP_I.pmpmtmmpu	3.391e+43	5.84	5.84	1.884e+39	0.00929
6274	diHPCARP_I.ptmptpmu	1.563e+43	5.38	5.38	1.879e+39	0.00926
6275	diHPCARP_I.pptpmpmpu	5.440e+43	6.13	6.13	1.861e+39	0.00917
6276	diHPCARP_I.mpppttmmu	1.545e+44	6.76	6.76	1.841e+39	0.00907
6277	diHPCARP_I.tttptptpu	5.741e+43	6.17	6.17	1.840e+39	0.00907
6278	diHPCARP_I.ptmtmtmmu	3.287e+43	5.84	5.84	1.828e+39	0.00901
6279	diHPCARP_I.mppmpmpu	2.199e+43	5.61	5.61	1.811e+39	0.00892
6280	diHPCARP_I.tmmmpmtmu	3.430e+43	5.87	5.87	1.804e+39	0.00889
6281	diHPCARP_I.mmmmtmtpu	7.629e+43	6.36	6.36	1.783e+39	0.00879
6282	diHPCARP_I.mtptmptmu	2.095e+43	5.59	5.59	1.779e+39	0.00877
6283	diHPCARP_I.mptmtpptu	1.464e+44	6.75	6.75	1.777e+39	0.00875
6284	diHPCARP_I.ttptptttu	8.467e+43	6.43	6.43	1.753e+39	0.00864
6285	diHPCARP_I.tttmmtmpu	1.051e+44	6.57	6.57	1.731e+39	0.00853
6286	diHPCARP_I.tptmptpmu	1.095e+44	6.60	6.60	1.702e+39	0.00838
6287	diHPCARP_I.pmmmtmtmu	3.232e+43	5.87	5.87	1.698e+39	0.00837
6288	diHPCARP_I.tpptmttptu	5.212e+44	7.53	7.53	1.696e+39	0.00836
6289	diHPCARP_I.mptmmtmmu	2.219e+44	7.03	7.03	1.690e+39	0.00833
6290	diHPCARP_I.tmpmmtpmu	1.203e+43	5.30	5.30	1.651e+39	0.00813
6291	diHPCARP_I.pmtmptpmu	5.140e+43	6.18	6.18	1.617e+39	0.00797
6292	diHPCARP_I.tptpmpmpu	2.041e+43	5.64	5.64	1.594e+39	0.00786
6293	diHPCARP_I.mtpptmmpu	1.649e+44	6.89	6.89	1.587e+39	0.00782
6294	diHPCARP_I.mtmmpptmu	6.752e+43	6.36	6.36	1.563e+39	0.0077
6295	diHPCARP_I.ttmmpptptu	9.612e+43	6.59	6.59	1.533e+39	0.00755
6296	diHPCARP_I.mtmmpptmu	6.622e+43	6.37	6.37	1.513e+39	0.00745
6297	diHPCARP_I.ptptptptu	1.949e+43	5.64	5.64	1.509e+39	0.00744
6298	diHPCARP_I.mmpmmtmtu	3.622e+43	6.02	6.02	1.493e+39	0.00736
6299	diHPCARP_I.tmmppptmu	1.388e+43	5.46	5.46	1.474e+39	0.00726
6300	diHPCARP_I.tmtmptptmu	5.899e+43	6.33	6.33	1.442e+39	0.0071
6301	diHPCARP_I.tmpptptptu	3.361e+44	7.37	7.37	1.426e+39	0.00703
6302	diHPCARP_I.mttptmptmu	5.676e+43	6.32	6.32	1.405e+39	0.00692
6303	diHPCARP_I.pmtmmtpmu	2.597e+44	7.23	7.23	1.403e+39	0.00692
6304	diHPCARP_I.pptpmmmpu	1.619e+43	5.58	5.58	1.400e+39	0.0069
6305	diHPCARP_I.tpptmpmpu	3.920e+44	7.48	7.48	1.384e+39	0.00682
6306	diHPCARP_I.mpmmpmtmu	1.343e+43	5.47	5.47	1.379e+39	0.0068
6307	diHPCARP_I.tmtmptptmu	1.694e+43	5.62	5.62	1.372e+39	0.00676
6308	diHPCARP_I.mptmptmptu	3.360e+43	6.03	6.03	1.357e+39	0.00669
6309	diHPCARP_I.pttmtmptmu	1.563e+44	6.95	6.95	1.356e+39	0.00668
6310	diHPCARP_I.mmpmptttu	1.912e+44	7.08	7.08	1.331e+39	0.00656
6311	diHPCARP_I.tttptmptmu	1.141e+44	6.77	6.77	1.327e+39	0.00654
6312	diHPCARP_I.mmtmmpmtmu	9.027e+43	6.64	6.64	1.319e+39	0.0065

6313	diHPCARP_I.mttptmpu	3.627e+43	6.10	6.10	1.315e+39	0.00648
6314	diHPCARP_I.mtpttptmu	3.355e+43	6.05	6.05	1.314e+39	0.00647
6315	diHPCARP_I.tpptmtttu	5.475e+44	7.72	7.72	1.310e+39	0.00645
6316	diHPCARP_I.ttmptttu	7.242e+43	6.52	6.52	1.289e+39	0.00635
6317	diHPCARP_I.mtppttmpu	2.273e+43	5.83	5.83	1.279e+39	0.0063
6318	diHPCARP_I.mmmptmpu	1.184e+43	5.45	5.45	1.263e+39	0.00622
6319	diHPCARP_I.tppttptu	4.513e+44	7.62	7.62	1.258e+39	0.0062
6320	diHPCARP_I.pmppttptmu	3.153e+43	6.05	6.05	1.235e+39	0.00609
6321	diHPCARP_I.mptmtttmu	1.943e+44	7.13	7.13	1.235e+39	0.00609
6322	diHPCARP_I.mmtptttmu	1.954e+44	7.14	7.14	1.234e+39	0.00608
6323	diHPCARP_I.tttptttu	1.008e+44	6.74	6.74	1.232e+39	0.00607
6324	diHPCARP_I.tptpttptmu	3.866e+43	6.18	6.18	1.220e+39	0.00601
6325	diHPCARP_I.ppptmmmpu	4.545e+43	6.28	6.28	1.212e+39	0.00597
6326	diHPCARP_I.mmmptmpu	8.005e+42	5.26	5.26	1.181e+39	0.00582
6327	diHPCARP_I.mptmtttu	3.663e+44	7.56	7.56	1.146e+39	0.00565
6328	diHPCARP_I.ppmptttu	5.430e+43	6.42	6.42	1.138e+39	0.00561
6329	diHPCARP_I.pttpttptmu	2.006e+44	7.21	7.21	1.125e+39	0.00555
6330	diHPCARP_I.pmpmmmpu	7.025e+42	5.21	5.21	1.116e+39	0.0055
6331	diHPCARP_I.pmmptttu	4.120e+43	6.28	6.28	1.101e+39	0.00543
6332	diHPCARP_I.mmtptttu	8.174e+43	6.69	6.69	1.094e+39	0.00539
6333	diHPCARP_I.ptmtmptu	2.503e+43	5.99	5.99	1.085e+39	0.00535
6334	diHPCARP_I.mmpptttu	1.175e+44	6.91	6.91	1.082e+39	0.00533
6335	diHPCARP_I.tptmtttu	1.801e+44	7.17	7.17	1.080e+39	0.00532
6336	diHPCARP_I.ttpttptu	2.580e+43	6.02	6.02	1.063e+39	0.00524
6337	diHPCARP_I.pttptttu	2.254e+44	7.32	7.32	1.055e+39	0.0052
6338	diHPCARP_I.tmtttttu	1.477e+44	7.07	7.07	1.045e+39	0.00515
6339	diHPCARP_I.tpmmtttu	1.135e+44	6.91	6.91	1.044e+39	0.00514
6340	diHPCARP_I.tmtmptmu	1.298e+44	7.00	7.00	1.040e+39	0.00513
6341	diHPCARP_I.pmmptttu	7.614e+43	6.68	6.68	1.039e+39	0.00512
6342	diHPCARP_I.pmpptttu	9.510e+43	6.81	6.81	1.036e+39	0.0051
6343	diHPCARP_I.pptptttu	1.049e+44	6.87	6.87	1.031e+39	0.00508
6344	diHPCARP_I.tppptttu	1.733e+44	7.18	7.18	1.023e+39	0.00504
6345	diHPCARP_I.mmmptttu	3.306e+43	6.21	6.21	9.949e+38	0.0049
6346	diHPCARP_I.pttmtttu	2.387e+44	7.40	7.40	9.761e+38	0.00481
6347	diHPCARP_I.pttptttu	1.031e+44	6.91	6.91	9.589e+38	0.00473
6348	diHPCARP_I.tppptttu	2.839e+44	7.52	7.52	9.484e+38	0.00467
6349	diHPCARP_I.mmtmptttu	2.117e+43	5.98	5.98	9.358e+38	0.00461
6350	diHPCARP_I.tppptttu	4.996e+44	7.87	7.87	9.278e+38	0.00457
6351	diHPCARP_I.tpmptttu	1.819e+43	5.89	5.89	9.254e+38	0.00456
6352	diHPCARP_I.tpmptttu	2.796e+43	6.15	6.15	9.204e+38	0.00454
6353	diHPCARP_I.mttmptttu	5.281e+43	6.53	6.53	9.170e+38	0.00452
6354	diHPCARP_I.mptmptttu	1.344e+44	7.10	7.10	9.103e+38	0.00449
6355	diHPCARP_I.ptmmptttu	1.999e+44	7.33	7.33	9.066e+38	0.00447
6356	diHPCARP_I.ttpmptttu	1.577e+43	5.83	5.83	8.942e+38	0.00441
6357	diHPCARP_I.mptmptttu	1.935e+43	5.95	5.95	8.923e+38	0.0044
6358	diHPCARP_I.tptmptttu	5.057e+43	6.53	6.53	8.869e+38	0.00437
6359	diHPCARP_I.mtppmptttu	1.623e+44	7.24	7.24	8.691e+38	0.00428
6360	diHPCARP_I.mtmptttu	4.922e+43	6.53	6.53	8.668e+38	0.00427
6361	diHPCARP_I.mptmptttu	3.797e+43	6.37	6.37	8.652e+38	0.00426
6362	diHPCARP_I.ptmptttu	1.567e+44	7.22	7.22	8.599e+38	0.00424
6363	diHPCARP_I.tptmptttu	2.426e+44	7.48	7.48	8.577e+38	0.00423
6364	diHPCARP_I.tmtmptttu	7.656e+43	6.80	6.80	8.573e+38	0.00422
6365	diHPCARP_I.mmtppptttu	1.027e+44	6.97	6.97	8.549e+38	0.00421
6366	diHPCARP_I.mmtttttu	7.025e+44	8.13	8.13	8.449e+38	0.00416
6367	diHPCARP_I.pptmptttu	1.145e+44	7.04	7.04	8.444e+38	0.00416
6368	diHPCARP_I.ptmmptttu	2.123e+44	7.42	7.42	8.343e+38	0.00411
6369	diHPCARP_I.tppmptttu	4.962e+43	6.56	6.56	8.282e+38	0.00408
6370	diHPCARP_I.ptmptttu	1.010e+44	6.98	6.98	8.264e+38	0.00407
6371	diHPCARP_I.ttmptttu	1.915e+43	5.99	5.99	8.241e+38	0.00406
6372	diHPCARP_I.ppmptttu	2.200e+43	6.08	6.08	8.155e+38	0.00402
6373	diHPCARP_I.pmtppptttu	4.494e+43	6.51	6.51	8.134e+38	0.00401
6374	diHPCARP_I.mmpmptttu	1.221e+44	7.11	7.11	8.029e+38	0.00396
6375	diHPCARP_I.mmpmptttu	1.510e+43	5.87	5.87	7.930e+38	0.00391
6376	diHPCARP_I.mmtmptttu	3.676e+43	6.41	6.41	7.870e+38	0.00388
6377	diHPCARP_I.mttmptttu	7.538e+44	8.21	8.21	7.869e+38	0.00388
6378	diHPCARP_I.tmpmptttu	4.088e+43	6.48	6.48	7.777e+38	0.00383
6379	diHPCARP_I.ttmppptttu	1.993e+43	6.05	6.05	7.746e+38	0.00382
6380	diHPCARP_I.tptptttu	1.842e+44	7.38	7.38	7.734e+38	0.00381
6381	diHPCARP_I.ptmtmptttu	4.834e+43	6.60	6.60	7.581e+38	0.00374
6382	diHPCARP_I.pmtmptttu	8.471e+43	6.93	6.93	7.579e+38	0.00373
6383	diHPCARP_I.ppptmptttu	5.102e+44	8.00	8.00	7.561e+38	0.00373
6384	diHPCARP_I.tmtmptttu	2.584e+44	7.60	7.60	7.526e+38	0.00371

6385	diHPCARP_I.tmmptmpu	1.304e+43	5.82	5.82	7.450e+38	0.00367
6386	diHPCARP_I.pttpmtmmu	9.235e+43	7.00	7.00	7.402e+38	0.00365
6387	diHPCARP_I.ptmtptmpu	2.315e+44	7.54	7.54	7.390e+38	0.00364
6388	diHPCARP_I.mmpmppptu	8.758e+43	6.97	6.97	7.364e+38	0.00363
6389	diHPCARP_I.pppptmmu	9.420e+43	7.01	7.01	7.310e+38	0.0036
6390	diHPCARP_I.mmmmttttu	6.842e+44	8.20	8.20	7.294e+38	0.00359
6391	diHPCARP_I.ptptptttu	4.403e+43	6.56	6.56	7.284e+38	0.00359
6392	diHPCARP_I.tttptmpu	3.243e+43	6.39	6.39	7.185e+38	0.00354
6393	diHPCARP_I.ttpptmmu	9.048e+43	7.01	7.01	7.103e+38	0.0035
6394	diHPCARP_I.ttpptmmu	9.026e+43	7.01	7.01	7.079e+38	0.00349
6395	diHPCARP_I.ptmppptpu	1.217e+44	7.20	7.20	6.969e+38	0.00343
6396	diHPCARP_I.ttpptmpu	2.717e+44	7.68	7.68	6.956e+38	0.00343
6397	diHPCARP_I.tpmmtmpu	5.359e+43	6.72	6.72	6.785e+38	0.00334
6398	diHPCARP_I.mmtmtttu	1.895e+44	7.48	7.48	6.774e+38	0.00334
6399	diHPCARP_I.ptpmtmpu	4.136e+43	6.57	6.57	6.722e+38	0.00331
6400	diHPCARP_I.tpmtmpu	6.400e+43	6.84	6.84	6.708e+38	0.00331
6401	diHPCARP_I.mttmtmpu	1.549e+44	7.37	7.37	6.653e+38	0.00328
6402	diHPCARP_I.mttmtmpu	1.812e+44	7.47	7.47	6.534e+38	0.00322
6403	diHPCARP_I.ttmppmpu	3.881e+44	7.93	7.93	6.471e+38	0.00319
6404	diHPCARP_I.tptmtmpu	3.990e+43	6.58	6.58	6.380e+38	0.00314
6405	diHPCARP_I.pmtmtmmu	1.731e+44	7.46	7.46	6.323e+38	0.00312
6406	diHPCARP_I.mmmppppu	2.611e+43	6.34	6.34	6.266e+38	0.00309
6407	diHPCARP_I.tppttmpu	1.959e+44	7.55	7.55	6.239e+38	0.00307
6408	diHPCARP_I.mttmtmpu	7.281e+43	6.98	6.98	6.039e+38	0.00298
6409	diHPCARP_I.mmtppppu	1.755e+44	7.50	7.50	6.001e+38	0.00296
6410	diHPCARP_I.mptmpmpu	2.179e+43	6.26	6.26	5.965e+38	0.00294
6411	diHPCARP_I.ttpptptu	1.981e+44	7.58	7.58	5.914e+38	0.00291
6412	diHPCARP_I.mtppmpu	1.159e+44	7.27	7.27	5.837e+38	0.00288
6413	diHPCARP_I.mmtptmpu	7.294e+43	7.00	7.00	5.817e+38	0.00287
6414	diHPCARP_I.tmtmtmpu	4.288e+43	6.68	6.68	5.812e+38	0.00286
6415	diHPCARP_I.ptppmttu	2.830e+43	6.43	6.43	5.809e+38	0.00286
6416	diHPCARP_I.ppmptmpu	1.115e+43	5.88	5.88	5.777e+38	0.00285
6417	diHPCARP_I.ttpptttu	4.582e+44	8.10	8.10	5.771e+38	0.00284
6418	diHPCARP_I.ppmppmpu	2.455e+43	6.36	6.36	5.754e+38	0.00284
6419	diHPCARP_I.tpmtptmpu	1.180e+44	7.29	7.29	5.749e+38	0.00283
6420	diHPCARP_I.ttpppmpu	7.459e+43	7.02	7.02	5.746e+38	0.00283
6421	diHPCARP_I.tppmmtmpu	7.750e+43	7.04	7.04	5.723e+38	0.00282
6422	diHPCARP_I.ptmtttu	5.968e+43	6.89	6.89	5.716e+38	0.00282
6423	diHPCARP_I.mmtmtmpu	5.292e+43	6.82	6.82	5.667e+38	0.00279
6424	diHPCARP_I.ttpmtmmu	1.327e+44	7.37	7.37	5.653e+38	0.00279
6425	diHPCARP_I.mmmppmpu	1.086e+43	5.88	5.88	5.649e+38	0.00278
6426	diHPCARP_I.ttpmtmpu	8.875e+43	7.14	7.14	5.624e+38	0.00277
6427	diHPCARP_I.tmmptttu	5.998e+44	8.29	8.29	5.513e+38	0.00272
6428	diHPCARP_I.tmmppmmtu	3.634e+43	6.62	6.62	5.426e+38	0.00267
6429	diHPCARP_I.ttmmtmpu	7.371e+43	7.06	7.06	5.343e+38	0.00263
6430	diHPCARP_I.pppptmpu	9.274e+43	7.19	7.19	5.334e+38	0.00263
6431	diHPCARP_I.mptmmmpu	1.225e+44	7.37	7.37	5.231e+38	0.00258
6432	diHPCARP_I.ttmptmmu	2.224e+44	7.74	7.74	5.131e+38	0.00253
6433	diHPCARP_I.pmtmpppu	3.937e+43	6.71	6.71	5.125e+38	0.00253
6434	diHPCARP_I.tpmtmpu	6.226e+43	6.98	6.98	5.107e+38	0.00252
6435	diHPCARP_I.ttpmtptu	3.512e+44	8.01	8.01	5.107e+38	0.00252
6436	diHPCARP_I.ptmtmmu	3.035e+44	7.93	7.93	5.088e+38	0.00251
6437	diHPCARP_I.mptmtmpu	6.441e+44	8.39	8.39	5.017e+38	0.00247
6438	diHPCARP_I.pmpptmpu	4.294e+43	6.78	6.78	4.920e+38	0.00242
6439	diHPCARP_I.ptmtttu	1.352e+44	7.48	7.48	4.841e+38	0.00239
6440	diHPCARP_I.ptpmmttu	6.553e+43	7.05	7.05	4.829e+38	0.00238
6441	diHPCARP_I.tmmptttu	2.292e+44	7.79	7.79	4.819e+38	0.00237
6442	diHPCARP_I.pppmmtmpu	8.745e+43	7.22	7.22	4.812e+38	0.00237
6443	diHPCARP_I.mptmtmpu	4.159e+43	6.78	6.78	4.802e+38	0.00237
6444	diHPCARP_I.tpmppmpu	3.229e+43	6.63	6.63	4.751e+38	0.00234
6445	diHPCARP_I.tptmpmpu	2.561e+43	6.51	6.51	4.602e+38	0.00227
6446	diHPCARP_I.mttmtmpu	2.956e+43	6.60	6.60	4.593e+38	0.00226
6447	diHPCARP_I.mptmtmpu	4.348e+43	6.83	6.83	4.585e+38	0.00226
6448	diHPCARP_I.pppptmpu	4.893e+43	6.91	6.91	4.557e+38	0.00225
6449	diHPCARP_I.pmmtmmpu	9.235e+43	7.29	7.29	4.554e+38	0.00224
6450	diHPCARP_I.mmpmtmpu	5.678e+43	7.00	7.00	4.536e+38	0.00224
6451	diHPCARP_I.mmmptmpu	1.600e+43	6.24	6.24	4.531e+38	0.00223
6452	diHPCARP_I.ppmptttu	7.968e+43	7.20	7.20	4.530e+38	0.00223
6453	diHPCARP_I.mmmttttu	2.125e+44	7.79	7.79	4.526e+38	0.00223
6454	diHPCARP_I.ptmtmpu	7.820e+43	7.19	7.19	4.523e+38	0.00223
6455	diHPCARP_I.tttmtmpu	1.353e+44	7.53	7.53	4.440e+38	0.00219
6456	diHPCARP_I.tmmppppu	1.987e+43	6.38	6.38	4.437e+38	0.00219

6457	diHPCARP_I.ttttptppu	2.206e+44	7.82	7.82	4.426e+38	0.00218
6458	diHPCARP_I.ttppmpmmu	4.684e+43	6.90	6.90	4.385e+38	0.00216
6459	diHPCARP_I.pmmmtmtpu	9.225e+42	5.94	5.94	4.342e+38	0.00214
6460	diHPCARP_I.pttmppppu	8.190e+43	7.24	7.24	4.332e+38	0.00213
6461	diHPCARP_I.pppmtpmpu	2.365e+43	6.51	6.51	4.315e+38	0.00213
6462	diHPCARP_I.tppnmtpu	1.659e+44	7.67	7.67	4.307e+38	0.00212
6463	diHPCARP_I.ptmpptttu	1.567e+44	7.64	7.64	4.296e+38	0.00212
6464	diHPCARP_I.tmttppppu	1.659e+44	7.67	7.67	4.263e+38	0.0021
6465	diHPCARP_I.pppptmmu	1.094e+44	7.43	7.43	4.216e+38	0.00208
6466	diHPCARP_I.pptmpmpu	1.191e+43	6.12	6.12	4.157e+38	0.00205
6467	diHPCARP_I.pppmtpmpu	6.639e+43	7.14	7.14	4.154e+38	0.00205
6468	diHPCARP_I.tppmmpmpu	3.901e+43	6.83	6.83	4.152e+38	0.00205
6469	diHPCARP_I.mtmmpmtu	9.523e+43	7.36	7.36	4.125e+38	0.00203
6470	diHPCARP_I.ptmpptmpu	7.301e+43	7.21	7.21	4.114e+38	0.00203
6471	diHPCARP_I.mpttpttu	1.770e+44	7.74	7.74	4.040e+38	0.00199
6472	diHPCARP_I.ptmtmtpu	1.180e+44	7.52	7.52	3.955e+38	0.00195
6473	diHPCARP_I.ttpmptptu	3.773e+43	6.84	6.84	3.938e+38	0.00194
6474	diHPCARP_I.mmmtpttu	5.670e+44	8.46	8.46	3.890e+38	0.00192
6475	diHPCARP_I.mmmmtttu	2.884e+44	8.06	8.06	3.882e+38	0.00191
6476	diHPCARP_I.mppmtmpu	1.035e+44	7.45	7.45	3.876e+38	0.00191
6477	diHPCARP_I.tmttppppu	9.433e+43	7.40	7.40	3.847e+38	0.0019
6478	diHPCARP_I.mtmmtttu	9.019e+43	7.37	7.37	3.826e+38	0.00189
6479	diHPCARP_I.tmttpttu	2.153e+44	7.91	7.91	3.730e+38	0.00184
6480	diHPCARP_I.tpptptmpu	1.145e+44	7.54	7.54	3.710e+38	0.00183
6481	diHPCARP_I.mppppmpu	9.120e+43	7.40	7.40	3.691e+38	0.00182
6482	diHPCARP_I.ttttpttu	1.481e+44	7.70	7.70	3.646e+38	0.0018
6483	diHPCARP_I.tmmmpmtu	3.051e+43	6.76	6.76	3.627e+38	0.00179
6484	diHPCARP_I.tpptppppu	8.148e+43	7.35	7.35	3.612e+38	0.00178
6485	diHPCARP_I.ppptptmpu	1.815e+44	7.83	7.83	3.598e+38	0.00177
6486	diHPCARP_I.tppmppppu	1.483e+43	6.35	6.35	3.537e+38	0.00174
6487	diHPCARP_I.tttmtmpu	5.456e+43	7.13	7.13	3.511e+38	0.00173
6488	diHPCARP_I.pmmmtmtu	1.892e+43	6.50	6.50	3.494e+38	0.00172
6489	diHPCARP_I.mppmtmpu	2.319e+44	8.00	8.00	3.448e+38	0.0017
6490	diHPCARP_I.pptmpmpu	3.604e+43	6.89	6.89	3.448e+38	0.0017
6491	diHPCARP_I.tttmtmtu	6.198e+43	7.23	7.23	3.347e+38	0.00165
6492	diHPCARP_I.tmmtppppu	5.847e+43	7.20	7.20	3.343e+38	0.00165
6493	diHPCARP_I.pmpmtppu	1.140e+43	6.23	6.23	3.303e+38	0.00163
6494	diHPCARP_I.pmpptmpu	5.765e+43	7.20	7.20	3.287e+38	0.00162
6495	diHPCARP_I.tppmmttu	1.455e+44	7.75	7.75	3.264e+38	0.00161
6496	diHPCARP_I.tmpmtttu	4.763e+43	7.09	7.09	3.261e+38	0.00161
6497	diHPCARP_I.ptptmttu	3.583e+44	8.30	8.30	3.236e+38	0.00159
6498	diHPCARP_I.mmttpppu	2.689e+44	8.14	8.14	3.177e+38	0.00157
6499	diHPCARP_I.pmtmptmpu	2.223e+43	6.66	6.66	3.136e+38	0.00155
6500	diHPCARP_I.ptmtpttu	5.744e+44	8.60	8.60	3.112e+38	0.00153
6501	diHPCARP_I.mppmtttu	1.002e+45	8.93	8.93	3.110e+38	0.00153
6502	diHPCARP_I.mmtptttu	5.069e+44	8.54	8.54	3.070e+38	0.00151
6503	diHPCARP_I.mppptmpu	4.290e+44	8.45	8.45	3.023e+38	0.00149
6504	diHPCARP_I.mpmmtppu	2.784e+43	6.82	6.82	3.002e+38	0.00148
6505	diHPCARP_I.mttptppu	6.962e+43	7.37	7.37	2.987e+38	0.00147
6506	diHPCARP_I.tmpmpttu	5.122e+43	7.19	7.19	2.982e+38	0.00147
6507	diHPCARP_I.ptttmttu	2.221e+44	8.06	8.06	2.980e+38	0.00147
6508	diHPCARP_I.ptptmtmpu	2.917e+44	8.22	8.22	2.976e+38	0.00147
6509	diHPCARP_I.mmtmtmpu	2.495e+44	8.14	8.14	2.945e+38	0.00145
6510	diHPCARP_I.mmmppmtu	6.495e+43	7.34	7.34	2.942e+38	0.00145
6511	diHPCARP_I.pmmtptppu	6.882e+43	7.38	7.38	2.915e+38	0.00144
6512	diHPCARP_I.mttmmtmpu	1.330e+44	7.77	7.77	2.907e+38	0.00143
6513	diHPCARP_I.mtptttmpu	1.393e+44	7.80	7.80	2.903e+38	0.00143
6514	diHPCARP_I.tppmmttu	4.983e+43	7.19	7.19	2.871e+38	0.00141
6515	diHPCARP_I.mpmmttptu	1.888e+43	6.62	6.62	2.854e+38	0.00141
6516	diHPCARP_I.tmtptttu	1.386e+44	7.81	7.81	2.847e+38	0.0014
6517	diHPCARP_I.tptmtmtu	2.635e+44	8.19	8.19	2.829e+38	0.00139
6518	diHPCARP_I.mmpmpmpu	4.358e+43	7.12	7.12	2.811e+38	0.00139
6519	diHPCARP_I.tptppmpu	1.505e+45	9.24	9.24	2.800e+38	0.00138
6520	diHPCARP_I.mtptmpmpu	5.542e+43	7.27	7.27	2.793e+38	0.00138
6521	diHPCARP_I.mtpptttu	4.792e+44	8.57	8.57	2.747e+38	0.00135
6522	diHPCARP_I.tppmmpmpu	8.014e+43	7.51	7.51	2.724e+38	0.00134
6523	diHPCARP_I.pmmpppppu	1.817e+43	6.62	6.62	2.714e+38	0.00134
6524	diHPCARP_I.tmtptmpu	3.135e+44	8.33	8.33	2.696e+38	0.00133
6525	diHPCARP_I.tpptptmmu	1.214e+44	7.76	7.76	2.685e+38	0.00132
6526	diHPCARP_I.mtptmmpu	1.232e+44	7.77	7.77	2.684e+38	0.00132
6527	diHPCARP_I.pmtmmtppu	5.664e+43	7.31	7.31	2.666e+38	0.00131
6528	diHPCARP_I.pmmmtmpu	1.575e+43	6.56	6.56	2.640e+38	0.0013

6529	diHPCARP_I.ppttpttmu	9.399e+43	7.62	7.62	2.628e+38	0.0013
6530	diHPCARP_I.pptmtppmu	1.902e+44	8.04	8.04	2.628e+38	0.00129
6531	diHPCARP_I.tmtppmpmu	1.515e+44	7.91	7.91	2.627e+38	0.00129
6532	diHPCARP_I.mptmptpmu	7.017e+43	7.45	7.45	2.622e+38	0.00129
6533	diHPCARP_I.ppttmtmpu	6.611e+43	7.42	7.42	2.613e+38	0.00129
6534	diHPCARP_I.mptpmtpmu	6.742e+43	7.43	7.43	2.609e+38	0.00129
6535	diHPCARP_I.mmtptmttu	3.191e+44	8.36	8.36	2.599e+38	0.00128
6536	diHPCARP_I.pmptptpmu	2.399e+43	6.82	6.82	2.592e+38	0.00128
6537	diHPCARP_I.tpmptpmu	2.380e+43	6.81	6.81	2.585e+38	0.00127
6538	diHPCARP_I.tmttpttmu	2.834e+44	8.30	8.30	2.563e+38	0.00126
6539	diHPCARP_I.pmtmmmtmu	9.243e+43	7.63	7.63	2.556e+38	0.00126
6540	diHPCARP_I.ttmtmmttu	5.663e+43	7.34	7.34	2.537e+38	0.00125
6541	diHPCARP_I.tpmmmmtmpu	4.543e+43	7.21	7.21	2.522e+38	0.00124
6542	diHPCARP_I.tmpmppptu	7.205e+43	7.49	7.49	2.514e+38	0.00124
6543	diHPCARP_I.mmtmtmtu	1.172e+45	9.16	9.16	2.508e+38	0.00124
6544	diHPCARP_I.mmmpttttu	2.227e+44	8.17	8.17	2.500e+38	0.00123
6545	diHPCARP_I.mpptpttpu	7.706e+44	8.91	8.91	2.491e+38	0.00123
6546	diHPCARP_I.mmtmmpmmu	5.113e+44	8.67	8.67	2.483e+38	0.00122
6547	diHPCARP_I.mtmmpptpu	1.210e+44	7.81	7.81	2.467e+38	0.00122
6548	diHPCARP_I.mtptmtpmu	2.795e+43	6.94	6.94	2.454e+38	0.00121
6549	diHPCARP_I.pptpmtpmu	3.602e+43	7.09	7.09	2.452e+38	0.00121
6550	diHPCARP_I.mttmpttmu	5.226e+43	7.31	7.31	2.451e+38	0.00121
6551	diHPCARP_I.mptpmmpmu	5.584e+43	7.37	7.37	2.401e+38	0.00118
6552	diHPCARP_I.mtmmpmmu	1.035e+44	7.74	7.74	2.374e+38	0.00117
6553	diHPCARP_I.mpptmtttu	1.242e+45	9.23	9.23	2.360e+38	0.00116
6554	diHPCARP_I.pmppttmu	6.331e+43	7.46	7.46	2.337e+38	0.00115
6555	diHPCARP_I.ttmtmmpu	4.417e+43	7.25	7.25	2.325e+38	0.00115
6556	diHPCARP_I.ttmtmtpmu	5.085e+43	7.33	7.33	2.315e+38	0.00114
6557	diHPCARP_I.tmtmmtmmu	2.345e+44	8.25	8.25	2.307e+38	0.00114
6558	diHPCARP_I.ptpmtptpu	1.760e+44	8.08	8.08	2.289e+38	0.00113
6559	diHPCARP_I.ttptmtmtu	4.361e+43	7.25	7.25	2.269e+38	0.00112
6560	diHPCARP_I.ptppmpmmu	1.594e+43	6.66	6.66	2.254e+38	0.00111
6561	diHPCARP_I.pttmtmtu	1.023e+44	7.77	7.77	2.247e+38	0.00111
6562	diHPCARP_I.tptpttmu	6.459e+44	8.87	8.87	2.232e+38	0.0011
6563	diHPCARP_I.ppptmttmu	3.663e+44	8.54	8.54	2.201e+38	0.00108
6564	diHPCARP_I.mpptmtmmu	1.851e+44	8.13	8.13	2.198e+38	0.00108
6565	diHPCARP_I.tttmmpmtu	4.754e+44	8.70	8.70	2.189e+38	0.00108
6566	diHPCARP_I.ppptmtttu	5.278e+44	8.76	8.76	2.177e+38	0.00107
6567	diHPCARP_I.mmttpttmu	2.131e+44	8.22	8.22	2.174e+38	0.00107
6568	diHPCARP_I.ttmmpptmu	3.217e+43	7.10	7.10	2.150e+38	0.00106
6569	diHPCARP_I.mptmtppu	5.507e+44	8.80	8.80	2.124e+38	0.00105
6570	diHPCARP_I.mtmmtmpu	8.275e+43	7.68	7.68	2.105e+38	0.00104
6571	diHPCARP_I.mptmpmtu	5.465e+43	7.43	7.43	2.104e+38	0.00104
6572	diHPCARP_I.tptmtptmu	3.313e+44	8.51	8.51	2.095e+38	0.00103
6573	diHPCARP_I.tmpptmtu	1.460e+44	8.04	8.04	2.016e+38	0.000994
6574	diHPCARP_I.pmttpttmu	1.340e+44	7.99	7.99	2.012e+38	0.000991
6575	diHPCARP_I.mtmtmtmpu	9.125e+43	7.77	7.77	1.993e+38	0.000982
6576	diHPCARP_I.ptptmtttu	6.738e+44	8.96	8.96	1.992e+38	0.000982
6577	diHPCARP_I.ptmtpttmu	2.201e+44	8.30	8.30	1.990e+38	0.00098
6578	diHPCARP_I.tptmpmtmu	3.730e+43	7.24	7.24	1.989e+38	0.00098
6579	diHPCARP_I.ttptttmpu	2.910e+44	8.47	8.47	1.979e+38	0.000975
6580	diHPCARP_I.mmttptppu	1.011e+44	7.84	7.84	1.972e+38	0.000971
6581	diHPCARP_I.tppmmtttu	2.133e+44	8.28	8.28	1.969e+38	0.00097
6582	diHPCARP_I.ptptmmpu	3.629e+44	8.61	8.61	1.947e+38	0.000959
6583	diHPCARP_I.pmtmtpmu	1.812e+44	8.20	8.20	1.939e+38	0.000956
6584	diHPCARP_I.tttmtmpu	1.183e+44	7.94	7.94	1.931e+38	0.000952
6585	diHPCARP_I.pptmptppu	2.451e+43	7.01	7.01	1.924e+38	0.000948
6586	diHPCARP_I.mmmmpmtpu	8.603e+43	7.76	7.76	1.918e+38	0.000945
6587	diHPCARP_I.tmpmpttmu	8.670e+43	7.77	7.77	1.900e+38	0.000936
6588	diHPCARP_I.tptmptmmu	5.126e+43	7.46	7.46	1.889e+38	0.000931
6589	diHPCARP_I.tptmpmpu	1.178e+44	7.97	7.97	1.844e+38	0.000909
6590	diHPCARP_I.ptptmtmmu	1.061e+44	7.91	7.91	1.841e+38	0.000907
6591	diHPCARP_I.mppptptpu	6.337e+43	7.61	7.61	1.823e+38	0.000898
6592	diHPCARP_I.mpttptppu	2.586e+44	8.45	8.45	1.805e+38	0.00089
6593	diHPCARP_I.pmmtptmpu	3.527e+43	7.27	7.27	1.795e+38	0.000885
6594	diHPCARP_I.tpmttmmu	1.052e+44	7.92	7.92	1.792e+38	0.000883
6595	diHPCARP_I.ptttmtpu	1.380e+44	8.09	8.09	1.772e+38	0.000873
6596	diHPCARP_I.tttmtmpu	1.753e+44	8.23	8.23	1.772e+38	0.000873
6597	diHPCARP_I.mptptmtmu	1.667e+44	8.21	8.21	1.743e+38	0.000859
6598	diHPCARP_I.pppmpmpu	2.039e+43	6.96	6.96	1.734e+38	0.000855
6599	diHPCARP_I.tttmmtmpu	1.835e+44	8.27	8.27	1.734e+38	0.000855
6600	diHPCARP_I.mptmtmpu	3.321e+44	8.62	8.62	1.732e+38	0.000854

6601	diHPCARP_I.tmtmmpmmu	3.361e+44	8.63	8.63	1.729e+38	0.000852
6602	diHPCARP_I.mpptptmpu	1.051e+44	7.95	7.95	1.709e+38	0.000842
6603	diHPCARP_I.tmtptptmpu	4.434e+43	7.43	7.43	1.708e+38	0.000842
6604	diHPCARP_I.mtptpttpu	7.391e+43	7.74	7.74	1.706e+38	0.000841
6605	diHPCARP_I.tmttptppu	1.166e+44	8.02	8.02	1.666e+38	0.000821
6606	diHPCARP_I.mmpptmmu	1.432e+44	8.15	8.15	1.666e+38	0.000821
6607	diHPCARP_I.tmtptmpu	1.571e+44	8.21	8.21	1.643e+38	0.00081
6608	diHPCARP_I.mmttttppu	4.589e+44	8.85	8.85	1.629e+38	0.000803
6609	diHPCARP_I.tmtmttppu	6.196e+43	7.66	7.66	1.624e+38	0.0008
6610	diHPCARP_I.pppttttppu	3.886e+44	8.76	8.76	1.623e+38	0.0008
6611	diHPCARP_I.ppptpttpu	2.976e+44	8.60	8.60	1.613e+38	0.000795
6612	diHPCARP_I.mptmppppmu	3.532e+43	7.34	7.34	1.597e+38	0.000787
6613	diHPCARP_I.pptmpmtmu	2.961e+43	7.24	7.24	1.581e+38	0.000779
6614	diHPCARP_I.ttptmtttu	8.082e+44	9.21	9.21	1.576e+38	0.000777
6615	diHPCARP_I.mptmtttu	1.733e+44	8.30	8.30	1.570e+38	0.000774
6616	diHPCARP_I.tptmmpmpu	2.967e+43	7.25	7.25	1.559e+38	0.000768
6617	diHPCARP_I.tpmtttttu	5.167e+44	8.95	8.95	1.551e+38	0.000764
6618	diHPCARP_I.mpptppppmu	2.247e+43	7.09	7.09	1.534e+38	0.000756
6619	diHPCARP_I.tmtmptttu	1.064e+44	8.02	8.02	1.518e+38	0.000748
6620	diHPCARP_I.tmpmtttppu	5.339e+43	7.62	7.62	1.503e+38	0.000741
6621	diHPCARP_I.mtppppmpu	6.894e+43	7.78	7.78	1.483e+38	0.000731
6622	diHPCARP_I.tttpttpu	1.055e+44	8.05	8.05	1.444e+38	0.000711
6623	diHPCARP_I.tppppmtmu	8.337e+44	9.28	9.28	1.443e+38	0.000711
6624	diHPCARP_I.mmmmpmpu	3.210e+43	7.34	7.34	1.439e+38	0.000709
6625	diHPCARP_I.tttmmtppu	6.745e+43	7.79	7.79	1.425e+38	0.000702
6626	diHPCARP_I.tpmtptppu	8.693e+43	7.94	7.94	1.424e+38	0.000702
6627	diHPCARP_I.mttmmtttu	1.298e+44	8.19	8.19	1.408e+38	0.000694
6628	diHPCARP_I.ttmmttppu	3.460e+43	7.40	7.40	1.402e+38	0.000691
6629	diHPCARP_I.tppppmttu	5.060e+44	9.00	9.00	1.402e+38	0.000691
6630	diHPCARP_I.tmpmtttmu	7.215e+43	7.84	7.84	1.401e+38	0.00069
6631	diHPCARP_I.pmtmpmtmu	4.093e+43	7.51	7.51	1.395e+38	0.000687
6632	diHPCARP_I.mppmmmttu	4.439e+43	7.56	7.56	1.390e+38	0.000685
6633	diHPCARP_I.ppmtptmpu	7.949e+43	7.90	7.90	1.387e+38	0.000684
6634	diHPCARP_I.tptmtmtmu	2.117e+44	8.49	8.49	1.380e+38	0.00068
6635	diHPCARP_I.pmpptmpu	1.460e+43	6.90	6.90	1.376e+38	0.000678
6636	diHPCARP_I.mptppmtmu	1.453e+44	8.27	8.27	1.375e+38	0.000677
6637	diHPCARP_I.pppmmttppu	9.926e+43	8.04	8.04	1.374e+38	0.000677
6638	diHPCARP_I.mmtmmtmmu	3.301e+44	8.76	8.76	1.367e+38	0.000674
6639	diHPCARP_I.ppttmtttu	8.852e+43	7.99	7.99	1.349e+38	0.000665
6640	diHPCARP_I.mttpttttu	1.175e+44	8.15	8.15	1.347e+38	0.000664
6641	diHPCARP_I.tpttppmpu	1.608e+44	8.34	8.34	1.342e+38	0.000661
6642	diHPCARP_I.tptptmtmu	1.435e+44	8.28	8.28	1.332e+38	0.000656
6643	diHPCARP_I.mppptmpmpu	2.699e+44	8.66	8.66	1.323e+38	0.000652
6644	diHPCARP_I.ttmppptppu	6.976e+43	7.86	7.86	1.319e+38	0.00065
6645	diHPCARP_I.tmtmtttmu	9.420e+43	8.04	8.04	1.314e+38	0.000648
6646	diHPCARP_I.ttmpppttu	1.244e+44	8.21	8.21	1.307e+38	0.000644
6647	diHPCARP_I.pmtptmtmu	6.279e+43	7.80	7.80	1.303e+38	0.000642
6648	diHPCARP_I.ttttptmpu	1.461e+44	8.31	8.31	1.299e+38	0.00064
6649	diHPCARP_I.mtppmtmmu	4.761e+43	7.64	7.64	1.284e+38	0.000633
6650	diHPCARP_I.tpttppppmu	7.851e+43	7.94	7.94	1.282e+38	0.000632
6651	diHPCARP_I.mtmmpttppu	1.108e+44	8.15	8.15	1.278e+38	0.00063
6652	diHPCARP_I.ptmptppu	7.914e+43	7.95	7.95	1.275e+38	0.000628
6653	diHPCARP_I.mmpmnmmtmu	8.513e+43	8.00	8.00	1.273e+38	0.000627
6654	diHPCARP_I.ptppppmpu	8.230e+43	7.98	7.98	1.268e+38	0.000625
6655	diHPCARP_I.ttmmttppu	1.680e+44	8.41	8.41	1.251e+38	0.000617
6656	diHPCARP_I.pppmmtmmu	1.382e+43	6.92	6.92	1.250e+38	0.000616
6657	diHPCARP_I.mmpmptttu	4.329e+43	7.60	7.60	1.250e+38	0.000616
6658	diHPCARP_I.mmmmtmttu	1.833e+44	8.47	8.47	1.237e+38	0.000609
6659	diHPCARP_I.ttptmpmpu	1.086e+44	8.16	8.16	1.235e+38	0.000608
6660	diHPCARP_I.pptmppppmu	8.240e+43	8.00	8.00	1.231e+38	0.000607
6661	diHPCARP_I.tmtmtttmu	2.395e+44	8.63	8.63	1.230e+38	0.000606
6662	diHPCARP_I.mttptttppu	1.826e+44	8.47	8.47	1.225e+38	0.000604
6663	diHPCARP_I.pptptmpu	3.183e+44	8.81	8.81	1.209e+38	0.000596
6664	diHPCARP_I.tttmptmtu	1.504e+44	8.37	8.37	1.205e+38	0.000594
6665	diHPCARP_I.mptmmmtmu	1.141e+44	8.21	8.21	1.187e+38	0.000585
6666	diHPCARP_I.mtppppmpu	1.005e+44	8.14	8.14	1.184e+38	0.000583
6667	diHPCARP_I.pptptmpu	1.354e+44	8.32	8.32	1.183e+38	0.000583
6668	diHPCARP_I.mptmnmmpu	3.341e+44	8.86	8.86	1.181e+38	0.000582
6669	diHPCARP_I.ppptptttu	2.500e+44	8.69	8.69	1.172e+38	0.000578
6670	diHPCARP_I.mttmptttu	1.018e+44	8.16	8.16	1.166e+38	0.000575
6671	diHPCARP_I.mptptmtmu	8.671e+43	8.06	8.06	1.159e+38	0.000571
6672	diHPCARP_I.mmtmptttu	2.150e+44	8.61	8.61	1.153e+38	0.000568

6673	diHPCARP_I.pmmtpmpu	1.574e+44	8.42	8.42	1.150e+38	0.000566
6674	diHPCARP_I.tptmmmpu	3.199e+44	8.85	8.85	1.143e+38	0.000563
6675	diHPCARP_I.pppmmttu	1.165e+44	8.26	8.26	1.122e+38	0.000553
6676	diHPCARP_I.tttptmmu	7.308e+43	7.99	7.99	1.109e+38	0.000546
6677	diHPCARP_I.tmpmptmmu	5.087e+43	7.77	7.77	1.107e+38	0.000546
6678	diHPCARP_I.tmpmptmtu	1.070e+44	8.22	8.22	1.095e+38	0.000539
6679	diHPCARP_I.ttpmtpmpu	4.511e+43	7.71	7.71	1.094e+38	0.000539
6680	diHPCARP_I.mpppmmttu	2.518e+44	8.74	8.74	1.079e+38	0.000532
6681	diHPCARP_I.mmtmmtmtu	1.193e+45	9.67	9.67	1.079e+38	0.000532
6682	diHPCARP_I.pmmptmpu	1.142e+43	6.90	6.90	1.069e+38	0.000527
6683	diHPCARP_I.pptmtmmu	1.919e+44	8.59	8.59	1.069e+38	0.000527
6684	diHPCARP_I.ttptmttptu	2.359e+44	8.71	8.71	1.068e+38	0.000526
6685	diHPCARP_I.pmmtmmmtu	1.532e+43	7.08	7.08	1.065e+38	0.000525
6686	diHPCARP_I.mptmmttptu	4.157e+44	9.05	9.05	1.053e+38	0.000519
6687	diHPCARP_I.pmttmmpu	1.254e+44	8.35	8.35	1.045e+38	0.000515
6688	diHPCARP_I.mppptmmu	1.373e+44	8.40	8.40	1.043e+38	0.000514
6689	diHPCARP_I.ptttmtmmu	4.533e+44	9.11	9.11	1.038e+38	0.000512
6690	diHPCARP_I.tmtttptu	3.048e+44	8.88	8.88	1.036e+38	0.000511
6691	diHPCARP_I.tttmtmtu	1.395e+44	8.42	8.42	1.034e+38	0.000509
6692	diHPCARP_I.mptmtmmu	1.480e+44	8.45	8.45	1.031e+38	0.000508
6693	diHPCARP_I.pptmpmpu	2.768e+43	7.45	7.45	1.029e+38	0.000507
6694	diHPCARP_I.mppptmtu	1.091e+44	8.28	8.28	1.018e+38	0.000502
6695	diHPCARP_I.pppmmpmpu	5.269e+43	7.85	7.85	1.013e+38	0.000499
6696	diHPCARP_I.pttmtmmu	7.114e+43	8.03	8.03	1.002e+38	0.000494
6697	diHPCARP_I.mmpptpmu	5.218e+43	7.86	7.86	9.846e+37	0.000485
6698	diHPCARP_I.tptmtttu	1.089e+44	8.30	8.30	9.767e+37	0.000481
6699	diHPCARP_I.mptpmmmpu	5.277e+43	7.87	7.87	9.767e+37	0.000481
6700	diHPCARP_I.pmtmtttu	1.177e+44	8.36	8.36	9.569e+37	0.000472
6701	diHPCARP_I.mttptttu	1.206e+44	8.37	8.37	9.561e+37	0.000471
6702	diHPCARP_I.pmttpppu	1.153e+44	8.35	8.35	9.550e+37	0.000471
6703	diHPCARP_I.ptmptmtu	5.320e+43	7.89	7.89	9.544e+37	0.00047
6704	diHPCARP_I.pptmpmpu	3.689e+43	7.67	7.67	9.469e+37	0.000467
6705	diHPCARP_I.tmmppttu	4.840e+43	7.84	7.84	9.415e+37	0.000464
6706	diHPCARP_I.mmpptpppu	4.754e+43	7.83	7.83	9.377e+37	0.000462
6707	diHPCARP_I.mmtmptmmu	5.095e+44	9.25	9.25	9.355e+37	0.000461
6708	diHPCARP_I.pttptmpu	1.704e+44	8.59	8.59	9.353e+37	0.000461
6709	diHPCARP_I.pttmtppmu	2.136e+44	8.73	8.73	9.318e+37	0.000459
6710	diHPCARP_I.pptmptpu	2.532e+43	7.47	7.47	9.208e+37	0.000454
6711	diHPCARP_I.pptppmtu	7.888e+43	8.15	8.15	9.165e+37	0.000452
6712	diHPCARP_I.pptmptmtu	4.246e+44	9.15	9.15	9.107e+37	0.000449
6713	diHPCARP_I.tmmppptpu	2.367e+43	7.44	7.44	9.018e+37	0.000444
6714	diHPCARP_I.mmttpppu	7.934e+43	8.16	8.16	9.006e+37	0.000444
6715	diHPCARP_I.mmpmptptu	3.119e+43	7.61	7.61	8.965e+37	0.000442
6716	diHPCARP_I.pmtmpmpu	2.168e+44	8.76	8.76	8.958e+37	0.000441
6717	diHPCARP_I.pptmpmpu	1.442e+44	8.52	8.52	8.922e+37	0.00044
6718	diHPCARP_I.mttmtmpu	6.672e+43	8.06	8.06	8.916e+37	0.000439
6719	diHPCARP_I.pptmptmmu	3.132e+43	7.63	7.63	8.713e+37	0.000429
6720	diHPCARP_I.tmpmmpmpu	4.144e+43	7.80	7.80	8.653e+37	0.000426
6721	diHPCARP_I.pmmtmttu	1.737e+44	8.65	8.65	8.617e+37	0.000425
6722	diHPCARP_I.tmpptttu	1.729e+44	8.66	8.66	8.442e+37	0.000416
6723	diHPCARP_I.tptppmtu	9.369e+43	8.31	8.31	8.338e+37	0.000411
6724	diHPCARP_I.ptmpppmu	4.172e+43	7.82	7.82	8.325e+37	0.00041
6725	diHPCARP_I.mmpptttu	1.108e+44	8.41	8.41	8.275e+37	0.000408
6726	diHPCARP_I.tmmppttu	2.502e+44	8.90	8.90	8.221e+37	0.000405
6727	diHPCARP_I.mmpmptmtu	2.005e+44	8.77	8.77	8.135e+37	0.000401
6728	diHPCARP_I.mppptppmu	4.383e+43	7.87	7.87	8.128e+37	0.0004
6729	diHPCARP_I.mmtmtttu	5.071e+44	9.33	9.33	8.110e+37	0.0004
6730	diHPCARP_I.mtpmtmpu	5.354e+43	7.99	7.99	8.060e+37	0.000397
6731	diHPCARP_I.tpmpttpu	8.715e+43	8.29	8.29	7.997e+37	0.000394
6732	diHPCARP_I.ptpmmmpu	6.111e+43	8.08	8.08	7.991e+37	0.000394
6733	diHPCARP_I.tptmmmtu	8.811e+43	8.30	8.30	7.952e+37	0.000392
6734	diHPCARP_I.tptmptttu	2.789e+44	8.99	8.99	7.831e+37	0.000386
6735	diHPCARP_I.tttptttu	5.750e+44	9.43	9.43	7.821e+37	0.000385
6736	diHPCARP_I.mppptttu	5.071e+44	9.35	9.35	7.791e+37	0.000384
6737	diHPCARP_I.mmpmtttu	5.022e+43	7.98	7.98	7.742e+37	0.000381
6738	diHPCARP_I.tpmmpmtu	4.277e+43	7.89	7.89	7.673e+37	0.000378
6739	diHPCARP_I.mmmmtmtu	1.293e+44	8.55	8.55	7.597e+37	0.000374
6740	diHPCARP_I.mtptptptu	6.442e+43	8.14	8.14	7.566e+37	0.000373
6741	diHPCARP_I.tpppppmu	7.524e+43	8.24	8.24	7.516e+37	0.00037
6742	diHPCARP_I.tppppptu	4.753e+44	9.34	9.34	7.502e+37	0.00037
6743	diHPCARP_I.ptpmtmtu	1.341e+44	8.58	8.58	7.475e+37	0.000368
6744	diHPCARP_I.tptmtmpu	4.227e+44	9.27	9.27	7.440e+37	0.000367

6745	diHPCARP_I.pmtptmttu	2.236e+44	8.90	8.90	7.317e+37	0.000361
6746	diHPCARP_I.tpttmttptu	3.097e+44	9.10	9.10	7.249e+37	0.000357
6747	diHPCARP_I.pmmpttptu	1.956e+43	7.46	7.46	7.244e+37	0.000357
6748	diHPCARP_I.mtptmtmpu	1.577e+44	8.70	8.70	7.217e+37	0.000356
6749	diHPCARP_I.ptptmtmpu	7.580e+43	8.27	8.27	7.216e+37	0.000356
6750	diHPCARP_I.mtptmmmpu	3.246e+44	9.17	9.17	6.757e+37	0.000333
6751	diHPCARP_I.ppptppppu	8.361e+43	8.37	8.37	6.717e+37	0.000331
6752	diHPCARP_I.pppmtppu	5.774e+42	6.78	6.78	6.683e+37	0.000329
6753	diHPCARP_I.pmmtppppu	5.386e+43	8.11	8.11	6.673e+37	0.000329
6754	diHPCARP_I.pttptmttu	2.803e+44	9.09	9.09	6.656e+37	0.000328
6755	diHPCARP_I.tmmmpptu	2.103e+43	7.55	7.55	6.644e+37	0.000327
6756	diHPCARP_I.tpmmtmttu	7.923e+43	8.34	8.34	6.628e+37	0.000327
6757	diHPCARP_I.mptmtttu	2.781e+43	7.72	7.72	6.615e+37	0.000326
6758	diHPCARP_I.ttttmttptu	2.014e+44	8.90	8.90	6.572e+37	0.000324
6759	diHPCARP_I.tmmmpmttu	5.788e+43	8.16	8.16	6.545e+37	0.000323
6760	diHPCARP_I.mmpptttu	2.238e+44	8.98	8.98	6.473e+37	0.000319
6761	diHPCARP_I.mtptmpmpu	4.149e+43	7.97	7.97	6.454e+37	0.000318
6762	diHPCARP_I.mptpmtptu	1.466e+44	8.73	8.73	6.447e+37	0.000318
6763	diHPCARP_I.ptttmtptu	1.007e+44	8.50	8.50	6.427e+37	0.000317
6764	diHPCARP_I.tmttmtptu	2.038e+44	8.92	8.92	6.421e+37	0.000316
6765	diHPCARP_I.mpptmpmpu	1.087e+44	8.55	8.55	6.393e+37	0.000315
6766	diHPCARP_I.ptppptmpu	4.092e+43	7.97	7.97	6.356e+37	0.000313
6767	diHPCARP_I.pmtptttu	1.403e+44	8.71	8.71	6.344e+37	0.000313
6768	diHPCARP_I.pppmtppu	1.732e+43	7.48	7.48	6.124e+37	0.000302
6769	diHPCARP_I.pmmtmtttu	4.841e+43	8.10	8.10	6.098e+37	0.0003
6770	diHPCARP_I.ppppmttu	1.708e+44	8.85	8.85	6.056e+37	0.000298
6771	diHPCARP_I.pptmmmttu	6.465e+43	8.28	8.28	6.016e+37	0.000296
6772	diHPCARP_I.ptmpptptu	3.702e+44	9.33	9.33	5.949e+37	0.000293
6773	diHPCARP_I.ptmtptmtu	3.643e+44	9.33	9.33	5.851e+37	0.000288
6774	diHPCARP_I.tmppttptu	1.470e+44	8.79	8.79	5.769e+37	0.000284
6775	diHPCARP_I.ptmtptmtu	1.699e+44	8.89	8.89	5.685e+37	0.00028
6776	diHPCARP_I.pmmppptpu	2.088e+43	7.66	7.66	5.498e+37	0.000271
6777	diHPCARP_I.ptttmmmttu	2.493e+44	9.14	9.14	5.462e+37	0.000269
6778	diHPCARP_I.mmmpptttu	2.015e+44	9.02	9.02	5.421e+37	0.000267
6779	diHPCARP_I.ptttmpmpu	2.478e+44	9.14	9.14	5.408e+37	0.000266
6780	diHPCARP_I.pptmmpmtu	3.513e+44	9.35	9.35	5.380e+37	0.000265
6781	diHPCARP_I.mmpmpmttu	3.456e+43	7.97	7.97	5.363e+37	0.000264
6782	diHPCARP_I.tmtptptmu	4.723e+43	8.16	8.16	5.352e+37	0.000264
6783	diHPCARP_I.mptppmpu	8.604e+43	8.52	8.52	5.316e+37	0.000262
6784	diHPCARP_I.pppmmmmmpu	1.155e+43	7.33	7.33	5.309e+37	0.000262
6785	diHPCARP_I.pmmtmntptu	1.711e+43	7.57	7.57	5.212e+37	0.000257
6786	diHPCARP_I.mmmmpmmmttu	8.130e+43	8.50	8.50	5.185e+37	0.000255
6787	diHPCARP_I.pmptmtptu	6.213e+43	8.35	8.35	5.112e+37	0.000252
6788	diHPCARP_I.tmmmtptu	1.563e+44	8.91	8.91	5.082e+37	0.00025
6789	diHPCARP_I.mmppttptu	1.691e+44	8.95	8.95	5.077e+37	0.00025
6790	diHPCARP_I.mpttmtptu	7.173e+44	9.82	9.82	5.065e+37	0.00025
6791	diHPCARP_I.tmttppppu	8.337e+43	8.54	8.54	5.020e+37	0.000247
6792	diHPCARP_I.ptmmtmttu	9.522e+43	8.62	8.62	5.006e+37	0.000247
6793	diHPCARP_I.mmmppptpu	2.981e+43	7.93	7.93	4.998e+37	0.000246
6794	diHPCARP_I.tptmtmttu	1.063e+44	8.69	8.69	4.995e+37	0.000246
6795	diHPCARP_I.tptttmttu	2.691e+44	9.24	9.24	4.987e+37	0.000246
6796	diHPCARP_I.ptmtppmmu	1.998e+44	9.06	9.06	4.979e+37	0.000245
6797	diHPCARP_I.pmmtmpmtu	1.802e+43	7.63	7.63	4.959e+37	0.000244
6798	diHPCARP_I.tmtpttptu	8.105e+43	8.53	8.53	4.929e+37	0.000243
6799	diHPCARP_I.mmpmmmttu	1.295e+44	8.82	8.82	4.890e+37	0.000241
6800	diHPCARP_I.ptmpptptu	7.264e+43	8.48	8.48	4.843e+37	0.000239
6801	diHPCARP_I.pttppppu	1.794e+44	9.03	9.03	4.764e+37	0.000235
6802	diHPCARP_I.tmtptmttu	1.252e+44	8.82	8.82	4.742e+37	0.000234
6803	diHPCARP_I.mppmmmpu	1.558e+44	8.95	8.95	4.734e+37	0.000233
6804	diHPCARP_I.mppppmttu	4.667e+44	9.60	9.60	4.724e+37	0.000233
6805	diHPCARP_I.mppmppttu	1.429e+44	8.90	8.90	4.689e+37	0.000231
6806	diHPCARP_I.mpttmtptu	1.154e+44	8.78	8.78	4.668e+37	0.00023
6807	diHPCARP_I.tptptptu	1.056e+44	8.72	8.72	4.663e+37	0.00023
6808	diHPCARP_I.ppttmtptu	1.353e+45	10.24	10.24	4.659e+37	0.00023
6809	diHPCARP_I.pmpmtptu	4.608e+42	6.86	6.86	4.630e+37	0.000228
6810	diHPCARP_I.ptpttptu	1.123e+44	8.77	8.77	4.603e+37	0.000227
6811	diHPCARP_I.pmtmmmmu	6.731e+44	9.84	9.84	4.561e+37	0.000225
6812	diHPCARP_I.ptmppttu	1.291e+43	7.49	7.49	4.537e+37	0.000224
6813	diHPCARP_I.mtttptptu	4.410e+44	9.60	9.60	4.469e+37	0.00022
6814	diHPCARP_I.tptmpmpu	8.263e+43	8.61	8.61	4.429e+37	0.000218
6815	diHPCARP_I.pppmtptu	5.879e+43	8.41	8.41	4.392e+37	0.000216
6816	diHPCARP_I.pmmppmpu	9.263e+42	7.31	7.31	4.364e+37	0.000215

6817	diHPCARP_I_ppptmtmmu	8.305e+43	8.62	8.62	4.334e+37	0.000214
6818	diHPCARP_I_ttmpppmu	5.618e+43	8.39	8.39	4.309e+37	0.000212
6819	diHPCARP_I_mmttmptmu	1.335e+44	8.92	8.92	4.225e+37	0.000208
6820	diHPCARP_I_ptmtppmmu	2.611e+44	9.32	9.32	4.218e+37	0.000208
6821	diHPCARP_I_pptpttmtmu	5.251e+43	8.37	8.37	4.217e+37	0.000208
6822	diHPCARP_I_pmttptpmu	8.960e+43	8.69	8.69	4.217e+37	0.000208
6823	diHPCARP_I_mppmmpmmu	1.465e+43	7.61	7.61	4.216e+37	0.000208
6824	diHPCARP_I_ptpmtmmpu	5.536e+43	8.40	8.40	4.209e+37	0.000207
6825	diHPCARP_I_mtttptpmu	7.567e+43	8.59	8.59	4.184e+37	0.000206
6826	diHPCARP_I_mpttptmmu	1.842e+44	9.12	9.12	4.176e+37	0.000206
6827	diHPCARP_I_ppptmppmu	7.998e+43	8.63	8.63	4.145e+37	0.000204
6828	diHPCARP_I_ttmptttmu	9.440e+44	10.10	10.10	4.126e+37	0.000203
6829	diHPCARP_I_pptmmmpu	6.422e+43	8.50	8.50	4.096e+37	0.000202
6830	diHPCARP_I_pttptpmu	1.242e+44	8.91	8.91	4.004e+37	0.000197
6831	diHPCARP_I_mttptpmu	4.895e+43	8.36	8.36	3.999e+37	0.000197
6832	diHPCARP_I_ptmpmmpu	5.339e+43	8.41	8.41	3.963e+37	0.000195
6833	diHPCARP_I_mppmmttmu	1.254e+44	8.93	8.93	3.947e+37	0.000195
6834	diHPCARP_I_mmtpmmttu	2.583e+44	9.36	9.36	3.946e+37	0.000194
6835	diHPCARP_I_tpptmppmu	2.575e+43	7.99	7.99	3.888e+37	0.000192
6836	diHPCARP_I_mmmmtpmu	5.854e+43	8.48	8.48	3.869e+37	0.000191
6837	diHPCARP_I_mtmptmmpu	2.048e+44	9.23	9.23	3.848e+37	0.00019
6838	diHPCARP_I_pmttptpmu	2.125e+44	9.27	9.27	3.778e+37	0.000186
6839	diHPCARP_I_pmpmptmu	1.645e+43	7.75	7.75	3.702e+37	0.000182
6840	diHPCARP_I_tptmtmmpu	1.227e+44	8.95	8.95	3.689e+37	0.000182
6841	diHPCARP_I_tpptmmmpu	1.558e+44	9.10	9.10	3.649e+37	0.00018
6842	diHPCARP_I_tpmptpmu	7.764e+43	8.69	8.69	3.645e+37	0.00018
6843	diHPCARP_I_pmtpmmtmu	9.003e+43	8.78	8.78	3.602e+37	0.000178
6844	diHPCARP_I_mpttmppmu	1.024e+44	8.86	8.86	3.591e+37	0.000177
6845	diHPCARP_I_pptmtttmu	1.018e+45	10.24	10.24	3.542e+37	0.000175
6846	diHPCARP_I_ptmtptpmu	7.963e+43	8.74	8.74	3.411e+37	0.000168
6847	diHPCARP_I_mtmptmmpu	8.738e+43	8.80	8.80	3.385e+37	0.000167
6848	diHPCARP_I_mtmptppmu	6.694e+43	8.65	8.65	3.356e+37	0.000165
6849	diHPCARP_I_mppmtmptu	3.448e+44	9.63	9.63	3.342e+37	0.000165
6850	diHPCARP_I_ttmmtmmu	8.531e+43	8.81	8.81	3.284e+37	0.000162
6851	diHPCARP_I_tptppmmpu	5.073e+43	8.50	8.50	3.270e+37	0.000161
6852	diHPCARP_I_ttmptttmu	3.428e+44	9.64	9.64	3.268e+37	0.000161
6853	diHPCARP_I_ppmmtttmu	8.990e+43	8.84	8.84	3.265e+37	0.000161
6854	diHPCARP_I_mpttttmtu	2.053e+44	9.33	9.33	3.251e+37	0.00016
6855	diHPCARP_I_mmmmtmtpu	3.137e+44	9.59	9.59	3.249e+37	0.00016
6856	diHPCARP_I_ppptptmmu	1.041e+44	8.94	8.94	3.191e+37	0.000157
6857	diHPCARP_I_tmpmmtttu	5.787e+43	8.59	8.59	3.183e+37	0.000157
6858	diHPCARP_I_pmtpmmttu	2.319e+44	9.42	9.42	3.162e+37	0.000156
6859	diHPCARP_I_mmmmtmptu	8.804e+43	8.85	8.85	3.139e+37	0.000155
6860	diHPCARP_I_mptppppmu	2.120e+44	9.38	9.38	3.137e+37	0.000155
6861	diHPCARP_I_ttpmtptmu	6.376e+43	8.67	8.67	3.102e+37	0.000153
6862	diHPCARP_I_mmpmmpmmu	7.159e+43	8.74	8.74	3.100e+37	0.000153
6863	diHPCARP_I_mptmptpmu	6.558e+43	8.68	8.68	3.092e+37	0.000152
6864	diHPCARP_I_tpttppmmu	1.114e+44	9.00	9.00	3.081e+37	0.000152
6865	diHPCARP_I_tmtpmpttu	1.930e+44	9.33	9.33	3.059e+37	0.000151
6866	diHPCARP_I_mmmptmttu	8.425e+43	8.86	8.86	2.975e+37	0.000147
6867	diHPCARP_I_tpmptttmu	1.132e+44	9.04	9.04	2.963e+37	0.000146
6868	diHPCARP_I_pttpptpmu	8.878e+43	8.90	8.90	2.924e+37	0.000144
6869	diHPCARP_I_tttmptmmu	7.339e+43	8.79	8.79	2.923e+37	0.000144
6870	diHPCARP_I_tmtmtmmu	3.184e+44	9.66	9.66	2.907e+37	0.000143
6871	diHPCARP_I_mppmmpmmu	1.384e+44	9.17	9.17	2.899e+37	0.000143
6872	diHPCARP_I_mmtpmmtmu	1.614e+44	9.26	9.26	2.883e+37	0.000142
6873	diHPCARP_I_pmttptmmu	2.497e+44	9.53	9.53	2.872e+37	0.000142
6874	diHPCARP_I_tmttptmmu	3.617e+44	9.75	9.75	2.864e+37	0.000141
6875	diHPCARP_I_ttmppttmu	3.705e+43	8.39	8.39	2.856e+37	0.000141
6876	diHPCARP_I_tmtmptpmu	1.302e+44	9.14	9.14	2.845e+37	0.00014
6877	diHPCARP_I_ptmppppmu	7.838e+42	7.47	7.47	2.825e+37	0.000139
6878	diHPCARP_I_mptmmpmmu	6.040e+43	8.69	8.69	2.804e+37	0.000138
6879	diHPCARP_I_mmtpmmmmu	2.738e+44	9.59	9.59	2.803e+37	0.000138
6880	diHPCARP_I_pmtmtmmu	2.315e+44	9.50	9.50	2.788e+37	0.000137
6881	diHPCARP_I_tmmmtmtpu	1.618e+44	9.29	9.29	2.765e+37	0.000136
6882	diHPCARP_I_mtpmptpmu	3.383e+43	8.36	8.36	2.736e+37	0.000135
6883	diHPCARP_I_tmtpmmpmu	2.721e+44	9.61	9.61	2.726e+37	0.000134
6884	diHPCARP_I_ttpmppmu	1.600e+44	9.29	9.29	2.715e+37	0.000134
6885	diHPCARP_I_tmpmmpmmu	4.772e+43	8.57	8.57	2.705e+37	0.000133
6886	diHPCARP_I_tmpmmtptu	4.370e+43	8.52	8.52	2.699e+37	0.000133
6887	diHPCARP_I_tptmmpmmu	3.389e+43	8.38	8.38	2.684e+37	0.000132
6888	diHPCARP_I_mmpmptmttu	1.234e+44	9.15	9.15	2.656e+37	0.000131

6889	diHPCARP_I.ttttmtpmu	1.093e+44	9.09	9.09	2.630e+37	0.00013
6890	diHPCARP_I.pmtmpttptu	6.133e+43	8.75	8.75	2.606e+37	0.000128
6891	diHPCARP_I.ptptmptpu	1.232e+44	9.16	9.16	2.605e+37	0.000128
6892	diHPCARP_I.tmtptpppu	2.625e+43	8.24	8.24	2.599e+37	0.000128
6893	diHPCARP_I.mptmpmmpu	5.315e+43	8.67	8.67	2.589e+37	0.000128
6894	diHPCARP_I.tmtmptmtu	1.463e+44	9.27	9.27	2.576e+37	0.000127
6895	diHPCARP_I.tttmtpppu	1.004e+44	9.05	9.05	2.566e+37	0.000126
6896	diHPCARP_I.mppppmptpu	4.926e+44	10.00	10.00	2.549e+37	0.000126
6897	diHPCARP_I.mmtptptmu	4.388e+43	8.57	8.57	2.527e+37	0.000125
6898	diHPCARP_I.tpmmpmttu	2.016e+44	9.48	9.48	2.485e+37	0.000122
6899	diHPCARP_I.ptmpptmtu	5.626e+43	8.73	8.73	2.468e+37	0.000122
6900	diHPCARP_I.ptttmttptu	3.702e+44	9.86	9.86	2.425e+37	0.000119
6901	diHPCARP_I.mtpmmttptu	1.195e+44	9.19	9.19	2.417e+37	0.000119
6902	diHPCARP_I.ttmmtmtmu	2.252e+44	9.57	9.57	2.392e+37	0.000118
6903	diHPCARP_I.ttptmtptu	1.555e+44	9.35	9.35	2.390e+37	0.000118
6904	diHPCARP_I.tpmmpmpu	2.018e+43	8.14	8.14	2.382e+37	0.000117
6905	diHPCARP_I.pmpmpmtu	8.074e+42	7.59	7.59	2.375e+37	0.000117
6906	diHPCARP_I.mmtmpmmpu	2.090e+44	9.53	9.53	2.375e+37	0.000117
6907	diHPCARP_I.ttmmpmpu	7.778e+43	8.95	8.95	2.356e+37	0.000116
6908	diHPCARP_I.mttmtmtu	1.258e+44	9.24	9.24	2.338e+37	0.000115
6909	diHPCARP_I.tpmmttptu	2.006e+44	9.52	9.52	2.336e+37	0.000115
6910	diHPCARP_I.pptmmpu	2.522e+43	8.29	8.29	2.317e+37	0.000114
6911	diHPCARP_I.mmpmpmtu	8.260e+43	9.00	9.00	2.311e+37	0.000114
6912	diHPCARP_I.mmtmtmtu	1.498e+45	10.73	10.73	2.304e+37	0.000114
6913	diHPCARP_I.ttpmmtptu	3.380e+44	9.84	9.84	2.275e+37	0.000112
6914	diHPCARP_I.mtppptptu	1.017e+44	9.13	9.13	2.275e+37	0.000112
6915	diHPCARP_I.mptmttptu	9.622e+44	10.47	10.47	2.257e+37	0.000111
6916	diHPCARP_I.pptmmtptu	5.393e+43	8.76	8.76	2.253e+37	0.000111
6917	diHPCARP_I.mmtmptptu	1.078e+44	9.17	9.17	2.237e+37	0.00011
6918	diHPCARP_I.tmtmtmtu	5.684e+44	10.18	10.18	2.195e+37	0.000108
6919	diHPCARP_I.tpmmpmtu	8.541e+43	9.05	9.05	2.181e+37	0.000107
6920	diHPCARP_I.mmtmtmtu	4.890e+44	10.10	10.10	2.159e+37	0.000106
6921	diHPCARP_I.ttmppmpu	5.048e+43	8.75	8.75	2.146e+37	0.000106
6922	diHPCARP_I.mtppptptu	1.296e+44	9.32	9.32	2.123e+37	0.000105
6923	diHPCARP_I.ptpmtmpu	6.069e+43	8.86	8.86	2.119e+37	0.000104
6924	diHPCARP_I.tmmmtmtu	1.378e+44	9.35	9.35	2.112e+37	0.000104
6925	diHPCARP_I.mmtmptptu	3.449e+44	9.90	9.90	2.110e+37	0.000104
6926	diHPCARP_I.tmptttttu	2.181e+44	9.64	9.64	2.084e+37	0.000103
6927	diHPCARP_I.pmttptmtu	1.277e+44	9.33	9.33	2.050e+37	0.000101
6928	diHPCARP_I.pmtptptmu	2.162e+43	8.28	8.28	1.995e+37	9.83e-05
6929	diHPCARP_I.mmptttptu	1.186e+44	9.30	9.30	1.991e+37	9.81e-05
6930	diHPCARP_I.mmttptmtu	5.043e+44	10.17	10.17	1.973e+37	9.72e-05
6931	diHPCARP_I.mtpmtmmpu	9.453e+43	9.18	9.18	1.957e+37	9.64e-05
6932	diHPCARP_I.ttmtpttmtu	1.201e+44	9.32	9.32	1.957e+37	9.64e-05
6933	diHPCARP_I.mtttptmtu	1.789e+44	9.56	9.56	1.948e+37	9.6e-05
6934	diHPCARP_I.ttmmpmptu	1.099e+44	9.27	9.27	1.941e+37	9.56e-05
6935	diHPCARP_I.pmmpmpptu	3.695e+43	8.63	8.63	1.922e+37	9.47e-05
6936	diHPCARP_I.mpmtpmpu	1.087e+44	9.27	9.27	1.919e+37	9.45e-05
6937	diHPCARP_I.mmtmmpptu	6.876e+44	10.37	10.37	1.909e+37	9.41e-05
6938	diHPCARP_I.tpmmtptmu	4.522e+43	8.75	8.75	1.899e+37	9.36e-05
6939	diHPCARP_I.mtmtpppmu	7.456e+43	9.05	9.05	1.895e+37	9.34e-05
6940	diHPCARP_I.mmttppmmpu	5.060e+44	10.20	10.20	1.892e+37	9.32e-05
6941	diHPCARP_I.mppmmpmpu	3.959e+43	8.69	8.69	1.863e+37	9.18e-05
6942	diHPCARP_I.pmttptttu	2.921e+44	9.88	9.88	1.861e+37	9.17e-05
6943	diHPCARP_I.ttmttptpu	6.144e+43	8.95	8.95	1.846e+37	9.1e-05
6944	diHPCARP_I.pptmtptmu	2.244e+44	9.74	9.74	1.817e+37	8.95e-05
6945	diHPCARP_I.pmptmtptu	6.839e+43	9.03	9.03	1.806e+37	8.9e-05
6946	diHPCARP_I.tmttptmtu	7.265e+44	10.44	10.44	1.800e+37	8.87e-05
6947	diHPCARP_I.mmttppmmpu	6.548e+44	10.39	10.39	1.780e+37	8.77e-05
6948	diHPCARP_I.mtmmpmptu	2.480e+44	9.82	9.82	1.743e+37	8.59e-05
6949	diHPCARP_I.mtmmttptu	6.503e+43	9.03	9.03	1.722e+37	8.49e-05
6950	diHPCARP_I.mtttpttmtu	1.796e+44	9.64	9.64	1.719e+37	8.47e-05
6951	diHPCARP_I.ttttmtmtu	3.130e+44	9.97	9.97	1.718e+37	8.46e-05
6952	diHPCARP_I.ttttppmmpu	3.212e+44	9.98	9.98	1.714e+37	8.45e-05
6953	diHPCARP_I.tmtmmpmtu	2.600e+44	9.87	9.87	1.685e+37	8.3e-05
6954	diHPCARP_I.ptmmpmttu	1.939e+44	9.69	9.69	1.684e+37	8.3e-05
6955	diHPCARP_I.pmtmmttptu	2.661e+44	9.88	9.88	1.682e+37	8.29e-05
6956	diHPCARP_I.tpttptmtu	1.763e+44	9.65	9.65	1.650e+37	8.13e-05
6957	diHPCARP_I.tpptmmpu	1.564e+44	9.59	9.59	1.621e+37	7.99e-05
6958	diHPCARP_I.tmptmtmtu	1.601e+44	9.60	9.60	1.618e+37	7.97e-05
6959	diHPCARP_I.ttttmmmtu	3.073e+44	9.99	9.99	1.613e+37	7.95e-05
6960	diHPCARP_I.pmmpmptmu	2.431e+43	8.48	8.48	1.612e+37	7.94e-05

6961	diHPCARP_I.ppttppmu	1.524e+44	9.58	9.58	1.591e+37	7.84e-05
6962	diHPCARP_I.pmttppmtu	1.251e+45	10.84	10.84	1.590e+37	7.84e-05
6963	diHPCARP_I.pmmppmtpu	4.853e+42	7.54	7.54	1.569e+37	7.73e-05
6964	diHPCARP_I.ttttppptpu	2.322e+44	9.85	9.85	1.544e+37	7.61e-05
6965	diHPCARP_I.mmpmtmtu	2.371e+44	9.87	9.87	1.532e+37	7.55e-05
6966	diHPCARP_I.mppmpppmu	1.458e+43	8.21	8.21	1.528e+37	7.53e-05
6967	diHPCARP_I.tptmmmmmu	2.924e+44	10.00	10.00	1.521e+37	7.5e-05
6968	diHPCARP_I.mmpmtmtpu	7.866e+43	9.22	9.22	1.511e+37	7.44e-05
6969	diHPCARP_I.pptpmtpu	4.329e+43	8.88	8.88	1.462e+37	7.21e-05
6970	diHPCARP_I.tmttppmmu	4.749e+44	10.32	10.32	1.448e+37	7.14e-05
6971	diHPCARP_I.tppmpppmu	1.795e+43	8.37	8.37	1.442e+37	7.11e-05
6972	diHPCARP_I.mttmtmtmu	1.975e+44	9.80	9.80	1.436e+37	7.08e-05
6973	diHPCARP_I.ptttpttptu	4.385e+44	10.28	10.28	1.426e+37	7.03e-05
6974	diHPCARP_I.pmtttmtu	3.168e+44	10.09	10.09	1.405e+37	6.92e-05
6975	diHPCARP_I.pmppttttu	2.405e+44	9.93	9.93	1.402e+37	6.91e-05
6976	diHPCARP_I.tmpmmttu	9.781e+43	9.41	9.41	1.356e+37	6.68e-05
6977	diHPCARP_I.pptmtttmu	9.453e+43	9.40	9.40	1.350e+37	6.65e-05
6978	diHPCARP_I.pptttttmu	4.292e+44	10.30	10.30	1.346e+37	6.63e-05
6979	diHPCARP_I.ttptpppmu	1.094e+44	9.49	9.49	1.333e+37	6.57e-05
6980	diHPCARP_I.pppmpppmu	1.608e+43	8.35	8.35	1.333e+37	6.57e-05
6981	diHPCARP_I.tmtttmtmu	4.513e+44	10.34	10.34	1.332e+37	6.56e-05
6982	diHPCARP_I.ptmppmmu	1.266e+44	9.58	9.58	1.321e+37	6.51e-05
6983	diHPCARP_I.pptmtmtmu	3.204e+43	8.77	8.77	1.313e+37	6.47e-05
6984	diHPCARP_I.mmpmpttptu	7.637e+43	9.29	9.29	1.302e+37	6.42e-05
6985	diHPCARP_I.tmpmmttptu	4.288e+43	8.96	8.96	1.282e+37	6.32e-05
6986	diHPCARP_I.mtmpppttptu	1.371e+44	9.65	9.65	1.280e+37	6.31e-05
6987	diHPCARP_I.ppttpttptu	1.700e+44	9.79	9.79	1.258e+37	6.2e-05
6988	diHPCARP_I.tmptmttptu	2.741e+44	10.09	10.09	1.230e+37	6.06e-05
6989	diHPCARP_I.tmmmpmmmu	5.602e+43	9.14	9.14	1.230e+37	6.06e-05
6990	diHPCARP_I.mmtppmmu	2.651e+44	10.07	10.07	1.229e+37	6.05e-05
6991	diHPCARP_I.mtmtmttptu	1.090e+44	9.54	9.54	1.221e+37	6.01e-05
6992	diHPCARP_I.pppmmttptu	2.642e+43	8.70	8.70	1.219e+37	6.01e-05
6993	diHPCARP_I.ttttptpmu	1.096e+44	9.56	9.56	1.195e+37	5.89e-05
6994	diHPCARP_I.mptmmppu	1.721e+44	9.83	9.83	1.191e+37	5.87e-05
6995	diHPCARP_I.mpttptpmu	4.028e+44	10.34	10.34	1.183e+37	5.83e-05
6996	diHPCARP_I.tmpmmttptu	7.532e+43	9.34	9.34	1.181e+37	5.82e-05
6997	diHPCARP_I.tttmtptu	2.994e+44	10.17	10.17	1.168e+37	5.75e-05
6998	diHPCARP_I.tmtmpttptu	3.643e+44	10.29	10.29	1.161e+37	5.72e-05
6999	diHPCARP_I.tttmpttptu	2.328e+44	10.03	10.03	1.154e+37	5.69e-05
7000	diHPCARP_I.tmmmtppmu	5.209e+43	9.14	9.14	1.149e+37	5.66e-05
7001	diHPCARP_I.mpttpppmu	1.962e+44	9.93	9.93	1.147e+37	5.65e-05
7002	diHPCARP_I.mmpmtppptu	1.642e+44	9.84	9.84	1.113e+37	5.49e-05
7003	diHPCARP_I.mtpttmtmu	3.479e+43	8.92	8.92	1.106e+37	5.45e-05
7004	diHPCARP_I.pmmmpmttptu	6.894e+43	9.33	9.33	1.105e+37	5.44e-05
7005	diHPCARP_I.tppppmmmu	3.043e+44	10.22	10.22	1.084e+37	5.34e-05
7006	diHPCARP_I.tttpttptmu	9.201e+43	9.52	9.52	1.076e+37	5.3e-05
7007	diHPCARP_I.mptmmpmmu	1.265e+43	8.34	8.34	1.068e+37	5.26e-05
7008	diHPCARP_I.mtppttmtu	5.718e+43	9.24	9.24	1.054e+37	5.19e-05
7009	diHPCARP_I.ttttptmmu	5.024e+44	10.54	10.54	1.053e+37	5.19e-05
7010	diHPCARP_I.tmttppmmu	3.102e+44	10.25	10.25	1.052e+37	5.18e-05
7011	diHPCARP_I.mmmmtmmu	2.658e+44	10.17	10.17	1.045e+37	5.15e-05
7012	diHPCARP_I.ptmtmtptu	1.517e+44	9.84	9.84	1.033e+37	5.09e-05
7013	diHPCARP_I.mmpmmttptu	3.932e+43	9.03	9.03	1.032e+37	5.08e-05
7014	diHPCARP_I.mmpmmtttu	6.362e+43	9.32	9.32	1.030e+37	5.07e-05
7015	diHPCARP_I.mtptmttptu	3.033e+44	10.26	10.26	1.011e+37	4.98e-05
7016	diHPCARP_I.pptmttptu	2.781e+44	10.22	10.22	1.005e+37	4.95e-05
7017	diHPCARP_I.mtptmttptu	1.000e+44	9.62	9.62	9.868e+36	4.86e-05
7018	diHPCARP_I.tmtmmttptu	2.452e+44	10.15	10.15	9.864e+36	4.86e-05
7019	diHPCARP_I.ttttppppu	7.778e+43	9.48	9.48	9.705e+36	4.78e-05
7020	diHPCARP_I.pmttmttptu	1.259e+44	9.77	9.77	9.612e+36	4.74e-05
7021	diHPCARP_I.ttttmttptu	3.464e+44	10.37	10.37	9.605e+36	4.73e-05
7022	diHPCARP_I.mppmmpmmu	1.082e+44	9.69	9.69	9.427e+36	4.65e-05
7023	diHPCARP_I.pptmtmtmu	1.133e+44	9.73	9.73	9.302e+36	4.58e-05
7024	diHPCARP_I.ttmppppptu	7.359e+43	9.47	9.47	9.298e+36	4.58e-05
7025	diHPCARP_I.pptmttttu	2.919e+44	10.29	10.29	9.266e+36	4.57e-05
7026	diHPCARP_I.mtmptmtmu	1.217e+44	9.77	9.77	9.223e+36	4.54e-05
7027	diHPCARP_I.mtmtptpmu	6.156e+43	9.37	9.37	9.205e+36	4.54e-05
7028	diHPCARP_I.mtmtptmtu	7.965e+44	10.93	10.93	8.693e+36	4.28e-05
7029	diHPCARP_I.ttttmtmmu	2.082e+44	10.13	10.13	8.671e+36	4.27e-05
7030	diHPCARP_I.mtmtmtttu	7.794e+43	9.55	9.55	8.601e+36	4.24e-05
7031	diHPCARP_I.mpttmtmtu	1.644e+44	10.01	10.01	8.434e+36	4.16e-05
7032	diHPCARP_I.mmpmttttptu	7.076e+44	10.88	10.88	8.420e+36	4.15e-05

7033	diHPCARP_I.tmpmpmtptu	7.039e+43	9.52	9.52	8.203e+36	4.04e-05
7034	diHPCARP_I.tttptmtmu	2.990e+44	10.38	10.38	8.158e+36	4.02e-05
7035	diHPCARP_I.tmtmpmtu	1.624e+44	10.03	10.03	8.002e+36	3.94e-05
7036	diHPCARP_I.tmpmpmttu	6.907e+43	9.53	9.53	7.892e+36	3.89e-05
7037	diHPCARP_I.pmmmtmtu	7.892e+43	9.61	9.61	7.885e+36	3.89e-05
7038	diHPCARP_I.ttptmtptu	2.656e+44	10.33	10.33	7.862e+36	3.87e-05
7039	diHPCARP_I.mpmpmtptu	2.244e+43	8.86	8.86	7.857e+36	3.87e-05
7040	diHPCARP_I.ttmtptmtu	2.085e+44	10.20	10.20	7.768e+36	3.83e-05
7041	diHPCARP_I.pmpppmtu	2.490e+44	10.31	10.31	7.742e+36	3.81e-05
7042	diHPCARP_I.tpmtmtmpu	1.040e+44	9.79	9.79	7.720e+36	3.8e-05
7043	diHPCARP_I.pmttmppu	1.083e+44	9.81	9.81	7.696e+36	3.79e-05
7044	diHPCARP_I.pmtmtmtu	1.247e+44	9.90	9.90	7.614e+36	3.75e-05
7045	diHPCARP_I.mmpptttu	2.406e+44	10.31	10.31	7.444e+36	3.67e-05
7046	diHPCARP_I.mtppptpu	1.350e+45	11.34	11.34	7.431e+36	3.66e-05
7047	diHPCARP_I.mtmttptu	2.978e+44	10.44	10.44	7.391e+36	3.64e-05
7048	diHPCARP_I.tprmpmptu	5.082e+43	9.39	9.39	7.305e+36	3.6e-05
7049	diHPCARP_I.tpptmttu	5.949e+44	10.86	10.86	7.239e+36	3.57e-05
7050	diHPCARP_I.ptmmmtptu	6.996e+43	9.60	9.60	7.130e+36	3.51e-05
7051	diHPCARP_I.pptmpmtu	8.130e+43	9.69	9.69	7.127e+36	3.51e-05
7052	diHPCARP_I.tptpmttu	1.187e+44	9.92	9.92	7.029e+36	3.46e-05
7053	diHPCARP_I.mmpptttmu	1.509e+44	10.06	10.06	7.022e+36	3.46e-05
7054	diHPCARP_I.mpttmtmu	2.228e+44	10.30	10.30	6.978e+36	3.44e-05
7055	diHPCARP_I.mtmppmtu	3.900e+43	9.27	9.27	6.879e+36	3.39e-05
7056	diHPCARP_I.tprmtptu	3.234e+43	9.16	9.16	6.832e+36	3.37e-05
7057	diHPCARP_I.tptptmtu	1.332e+44	10.01	10.01	6.830e+36	3.37e-05
7058	diHPCARP_I.mptmmmtu	2.793e+44	10.45	10.45	6.808e+36	3.35e-05
7059	diHPCARP_I.mtmtptmu	2.290e+44	10.35	10.35	6.654e+36	3.28e-05
7060	diHPCARP_I.ptmppmtu	1.369e+44	10.04	10.04	6.609e+36	3.26e-05
7061	diHPCARP_I.mmpmmttu	5.276e+43	9.48	9.48	6.600e+36	3.25e-05
7062	diHPCARP_I.ptpmtptu	1.994e+44	10.27	10.27	6.582e+36	3.24e-05
7063	diHPCARP_I.tmtptmtu	4.171e+44	10.72	10.72	6.501e+36	3.2e-05
7064	diHPCARP_I.mmtmtttu	4.043e+44	10.70	10.70	6.443e+36	3.17e-05
7065	diHPCARP_I.mtpmmttu	4.578e+44	10.78	10.78	6.434e+36	3.17e-05
7066	diHPCARP_I.mppppmtu	2.322e+44	10.37	10.37	6.431e+36	3.17e-05
7067	diHPCARP_I.tptmmpu	9.346e+43	9.83	9.83	6.419e+36	3.16e-05
7068	diHPCARP_I.pmpptttu	1.503e+44	10.12	10.12	6.372e+36	3.14e-05
7069	diHPCARP_I.tpttmtu	1.900e+44	10.26	10.26	6.356e+36	3.13e-05
7070	diHPCARP_I.tmpmmttu	4.401e+43	9.39	9.39	6.346e+36	3.13e-05
7071	diHPCARP_I.tmttppmtu	9.906e+43	9.88	9.88	6.326e+36	3.12e-05
7072	diHPCARP_I.tmmpmttu	1.401e+44	10.09	10.09	6.263e+36	3.09e-05
7073	diHPCARP_I.mppmmttu	8.825e+43	9.82	9.82	6.155e+36	3.03e-05
7074	diHPCARP_I.ttmpppmu	6.780e+43	9.68	9.68	6.033e+36	2.97e-05
7075	diHPCARP_I.pmpptptu	7.569e+43	9.74	9.74	6.033e+36	2.97e-05
7076	diHPCARP_I.mpttpttu	1.315e+45	11.45	11.45	5.964e+36	2.94e-05
7077	diHPCARP_I.ttpmmttu	7.384e+43	9.74	9.74	5.944e+36	2.93e-05
7078	diHPCARP_I.tmpmmttu	4.173e+43	9.40	9.40	5.931e+36	2.92e-05
7079	diHPCARP_I.mtpppttu	2.721e+44	10.52	10.52	5.859e+36	2.89e-05
7080	diHPCARP_I.ttmtpttu	7.196e+43	9.74	9.74	5.777e+36	2.85e-05
7081	diHPCARP_I.pptmmttu	4.640e+44	10.85	10.85	5.773e+36	2.84e-05
7082	diHPCARP_I.pptttmtu	6.237e+43	9.66	9.66	5.767e+36	2.84e-05
7083	diHPCARP_I.tmppppmu	5.661e+44	10.97	10.97	5.739e+36	2.83e-05
7084	diHPCARP_I.mmpmtmtu	9.198e+43	9.89	9.89	5.737e+36	2.83e-05
7085	diHPCARP_I.ppttppmu	3.701e+44	10.72	10.72	5.716e+36	2.82e-05
7086	diHPCARP_I.pmpmmttu	2.552e+43	9.13	9.13	5.705e+36	2.81e-05
7087	diHPCARP_I.tmpmmpmtu	4.952e+43	9.54	9.54	5.532e+36	2.73e-05
7088	diHPCARP_I.tpptpmtu	2.601e+44	10.53	10.53	5.531e+36	2.73e-05
7089	diHPCARP_I.pmpptttu	7.296e+43	9.78	9.78	5.519e+36	2.72e-05
7090	diHPCARP_I.pptpmtu	3.121e+43	9.27	9.27	5.500e+36	2.71e-05
7091	diHPCARP_I.mtmtppmu	1.922e+44	10.36	10.36	5.473e+36	2.7e-05
7092	diHPCARP_I.mttmtptu	3.770e+44	10.77	10.77	5.418e+36	2.67e-05
7093	diHPCARP_I.mtptppmu	1.042e+44	10.01	10.01	5.309e+36	2.62e-05
7094	diHPCARP_I.pptmmttu	7.319e+43	9.81	9.81	5.258e+36	2.59e-05
7095	diHPCARP_I.mptmmttu	1.458e+44	10.22	10.22	5.258e+36	2.59e-05
7096	diHPCARP_I.mmpptpmu	5.968e+44	11.06	11.06	5.199e+36	2.56e-05
7097	diHPCARP_I.mpttmttu	5.611e+44	11.03	11.03	5.166e+36	2.55e-05
7098	diHPCARP_I.tmpptptu	4.934e+44	10.96	10.96	5.155e+36	2.54e-05
7099	diHPCARP_I.pmpptptu	1.969e+44	10.41	10.41	5.127e+36	2.53e-05
7100	diHPCARP_I.mtmtmttu	1.188e+44	10.11	10.11	5.109e+36	2.52e-05
7101	diHPCARP_I.mtmpppmu	3.115e+43	9.33	9.33	5.004e+36	2.47e-05
7102	diHPCARP_I.ptmmtptu	1.030e+44	10.05	10.05	4.924e+36	2.43e-05
7103	diHPCARP_I.ppttpttu	7.704e+43	9.88	9.88	4.911e+36	2.42e-05
7104	diHPCARP_I.mpttmttu	1.636e+44	10.33	10.33	4.866e+36	2.4e-05

7105	diHPCARP_I.pmmmtmtptu	6.896e+43	9.83	9.83	4.735e+36	2.33e-05
7106	diHPCARP_I.mttttmttu	1.763e+44	10.40	10.40	4.711e+36	2.32e-05
7107	diHPCARP_I.tptmmmttu	3.143e+44	10.74	10.74	4.689e+36	2.31e-05
7108	diHPCARP_I.mprnmtmptu	4.325e+43	9.57	9.57	4.609e+36	2.27e-05
7109	diHPCARP_I.pppmmmttu	1.134e+44	10.15	10.15	4.575e+36	2.25e-05
7110	diHPCARP_I.ttttpttptu	3.850e+44	10.89	10.89	4.511e+36	2.22e-05
7111	diHPCARP_I.tmttmmttu	4.295e+44	10.96	10.96	4.425e+36	2.18e-05
7112	diHPCARP_I.tmmttmmtu	3.153e+44	10.79	10.79	4.346e+36	2.14e-05
7113	diHPCARP_I.mmmppmttu	9.798e+43	10.10	10.10	4.266e+36	2.1e-05
7114	diHPCARP_I.mmppppttu	5.058e+44	11.09	11.09	4.218e+36	2.08e-05
7115	diHPCARP_I.tpptpmttu	5.088e+44	11.10	11.10	4.197e+36	2.07e-05
7116	diHPCARP_I.mmpmtmttu	2.287e+44	10.63	10.63	4.151e+36	2.05e-05
7117	diHPCARP_I.tmtmpmttu	1.192e+44	10.25	10.25	4.051e+36	2e-05
7118	diHPCARP_I.tmmmpmmttu	7.492e+43	9.98	9.98	4.004e+36	1.97e-05
7119	diHPCARP_I.mppmmmpmttu	4.358e+43	9.66	9.66	3.976e+36	1.96e-05
7120	diHPCARP_I.pppmmttu	6.045e+43	9.86	9.86	3.959e+36	1.95e-05
7121	diHPCARP_I.pptpmttu	8.564e+43	10.08	10.08	3.873e+36	1.91e-05
7122	diHPCARP_I.mtmtmpppu	1.524e+44	10.43	10.43	3.861e+36	1.9e-05
7123	diHPCARP_I.tptmmmttu	1.311e+44	10.34	10.34	3.826e+36	1.89e-05
7124	diHPCARP_I.ttmppmttu	9.226e+43	10.13	10.13	3.821e+36	1.88e-05
7125	diHPCARP_I.pmpmmttu	6.076e+43	9.90	9.90	3.761e+36	1.85e-05
7126	diHPCARP_I.tppmmpmttu	1.125e+44	10.27	10.27	3.732e+36	1.84e-05
7127	diHPCARP_I.ttmpppttu	8.855e+42	8.76	8.76	3.670e+36	1.81e-05
7128	diHPCARP_I.ppptpmttu	2.222e+44	10.69	10.69	3.653e+36	1.8e-05
7129	diHPCARP_I.pmmppmttu	1.630e+43	9.13	9.13	3.635e+36	1.79e-05
7130	diHPCARP_I.pmmmpmmttu	6.168e+43	9.92	9.92	3.633e+36	1.79e-05
7131	diHPCARP_I.tmppppttu	3.995e+44	11.04	11.04	3.630e+36	1.79e-05
7132	diHPCARP_I.mtmtmptu	6.978e+43	10.03	10.03	3.437e+36	1.69e-05
7133	diHPCARP_I.mppmtmttu	1.028e+45	11.64	11.64	3.432e+36	1.69e-05
7134	diHPCARP_I.pppmmmpmttu	3.266e+43	9.59	9.59	3.352e+36	1.65e-05
7135	diHPCARP_I.mptppmmttu	9.737e+44	11.62	11.62	3.347e+36	1.65e-05
7136	diHPCARP_I.ptpmttu	1.480e+44	10.50	10.50	3.331e+36	1.64e-05
7137	diHPCARP_I.pppmmmttu	3.085e+43	9.58	9.58	3.248e+36	1.6e-05
7138	diHPCARP_I.mpptpmttu	9.374e+43	10.24	10.24	3.232e+36	1.59e-05
7139	diHPCARP_I.mmpmmttu	5.214e+43	9.90	9.90	3.208e+36	1.58e-05
7140	diHPCARP_I.mmttpttptu	1.900e+45	12.05	12.05	3.145e+36	1.55e-05
7141	diHPCARP_I.mmpptpmttu	1.794e+44	10.65	10.65	3.141e+36	1.55e-05
7142	diHPCARP_I.mmpmmttu	4.144e+43	9.79	9.79	3.073e+36	1.51e-05
7143	diHPCARP_I.ttmtpmttu	8.866e+43	10.24	10.24	3.052e+36	1.5e-05
7144	diHPCARP_I.pmpppmttu	8.635e+44	11.60	11.60	3.050e+36	1.5e-05
7145	diHPCARP_I.pppppmttu	1.927e+44	10.71	10.71	3.047e+36	1.5e-05
7146	diHPCARP_I.tmmtmtptu	1.916e+44	10.71	10.71	3.009e+36	1.48e-05
7147	diHPCARP_I.ppppmttu	2.306e+44	10.83	10.83	2.984e+36	1.47e-05
7148	diHPCARP_I.mtmtmptu	1.760e+44	10.67	10.67	2.976e+36	1.47e-05
7149	diHPCARP_I.ttpptpmttu	1.615e+44	10.62	10.62	2.956e+36	1.46e-05
7150	diHPCARP_I.mtmtppmttu	2.292e+44	10.84	10.84	2.931e+36	1.44e-05
7151	diHPCARP_I.ttmtpppmttu	7.813e+43	10.19	10.19	2.924e+36	1.44e-05
7152	diHPCARP_I.pmmtpmttu	1.505e+44	10.59	10.59	2.905e+36	1.43e-05
7153	diHPCARP_I.tpttptmttu	2.856e+44	10.98	10.98	2.870e+36	1.41e-05
7154	diHPCARP_I.mtmtppmttu	1.169e+44	10.46	10.46	2.822e+36	1.39e-05
7155	diHPCARP_I.tppmmmttu	2.426e+44	10.89	10.89	2.816e+36	1.39e-05
7156	diHPCARP_I.pmpmtmttu	3.098e+44	11.04	11.04	2.788e+36	1.37e-05
7157	diHPCARP_I.pptmmttu	8.204e+43	10.28	10.28	2.678e+36	1.32e-05
7158	diHPCARP_I.tmppppttu	3.616e+44	11.16	11.16	2.668e+36	1.31e-05
7159	diHPCARP_I.mtmmtptu	3.394e+43	9.77	9.77	2.608e+36	1.29e-05
7160	diHPCARP_I.pmpptmttu	6.818e+43	10.19	10.19	2.592e+36	1.28e-05
7161	diHPCARP_I.mtmtmttu	1.114e+44	10.48	10.48	2.565e+36	1.26e-05
7162	diHPCARP_I.pppmmmttu	1.016e+44	10.43	10.43	2.547e+36	1.26e-05
7163	diHPCARP_I.pmpmpmttu	2.318e+44	10.93	10.93	2.518e+36	1.24e-05
7164	diHPCARP_I.pmtppmttu	1.044e+45	11.83	11.83	2.507e+36	1.24e-05
7165	diHPCARP_I.pmtmpttu	7.258e+43	10.24	10.24	2.499e+36	1.23e-05
7166	diHPCARP_I.pmppppttu	1.533e+44	10.72	10.72	2.393e+36	1.18e-05
7167	diHPCARP_I.tttmpttu	7.726e+44	11.68	11.68	2.379e+36	1.17e-05
7168	diHPCARP_I.tmmppmttu	1.439e+44	10.70	10.70	2.323e+36	1.14e-05
7169	diHPCARP_I.ptpmttu	1.667e+44	10.79	10.79	2.308e+36	1.14e-05
7170	diHPCARP_I.pmpmtmttu	7.503e+44	11.69	11.69	2.290e+36	1.13e-05
7171	diHPCARP_I.ptmtmptu	1.819e+44	10.85	10.85	2.257e+36	1.11e-05
7172	diHPCARP_I.mtmtppmttu	4.022e+44	11.33	11.33	2.252e+36	1.11e-05
7173	diHPCARP_I.pppmmpmttu	1.987e+43	9.55	9.55	2.197e+36	1.08e-05
7174	diHPCARP_I.tptmmttu	5.034e+44	11.48	11.48	2.182e+36	1.08e-05
7175	diHPCARP_I.mptmmttu	1.145e+45	11.99	11.99	2.106e+36	1.04e-05
7176	diHPCARP_I.ppptpmttu	1.675e+44	10.85	10.85	2.099e+36	1.03e-05

7177	diHPCARP_I.ttmttpttu	1.443e+44	10.78	10.78	2.032e+36	1e-05
7178	diHPCARP_I.mpmntmpu	2.058e+43	9.62	9.62	2.009e+36	9.9e-06
7179	diHPCARP_I.pmpptppu	1.393e+44	10.77	10.77	1.995e+36	9.83e-06
7180	diHPCARP_I.mmpmppttu	1.105e+44	10.63	10.63	1.990e+36	9.81e-06
7181	diHPCARP_I.pmpptttu	6.114e+44	11.65	11.65	1.989e+36	9.8e-06
7182	diHPCARP_I.tmttpttu	4.772e+44	11.51	11.51	1.978e+36	9.75e-06
7183	diHPCARP_I.tpmmmmpu	5.339e+43	10.20	10.20	1.965e+36	9.68e-06
7184	diHPCARP_I.mmttpttu	9.320e+44	11.91	11.91	1.958e+36	9.65e-06
7185	diHPCARP_I.ppptmmtu	2.701e+44	11.18	11.18	1.938e+36	9.55e-06
7186	diHPCARP_I.pmtpmmmu	7.704e+43	10.44	10.44	1.916e+36	9.44e-06
7187	diHPCARP_I.ttptpttu	3.552e+44	11.37	11.37	1.852e+36	9.13e-06
7188	diHPCARP_I.pmttmmmu	5.777e+44	11.67	11.67	1.815e+36	8.94e-06
7189	diHPCARP_I.pmttppmu	7.341e+44	11.82	11.82	1.809e+36	8.91e-06
7190	diHPCARP_I.tpmtpmpu	8.739e+43	10.57	10.57	1.756e+36	8.65e-06
7191	diHPCARP_I.mmpmpptu	1.380e+44	10.84	10.84	1.751e+36	8.63e-06
7192	diHPCARP_I.mtmtpttu	1.523e+44	10.90	10.90	1.744e+36	8.59e-06
7193	diHPCARP_I.pmtptttu	6.524e+43	10.40	10.40	1.738e+36	8.57e-06
7194	diHPCARP_I.tmpmtmtu	2.240e+44	11.13	11.13	1.735e+36	8.55e-06
7195	diHPCARP_I.mmttmttu	6.125e+44	11.73	11.73	1.733e+36	8.54e-06
7196	diHPCARP_I.tpmppmmu	7.844e+43	10.51	10.51	1.729e+36	8.52e-06
7197	diHPCARP_I.tmtppptu	9.905e+43	10.65	10.65	1.729e+36	8.52e-06
7198	diHPCARP_I.tpmppmmtu	7.890e+43	10.52	10.52	1.714e+36	8.44e-06
7199	diHPCARP_I.mtmtpttu	2.128e+44	11.11	11.11	1.712e+36	8.43e-06
7200	diHPCARP_I.mmpppptu	2.008e+44	11.08	11.08	1.695e+36	8.35e-06
7201	diHPCARP_I.mmpptmtu	2.825e+44	11.29	11.29	1.691e+36	8.33e-06
7202	diHPCARP_I.mpmmmmtu	4.699e+43	10.22	10.22	1.681e+36	8.28e-06
7203	diHPCARP_I.mtmtpttu	1.384e+43	9.50	9.50	1.662e+36	8.19e-06
7204	diHPCARP_I.mtmtpppu	1.457e+44	10.91	10.91	1.649e+36	8.13e-06
7205	diHPCARP_I.mtmtpttu	2.000e+44	11.11	11.11	1.611e+36	7.94e-06
7206	diHPCARP_I.pmpptmtu	1.317e+44	10.87	10.87	1.584e+36	7.81e-06
7207	diHPCARP_I.pmpmpmtu	7.589e+43	10.54	10.54	1.579e+36	7.78e-06
7208	diHPCARP_I.tmpmtmtu	8.761e+43	10.64	10.64	1.545e+36	7.61e-06
7209	diHPCARP_I.tptpmmmu	1.538e+44	10.98	10.98	1.537e+36	7.58e-06
7210	diHPCARP_I.mtptmptu	3.039e+44	11.39	11.39	1.529e+36	7.54e-06
7211	diHPCARP_I.tmtptpmtu	1.271e+44	10.87	10.87	1.526e+36	7.52e-06
7212	diHPCARP_I.tmttpttu	5.903e+44	11.81	11.81	1.471e+36	7.25e-06
7213	diHPCARP_I.tmttmttu	4.375e+44	11.64	11.64	1.444e+36	7.12e-06
7214	diHPCARP_I.mtttmttu	3.187e+44	11.46	11.46	1.441e+36	7.1e-06
7215	diHPCARP_I.ttmtppptu	1.271e+44	10.91	10.91	1.439e+36	7.09e-06
7216	diHPCARP_I.tpmmtmtu	7.690e+43	10.62	10.62	1.402e+36	6.91e-06
7217	diHPCARP_I.ppttmttu	7.677e+43	10.62	10.62	1.397e+36	6.88e-06
7218	diHPCARP_I.mptmmttu	2.991e+43	10.06	10.06	1.397e+36	6.88e-06
7219	diHPCARP_I.pmmtpttu	2.274e+44	11.28	11.28	1.386e+36	6.83e-06
7220	diHPCARP_I.pmtpmmmu	1.603e+44	11.10	11.10	1.323e+36	6.52e-06
7221	diHPCARP_I.tmmpmmtu	3.083e+44	11.49	11.49	1.313e+36	6.47e-06
7222	diHPCARP_I.ttmtmptu	1.049e+44	10.86	10.86	1.297e+36	6.39e-06
7223	diHPCARP_I.pmttmttu	2.831e+44	11.45	11.45	1.284e+36	6.32e-06
7224	diHPCARP_I.mmttmttu	5.925e+44	11.90	11.90	1.280e+36	6.31e-06
7225	diHPCARP_I.pppppmmu	1.040e+44	10.88	10.88	1.229e+36	6.06e-06
7226	diHPCARP_I.mptmtttu	9.848e+43	10.88	10.88	1.163e+36	5.73e-06
7227	diHPCARP_I.pmpptttu	9.827e+43	10.89	10.89	1.152e+36	5.68e-06
7228	diHPCARP_I.tppmmmtu	2.028e+44	11.34	11.34	1.117e+36	5.5e-06
7229	diHPCARP_I.mptmpttu	4.367e+44	11.80	11.80	1.114e+36	5.49e-06
7230	diHPCARP_I.mppmtmtu	6.788e+44	12.06	12.06	1.112e+36	5.48e-06
7231	diHPCARP_I.tpttpppu	2.665e+44	11.52	11.52	1.087e+36	5.36e-06
7232	diHPCARP_I.pmpptttu	3.213e+44	11.63	11.63	1.082e+36	5.33e-06
7233	diHPCARP_I.pmptmttu	2.808e+44	11.55	11.55	1.081e+36	5.33e-06
7234	diHPCARP_I.mpptmmtu	1.116e+44	11.00	11.00	1.080e+36	5.32e-06
7235	diHPCARP_I.mtttptmu	2.729e+44	11.54	11.54	1.079e+36	5.31e-06
7236	diHPCARP_I.mmpptptmu	3.936e+44	11.79	11.79	1.019e+36	5.02e-06
7237	diHPCARP_I.ttmtpttu	2.601e+44	11.55	11.55	1.004e+36	4.95e-06
7238	diHPCARP_I.ptptmmtu	2.896e+44	11.62	11.62	9.871e+35	4.86e-06
7239	diHPCARP_I.mptpmmmu	1.192e+44	11.10	11.10	9.728e+35	4.79e-06
7240	diHPCARP_I.pmpttttu	8.281e+44	12.27	12.27	9.554e+35	4.71e-06
7241	diHPCARP_I.pmptmttu	1.349e+44	11.22	11.22	9.107e+35	4.49e-06
7242	diHPCARP_I.mpttpppu	2.771e+44	11.65	11.65	9.097e+35	4.48e-06
7243	diHPCARP_I.pmpptmtu	3.637e+44	11.82	11.82	8.857e+35	4.36e-06
7244	diHPCARP_I.tmtptttu	3.921e+44	11.88	11.88	8.743e+35	4.31e-06
7245	diHPCARP_I.tpttmmmu	2.744e+44	11.66	11.66	8.732e+35	4.3e-06
7246	diHPCARP_I.pmpmmttu	6.407e+44	12.17	12.17	8.694e+35	4.28e-06
7247	diHPCARP_I.pmmtmttu	1.556e+44	11.38	11.38	8.019e+35	3.95e-06
7248	diHPCARP_I.ttmmmpptu	1.254e+44	11.26	11.26	7.887e+35	3.89e-06

7249	diHPCARP_I.mtmpptttu	1.240e+43	9.88	9.88	7.846e+35	3.87e-06
7250	diHPCARP_I.pmmmppttu	7.466e+43	10.96	10.96	7.768e+35	3.83e-06
7251	diHPCARP_I.tmtptmtu	7.743e+44	12.36	12.36	7.662e+35	3.78e-06
7252	diHPCARP_I.ttmtmppmu	1.301e+44	11.31	11.31	7.526e+35	3.71e-06
7253	diHPCARP_I.pptmmppu	1.040e+44	11.19	11.19	7.378e+35	3.64e-06
7254	diHPCARP_I.pptmpmpmu	9.593e+43	11.14	11.14	7.371e+35	3.63e-06
7255	diHPCARP_I.pmppttmmu	4.458e+44	12.08	12.08	7.038e+35	3.47e-06
7256	diHPCARP_I.tpmtmmppu	8.523e+43	11.11	11.11	6.840e+35	3.37e-06
7257	diHPCARP_I.tpptmmmmu	3.664e+44	12.00	12.00	6.625e+35	3.26e-06
7258	diHPCARP_I.mpttmmppu	4.578e+44	12.15	12.15	6.441e+35	3.17e-06
7259	diHPCARP_I.mpttmmmmu	3.621e+44	12.03	12.03	6.264e+35	3.09e-06
7260	diHPCARP_I.ttmmmtptu	7.203e+43	11.08	11.08	6.109e+35	3.01e-06
7261	diHPCARP_I.mtppmptu	2.394e+44	11.80	11.80	6.088e+35	3e-06
7262	diHPCARP_I.mmpptptu	3.679e+44	12.06	12.06	6.038e+35	2.98e-06
7263	diHPCARP_I.pmmppmmtu	4.249e+43	10.78	10.78	6.003e+35	2.96e-06
7264	diHPCARP_I.tpmtpppmu	1.450e+44	11.53	11.53	5.768e+35	2.84e-06
7265	diHPCARP_I.tpptpmmmu	4.155e+44	12.16	12.16	5.714e+35	2.82e-06
7266	diHPCARP_I.ttpmtpmmu	7.558e+43	11.15	11.15	5.682e+35	2.8e-06
7267	diHPCARP_I.mtppppmmu	1.841e+44	11.69	11.69	5.586e+35	2.75e-06
7268	diHPCARP_I.mptmmmtptu	5.105e+44	12.30	12.30	5.549e+35	2.73e-06
7269	diHPCARP_I.tpptpmmmu	3.722e+44	12.16	12.16	5.149e+35	2.54e-06
7270	diHPCARP_I.pptmttptu	1.757e+44	11.72	11.72	5.074e+35	2.5e-06
7271	diHPCARP_I.ttmmmpmmu	5.403e+43	11.02	11.02	5.062e+35	2.49e-06
7272	diHPCARP_I.tmtptptu	3.823e+44	12.19	12.19	5.058e+35	2.49e-06
7273	diHPCARP_I.ttptmpmmu	1.883e+44	11.77	11.77	5.043e+35	2.49e-06
7274	diHPCARP_I.ptmppmpmu	5.670e+43	11.07	11.07	4.919e+35	2.42e-06
7275	diHPCARP_I.mppmmmttu	3.191e+44	12.10	12.10	4.892e+35	2.41e-06
7276	diHPCARP_I.mtptptptu	5.163e+44	12.39	12.39	4.827e+35	2.38e-06
7277	diHPCARP_I.mttmtttu	5.285e+44	12.41	12.41	4.775e+35	2.35e-06
7278	diHPCARP_I.pmtmtttu	4.939e+45	13.76	13.76	4.681e+35	2.31e-06
7279	diHPCARP_I.mtppmpmmu	6.753e+43	11.20	11.20	4.676e+35	2.3e-06
7280	diHPCARP_I.ttmmmtptu	6.899e+43	11.22	11.22	4.643e+35	2.29e-06
7281	diHPCARP_I.pmptmmtptu	1.420e+45	13.03	13.03	4.581e+35	2.26e-06
7282	diHPCARP_I.pmmppmttu	3.066e+43	10.77	10.77	4.393e+35	2.16e-06
7283	diHPCARP_I.mtpttmmtu	1.173e+45	12.95	12.95	4.319e+35	2.13e-06
7284	diHPCARP_I.mppmmptptu	2.835e+44	12.11	12.11	4.304e+35	2.12e-06
7285	diHPCARP_I.pptmtmttu	1.123e+45	12.93	12.93	4.284e+35	2.11e-06
7286	diHPCARP_I.tttmmpmmu	2.460e+44	12.04	12.04	4.155e+35	2.05e-06
7287	diHPCARP_I.pmttpttu	2.031e+44	11.97	11.97	3.881e+35	1.91e-06
7288	diHPCARP_I.mmpmmmtptu	6.320e+43	11.29	11.29	3.779e+35	1.86e-06
7289	diHPCARP_I.tpmmtmpmu	4.263e+43	11.11	11.11	3.424e+35	1.69e-06
7290	diHPCARP_I.tmtptppmu	6.966e+43	11.43	11.43	3.297e+35	1.62e-06
7291	diHPCARP_I.mtmtptmtu	1.221e+44	11.80	11.80	3.110e+35	1.53e-06
7292	diHPCARP_I.mppptpmmmu	3.825e+44	12.48	12.48	3.106e+35	1.53e-06
7293	diHPCARP_I.mtptmpmmu	3.034e+44	12.34	12.34	3.096e+35	1.53e-06
7294	diHPCARP_I.pmptmtmmu	3.255e+44	12.43	12.43	2.884e+35	1.42e-06
7295	diHPCARP_I.pptpmpmmu	8.863e+43	11.65	11.65	2.884e+35	1.42e-06
7296	diHPCARP_I.mppmtmmmmu	3.185e+44	12.44	12.44	2.763e+35	1.36e-06
7297	diHPCARP_I.mmpmmpttu	2.689e+43	10.99	10.99	2.646e+35	1.3e-06
7298	diHPCARP_I.tpmttmttu	5.932e+44	12.88	12.88	2.441e+35	1.2e-06
7299	diHPCARP_I.mptmpmpmu	5.664e+43	11.48	11.48	2.440e+35	1.2e-06
7300	diHPCARP_I.tpmtmmtmu	9.799e+43	11.86	11.86	2.249e+35	1.11e-06
7301	diHPCARP_I.mtptmpmmu	9.810e+43	11.87	11.87	2.204e+35	1.09e-06
7302	diHPCARP_I.mttmpttu	8.845e+44	13.21	13.21	2.103e+35	1.04e-06
7303	diHPCARP_I.pmpmmmmmu	1.940e+43	10.94	10.94	2.084e+35	1.03e-06
7304	diHPCARP_I.pmptmtptu	2.758e+44	12.57	12.57	1.922e+35	9.47e-07
7305	diHPCARP_I.mpttpmmmu	3.498e+44	12.74	12.74	1.836e+35	9.04e-07
7306	diHPCARP_I.tmtptpttu	5.443e+44	13.06	13.06	1.660e+35	8.18e-07
7307	diHPCARP_I.tttmpmmmu	1.168e+44	12.15	12.15	1.646e+35	8.11e-07
7308	diHPCARP_I.pmttmmptu	9.210e+44	13.39	13.39	1.622e+35	7.99e-07
7309	diHPCARP_I.mmpmtptu	4.892e+44	13.01	13.01	1.618e+35	7.97e-07
7310	diHPCARP_I.tmtptptu	6.547e+44	13.21	13.21	1.548e+35	7.63e-07
7311	diHPCARP_I.pmtmmmtptu	7.888e+43	11.95	11.95	1.546e+35	7.62e-07
7312	diHPCARP_I.tpmtmttu	2.447e+44	12.72	12.72	1.322e+35	6.52e-07
7313	diHPCARP_I.pppmpmttu	8.693e+44	13.50	13.50	1.269e+35	6.25e-07
7314	diHPCARP_I.tpttmmptu	3.019e+44	12.89	12.89	1.224e+35	6.03e-07
7315	diHPCARP_I.pmtppmttu	1.475e+44	12.53	12.53	1.096e+35	5.4e-07
7316	diHPCARP_I.mpttmmptu	7.025e+44	13.47	13.47	1.084e+35	5.34e-07
7317	diHPCARP_I.pppmmmpmu	1.914e+43	11.33	11.33	1.061e+35	5.23e-07
7318	diHPCARP_I.pmpmtmttu	9.750e+43	12.31	12.31	1.055e+35	5.2e-07
7319	diHPCARP_I.tmpmmpppu	2.743e+43	11.55	11.55	1.052e+35	5.18e-07
7320	diHPCARP_I.pppptmptu	4.298e+43	11.83	11.83	1.041e+35	5.13e-07

7321	diHPCARP_I_ppmtmmtmu	7.457e+43	12.17	12.17	1.014e+35	5e-07
7322	diHPCARP_I_tpmtpmpu	9.228e+43	12.33	12.33	9.565e+34	4.71e-07
7323	diHPCARP_I_ttmppmpmu	6.139e+43	12.12	12.12	9.065e+34	4.47e-07
7324	diHPCARP_I_mpmmpmttu	9.040e+43	12.37	12.37	8.800e+34	4.34e-07
7325	diHPCARP_I_pptpmmmu	4.217e+43	11.94	11.94	8.481e+34	4.18e-07
7326	diHPCARP_I_pptmmttu	4.333e+44	13.38	13.38	7.799e+34	3.84e-07
7327	diHPCARP_I_ppptmmttu	1.139e+44	12.60	12.60	7.555e+34	3.72e-07
7328	diHPCARP_I_ppttpmpu	1.843e+44	12.92	12.92	7.083e+34	3.49e-07
7329	diHPCARP_I_pmmptmmtu	8.877e+43	12.54	12.54	6.518e+34	3.21e-07
7330	diHPCARP_I_tpmmmmpu	3.278e+43	11.97	11.97	6.207e+34	3.06e-07
7331	diHPCARP_I_pppmmttu	4.086e+43	12.13	12.13	5.926e+34	2.92e-07
7332	diHPCARP_I_ttttppmu	2.243e+44	13.16	13.16	5.823e+34	2.87e-07
7333	diHPCARP_I_mpmtpmtu	4.438e+43	12.24	12.24	5.405e+34	2.66e-07
7334	diHPCARP_I_ttttppmu	3.162e+44	13.41	13.41	5.346e+34	2.63e-07
7335	diHPCARP_I_mmpmmmttu	1.013e+44	12.77	12.77	5.082e+34	2.5e-07
7336	diHPCARP_I_mpmtpmpu	3.274e+43	12.11	12.11	4.922e+34	2.43e-07
7337	diHPCARP_I_ppptpmmu	1.185e+44	12.93	12.93	4.513e+34	2.22e-07
7338	diHPCARP_I_mtpptpmu	2.962e+44	13.53	13.53	4.153e+34	2.05e-07
7339	diHPCARP_I_mmpmmmttu	1.543e+44	13.25	13.25	3.450e+34	1.7e-07
7340	diHPCARP_I_mpmtpmpu	1.935e+44	13.50	13.50	2.856e+34	1.41e-07
7341	diHPCARP_I_tpmmmppu	3.754e+43	12.54	12.54	2.741e+34	1.35e-07
7342	diHPCARP_I_ppttmmpu	1.573e+44	13.43	13.43	2.580e+34	1.27e-07
7343	diHPCARP_I_mmpmtmpu	3.379e+44	13.93	13.93	2.387e+34	1.18e-07
7344	diHPCARP_I_ppmpttpu	2.420e+43	12.42	12.42	2.150e+34	1.06e-07
7345	diHPCARP_I_mpttpmtu	8.622e+44	14.58	14.58	2.061e+34	1.02e-07
7346	diHPCARP_I_tpmppmpu	7.297e+43	13.15	13.15	1.914e+34	9.43e-08
7347	diHPCARP_I_tmpmmmttu	1.247e+44	13.48	13.48	1.882e+34	9.27e-08
7348	diHPCARP_I_tpmmtmmtu	1.779e+44	13.71	13.71	1.837e+34	9.05e-08
7349	diHPCARP_I_mmpmmmmu	8.201e+43	13.26	13.26	1.795e+34	8.84e-08
7350	diHPCARP_I_tpmmmmttu	1.412e+44	13.81	13.81	1.239e+34	6.1e-08
7351	diHPCARP_I_mmpmmmpu	9.388e+43	13.70	13.70	9.876e+33	4.87e-08
7352	diHPCARP_I_mmpmmptu	1.179e+44	14.05	14.05	6.861e+33	3.38e-08
7353	diHPCARP_I_tpmmmmmu	9.757e+43	14.31	14.31	3.664e+33	1.81e-08
7354	diHPCARP_I_mmpmmpttu	1.258e+44	14.58	14.58	3.006e+33	1.48e-08
7355	diHPCARP_I_tpmmmmpu	1.321e+44	14.66	14.66	2.760e+33	1.36e-08
7356	diHPCARP_I_tpmmmpttu	1.361e+44	14.75	14.75	2.440e+33	1.2e-08
7357	diHPCARP_I_ppmtmmtu	7.255e+43	14.49	14.49	2.035e+33	1e-08
7358	diHPCARP_I_ppmmmmmu	5.289e+43	14.31	14.31	1.973e+33	9.72e-09
7359	diHPCARP_I_mmpmmmpu	5.351e+43	14.94	14.94	7.029e+32	3.46e-09
7360	diHPCARP_I_tpmmpmpu	6.901e+43	15.20	15.20	5.832e+32	2.87e-09
7361	diHPCARP_I_mpmmtppu	5.309e+43	15.05	15.05	5.769e+32	2.84e-09
7362	Total				2.029e+43	100

7363
7364
7365
7366 (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-Ib)
7367 =====

7368
7369 Population analysis at 300K. Vibrational scaling: 0.971.
7370 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
7371 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
7372 %: contribution to the population (with current data set assumed 100%)
7373 Compound Qtot Erel Erel2 n*Q*MB %
7374 -----

7375	diHPCARP_Ib.ptppmpmu	1.045e+43	0.00	0.00	1.045e+43	45.7
7376	diHPCARP_Ib.ptppmtmu	9.193e+42	0.88	0.88	2.102e+42	9.19
7377	diHPCARP_Ib.ppmpttmu	2.296e+43	1.75	1.75	1.225e+42	5.35
7378	diHPCARP_Ib.pttmptmu	1.057e+44	2.68	2.68	1.179e+42	5.15
7379	diHPCARP_Ib.pttmmtmu	6.925e+43	2.49	2.49	1.059e+42	4.63
7380	diHPCARP_Ib.ptmmptmu	2.508e+43	2.37	2.37	4.719e+41	2.06
7381	diHPCARP_Ib.pttpptmu	1.502e+44	3.49	3.49	4.279e+41	1.87
7382	diHPCARP_Ib.ptmmmtmu	3.301e+43	2.62	2.62	4.069e+41	1.78
7383	diHPCARP_Ib.pttpmtmu	3.734e+43	2.82	2.82	3.280e+41	1.43
7384	diHPCARP_Ib.ptppmttu	2.054e+43	2.63	2.63	2.488e+41	1.09
7385	diHPCARP_Ib.ppmpttmu	2.107e+43	2.66	2.66	2.437e+41	1.07
7386	diHPCARP_Ib.pptmpmpu	1.523e+44	3.99	3.99	1.888e+41	0.825
7387	diHPCARP_Ib.pmmmmmttu	3.668e+43	3.26	3.26	1.546e+41	0.676
7388	diHPCARP_Ib.tmmppmttu	2.091e+43	2.99	2.99	1.383e+41	0.605
7389	diHPCARP_Ib.pppppptu	6.572e+43	3.71	3.71	1.305e+41	0.57
7390	diHPCARP_Ib.pptmpmtu	1.539e+43	2.85	2.85	1.285e+41	0.562
7391	diHPCARP_Ib.ppmptmpu	1.407e+43	2.83	2.83	1.231e+41	0.538
7392	diHPCARP_Ib.pppppmpu	7.627e+43	3.88	3.88	1.135e+41	0.496

7393	diHPCARP_Ib.ptmtptmmu	1.036e+44	4.10	4.10	1.076e+41	0.47
7394	diHPCARP_Ib.ptttptmmu	7.849e+43	3.96	3.96	1.027e+41	0.449
7395	diHPCARP_Ib.tmpmmpmu	1.148e+43	2.84	2.84	9.848e+40	0.431
7396	diHPCARP_Ib.ptttmtmmu	8.108e+43	4.03	4.03	9.365e+40	0.409
7397	diHPCARP_Ib.ptpmpmmu	1.186e+43	2.92	2.92	8.806e+40	0.385
7398	diHPCARP_Ib.pttmpttmu	8.111e+43	4.07	4.07	8.785e+40	0.384
7399	diHPCARP_Ib.pmpmpppu	1.471e+43	3.09	3.09	8.198e+40	0.358
7400	diHPCARP_Ib.mmmmpmtmu	2.774e+43	3.47	3.47	8.161e+40	0.357
7401	diHPCARP_Ib.tmmmpmmu	2.325e+43	3.40	3.40	7.726e+40	0.338
7402	diHPCARP_Ib.pmpmptmmu	1.177e+43	3.02	3.02	7.419e+40	0.324
7403	diHPCARP_Ib.pptmmpmpu	8.618e+43	4.21	4.21	7.373e+40	0.322
7404	diHPCARP_Ib.pptmpttmu	2.437e+43	3.48	3.48	7.162e+40	0.313
7405	diHPCARP_Ib.ptmtmtmmu	1.450e+44	4.55	4.55	7.082e+40	0.31
7406	diHPCARP_Ib.ptmpptmmu	4.807e+43	3.90	3.90	6.909e+40	0.302
7407	diHPCARP_Ib.pmmmmmpu	4.481e+43	3.87	3.87	6.825e+40	0.298
7408	diHPCARP_Ib.ptpmpmtmu	1.816e+43	3.33	3.33	6.805e+40	0.298
7409	diHPCARP_Ib.tmmmmmtmu	5.137e+43	4.05	4.05	5.758e+40	0.252
7410	diHPCARP_Ib.tpmpmmtmu	1.069e+43	3.13	3.13	5.608e+40	0.245
7411	diHPCARP_Ib.ppmmpmpu	8.874e+42	3.03	3.03	5.528e+40	0.242
7412	diHPCARP_Ib.ptmpmmtmu	3.576e+43	3.87	3.87	5.421e+40	0.237
7413	diHPCARP_Ib.tmtmpttmu	3.447e+43	3.88	3.88	5.177e+40	0.226
7414	diHPCARP_Ib.mmmmpmtmu	2.047e+43	3.57	3.57	5.175e+40	0.226
7415	diHPCARP_Ib.mmpmppppu	1.172e+43	3.26	3.26	4.978e+40	0.218
7416	diHPCARP_Ib.ppmmmmtmu	2.451e+43	3.74	3.74	4.596e+40	0.201
7417	diHPCARP_Ib.ptppptmmu	3.807e+44	5.40	5.40	4.464e+40	0.195
7418	diHPCARP_Ib.mpmmpmtmu	1.762e+43	3.66	3.66	3.782e+40	0.165
7419	diHPCARP_Ib.ppppmtmu	8.377e+43	4.60	4.60	3.714e+40	0.162
7420	diHPCARP_Ib.tmtmmpmpu	9.028e+43	4.67	4.67	3.567e+40	0.156
7421	diHPCARP_Ib.ptmptpmu	1.649e+44	5.03	5.03	3.556e+40	0.155
7422	diHPCARP_Ib.ptmpptmpu	4.785e+43	4.31	4.31	3.467e+40	0.152
7423	diHPCARP_Ib.tmmmpmtmu	2.105e+43	3.91	3.91	3.009e+40	0.132
7424	diHPCARP_Ib.tmtmppppu	1.023e+44	4.85	4.85	2.979e+40	0.13
7425	diHPCARP_Ib.pmmmpmpu	2.388e+43	3.99	3.99	2.951e+40	0.129
7426	diHPCARP_Ib.ptmmtmpu	9.523e+43	4.82	4.82	2.920e+40	0.128
7427	diHPCARP_Ib.ptppmtmu	1.367e+43	3.71	3.71	2.702e+40	0.118
7428	diHPCARP_Ib.pmtmptmu	2.512e+43	4.08	4.08	2.657e+40	0.116
7429	diHPCARP_Ib.tmmmpmtmu	2.722e+43	4.14	4.14	2.631e+40	0.115
7430	diHPCARP_Ib.pmppttmu	3.413e+43	4.28	4.28	2.614e+40	0.114
7431	diHPCARP_Ib.ppppmtmu	1.051e+44	4.95	4.95	2.600e+40	0.114
7432	diHPCARP_Ib.pmmmpmtmu	5.193e+43	4.55	4.55	2.536e+40	0.111
7433	diHPCARP_Ib.pmmmpmtmu	5.187e+43	4.56	4.56	2.472e+40	0.108
7434	diHPCARP_Ib.pmmptmpu	1.268e+44	5.10	5.10	2.454e+40	0.107
7435	diHPCARP_Ib.tmtppppu	1.290e+44	5.12	5.12	2.384e+40	0.104
7436	diHPCARP_Ib.pmmmpmpu	1.088e+43	3.71	3.71	2.171e+40	0.0949
7437	diHPCARP_Ib.pmpmtmpu	4.153e+43	4.52	4.52	2.118e+40	0.0926
7438	diHPCARP_Ib.mptmptmu	8.343e+43	4.96	4.96	2.043e+40	0.0893
7439	diHPCARP_Ib.ptmmttmu	1.802e+44	5.42	5.42	2.019e+40	0.0883
7440	diHPCARP_Ib.pmmmttmu	1.783e+43	4.04	4.04	2.018e+40	0.0882
7441	diHPCARP_Ib.pptmptmu	7.398e+43	4.92	4.92	1.931e+40	0.0844
7442	diHPCARP_Ib.tmmmpmtmu	1.691e+43	4.05	4.05	1.882e+40	0.0823
7443	diHPCARP_Ib.tptmptmu	2.676e+43	4.33	4.33	1.866e+40	0.0816
7444	diHPCARP_Ib.ptpmpmtmu	1.475e+43	4.01	4.01	1.753e+40	0.0767
7445	diHPCARP_Ib.ptmmpmtmu	1.975e+44	5.57	5.57	1.737e+40	0.0759
7446	diHPCARP_Ib.pmmmtmpu	1.714e+43	4.12	4.12	1.708e+40	0.0747
7447	diHPCARP_Ib.tpppmtmu	1.562e+44	5.44	5.44	1.695e+40	0.0741
7448	diHPCARP_Ib.tmmmmmtmu	5.682e+43	4.84	4.84	1.684e+40	0.0736
7449	diHPCARP_Ib.tppppmmu	1.026e+44	5.20	5.20	1.683e+40	0.0736
7450	diHPCARP_Ib.tptmmpmmu	1.668e+44	5.50	5.50	1.635e+40	0.0715
7451	diHPCARP_Ib.ptppmtmu	1.477e+44	5.44	5.44	1.618e+40	0.0708
7452	diHPCARP_Ib.mptmmtmu	1.110e+44	5.28	5.28	1.591e+40	0.0695
7453	diHPCARP_Ib.tmmmpmpu	1.198e+43	3.95	3.95	1.586e+40	0.0693
7454	diHPCARP_Ib.tpmpmmtmu	1.303e+43	4.01	4.01	1.564e+40	0.0684
7455	diHPCARP_Ib.pppmmmtmu	2.219e+44	5.71	5.71	1.546e+40	0.0676
7456	diHPCARP_Ib.pmtmmtmu	9.758e+43	5.24	5.24	1.499e+40	0.0655
7457	diHPCARP_Ib.tmpmmpmmu	2.804e+43	4.49	4.49	1.493e+40	0.0653
7458	diHPCARP_Ib.tptmpttmu	8.286e+43	5.14	5.14	1.490e+40	0.0651
7459	diHPCARP_Ib.tmpmmtmu	3.872e+43	4.69	4.69	1.472e+40	0.0643
7460	diHPCARP_Ib.pmmmtmpu	1.796e+43	4.25	4.25	1.438e+40	0.0629
7461	diHPCARP_Ib.tpmpmtmu	1.827e+43	4.26	4.26	1.429e+40	0.0625
7462	diHPCARP_Ib.tmmmpmpu	1.946e+43	4.30	4.30	1.427e+40	0.0624
7463	diHPCARP_Ib.tmtmmpmmu	2.690e+44	5.89	5.89	1.386e+40	0.0606
7464	diHPCARP_Ib.tptmmpmmu	1.799e+44	5.66	5.66	1.349e+40	0.059

7465	diHPCARP_Ib.pppmptmmu	1.442e+43	4.17	4.17	1.321e+40	0.0577
7466	diHPCARP_Ib.tppmptmpu	2.137e+43	4.41	4.41	1.318e+40	0.0576
7467	diHPCARP_Ib.ptmmpptpmu	3.658e+43	4.76	4.76	1.253e+40	0.0548
7468	diHPCARP_Ib.pppmptpmu	1.911e+43	4.38	4.38	1.229e+40	0.0537
7469	diHPCARP_Ib.tmtmpmpmu	5.991e+43	5.07	5.07	1.211e+40	0.0529
7470	diHPCARP_Ib.tmmmpmtmu	2.132e+43	4.46	4.46	1.207e+40	0.0528
7471	diHPCARP_Ib.ppppmtmmu	4.917e+43	4.96	4.96	1.199e+40	0.0524
7472	diHPCARP_Ib.pmmtmmpmu	1.581e+43	4.30	4.30	1.163e+40	0.0509
7473	diHPCARP_Ib.pptpmmtpu	5.307e+43	5.07	5.07	1.077e+40	0.0471
7474	diHPCARP_Ib.tppmpttpu	5.753e+43	5.12	5.12	1.072e+40	0.0469
7475	diHPCARP_Ib.mpppmtppu	6.447e+43	5.20	5.20	1.048e+40	0.0458
7476	diHPCARP_Ib.tmtppmtmu	1.501e+44	5.71	5.71	1.045e+40	0.0457
7477	diHPCARP_Ib.pmmmpmtpu	4.148e+43	4.94	4.94	1.037e+40	0.0453
7478	diHPCARP_Ib.pttpptpmu	1.336e+44	5.65	5.65	1.015e+40	0.0444
7479	diHPCARP_Ib.mpppmtppu	9.455e+43	5.45	5.45	1.009e+40	0.0441
7480	diHPCARP_Ib.tptmpttpu	7.331e+43	5.31	5.31	9.960e+39	0.0435
7481	diHPCARP_Ib.pppmmpmpu	9.260e+42	4.08	4.08	9.890e+39	0.0432
7482	diHPCARP_Ib.pmmtpmmpu	9.967e+43	5.50	5.50	9.863e+39	0.0431
7483	diHPCARP_Ib.tmpmpmpmu	1.480e+43	4.38	4.38	9.487e+39	0.0415
7484	diHPCARP_Ib.mppmptmpu	8.291e+42	4.04	4.04	9.427e+39	0.0412
7485	diHPCARP_Ib.mpppmtppu	3.927e+43	4.97	4.97	9.401e+39	0.0411
7486	diHPCARP_Ib.mtppmtppu	1.557e+43	4.43	4.43	9.183e+39	0.0401
7487	diHPCARP_Ib.pppmtptmu	1.434e+44	5.77	5.77	9.050e+39	0.0396
7488	diHPCARP_Ib.pptppmpmu	5.546e+43	5.21	5.21	8.829e+39	0.0386
7489	diHPCARP_Ib.pptpmtpmu	4.982e+43	5.16	5.16	8.690e+39	0.038
7490	diHPCARP_Ib.pmtmptmmu	4.461e+43	5.10	5.10	8.590e+39	0.0376
7491	diHPCARP_Ib.mtppmttpu	2.361e+43	4.72	4.72	8.585e+39	0.0375
7492	diHPCARP_Ib.tppmptmmu	1.974e+43	4.62	4.62	8.469e+39	0.037
7493	diHPCARP_Ib.tmmtpmtmu	1.489e+44	5.85	5.85	8.202e+39	0.0359
7494	diHPCARP_Ib.ptppmmpmu	1.841e+43	4.60	4.60	8.158e+39	0.0357
7495	diHPCARP_Ib.ptppmmtpu	1.788e+43	4.60	4.60	7.970e+39	0.0348
7496	diHPCARP_Ib.pmmtmmpmu	2.728e+43	4.87	4.87	7.729e+39	0.0338
7497	diHPCARP_Ib.pppmtmtmu	1.542e+44	5.92	5.92	7.491e+39	0.0327
7498	diHPCARP_Ib.tmmmpmtmu	5.111e+43	5.27	5.27	7.444e+39	0.0325
7499	diHPCARP_Ib.mppmpttpu	1.648e+43	4.60	4.60	7.323e+39	0.032
7500	diHPCARP_Ib.tppmptmmu	1.854e+43	4.68	4.68	7.218e+39	0.0316
7501	diHPCARP_Ib.tpppmtmu	8.855e+44	6.99	6.99	7.114e+39	0.0311
7502	diHPCARP_Ib.pmmmpmmpu	3.412e+43	5.06	5.06	7.067e+39	0.0309
7503	diHPCARP_Ib.ptppmpppu	3.057e+43	5.00	5.00	6.968e+39	0.0305
7504	diHPCARP_Ib.tttmpttmu	1.780e+44	6.06	6.06	6.835e+39	0.0299
7505	diHPCARP_Ib.pmtmnpmpu	6.664e+43	5.49	5.49	6.692e+39	0.0293
7506	diHPCARP_Ib.ptmnpmpmu	1.982e+43	4.78	4.78	6.579e+39	0.0288
7507	diHPCARP_Ib.pmtmnpmpu	6.228e+43	5.46	5.46	6.567e+39	0.0287
7508	diHPCARP_Ib.ptppmptpu	5.065e+43	5.34	5.34	6.509e+39	0.0285
7509	diHPCARP_Ib.pmmmpmpmu	1.587e+43	4.67	4.67	6.271e+39	0.0274
7510	diHPCARP_Ib.tmtmmmpmu	1.566e+44	6.04	6.04	6.249e+39	0.0273
7511	diHPCARP_Ib.tpppmtmu	1.515e+45	7.40	7.40	6.200e+39	0.0271
7512	diHPCARP_Ib.mmtppmpmu	4.368e+43	5.28	5.28	6.195e+39	0.0271
7513	diHPCARP_Ib.pmmtpmmpu	6.301e+43	5.51	5.51	6.086e+39	0.0266
7514	diHPCARP_Ib.ptpmpmtmu	3.565e+43	5.18	5.18	6.050e+39	0.0264
7515	diHPCARP_Ib.pppmmpmu	3.088e+44	6.47	6.47	5.990e+39	0.0262
7516	diHPCARP_Ib.mmtmmpmpu	3.767e+43	5.22	5.22	5.978e+39	0.0261
7517	diHPCARP_Ib.mppmmttpu	8.891e+43	5.73	5.73	5.930e+39	0.0259
7518	diHPCARP_Ib.ppppmttmu	1.931e+43	4.83	4.83	5.882e+39	0.0257
7519	diHPCARP_Ib.mpppmtmmu	2.966e+43	5.09	5.09	5.846e+39	0.0256
7520	diHPCARP_Ib.pptmpmpmu	8.400e+43	5.71	5.71	5.834e+39	0.0255
7521	diHPCARP_Ib.mpppppppu	3.741e+43	5.24	5.24	5.709e+39	0.025
7522	diHPCARP_Ib.pmpmtmtmu	7.146e+43	5.63	5.63	5.675e+39	0.0248
7523	diHPCARP_Ib.tmmmpmmpu	3.840e+43	5.27	5.27	5.582e+39	0.0244
7524	diHPCARP_Ib.pptpmpmpu	3.844e+43	5.29	5.29	5.420e+39	0.0237
7525	diHPCARP_Ib.mmtmmpmpu	4.803e+43	5.42	5.42	5.367e+39	0.0235
7526	diHPCARP_Ib.pptmptpmu	6.779e+43	5.64	5.64	5.295e+39	0.0231
7527	diHPCARP_Ib.ptmmpmtpu	3.410e+43	5.24	5.24	5.175e+39	0.0226
7528	diHPCARP_Ib.tttmpttpu	6.050e+43	5.60	5.60	5.058e+39	0.0221
7529	diHPCARP_Ib.mmtmmpmpu	4.376e+43	5.41	5.41	5.040e+39	0.022
7530	diHPCARP_Ib.tptmmttmu	5.314e+44	6.90	6.90	5.026e+39	0.022
7531	diHPCARP_Ib.tppppmpmu	1.936e+44	6.31	6.31	4.911e+39	0.0215
7532	diHPCARP_Ib.mtppmtmpu	1.904e+43	4.93	4.93	4.899e+39	0.0214
7533	diHPCARP_Ib.mmmmpmtmu	5.739e+43	5.59	5.59	4.834e+39	0.0211
7534	diHPCARP_Ib.mmtppmtmu	6.504e+43	5.70	5.70	4.602e+39	0.0201
7535	diHPCARP_Ib.ppppmtmmu	2.051e+43	5.01	5.01	4.588e+39	0.0201
7536	diHPCARP_Ib.pmmmmmpmu	2.342e+43	5.09	5.09	4.581e+39	0.02

7537	diHPCARP_Ib.tpmmpmttmu	6.172e+43	5.68	5.68	4.527e+39	0.0198
7538	diHPCARP_Ib.pmtppmpppu	3.728e+43	5.38	5.38	4.496e+39	0.0197
7539	diHPCARP_Ib.ppppppttpu	1.997e+44	6.40	6.40	4.378e+39	0.0191
7540	diHPCARP_Ib.mmpmpmpmpu	1.900e+43	5.02	5.02	4.217e+39	0.0184
7541	diHPCARP_Ib.pppmptpmu	1.832e+43	5.03	5.03	3.939e+39	0.0172
7542	diHPCARP_Ib.pptppmpppu	9.818e+43	6.04	6.04	3.904e+39	0.0171
7543	diHPCARP_Ib.tptmpmpmu	2.260e+44	6.54	6.54	3.867e+39	0.0169
7544	diHPCARP_Ib.mmtmmpppu	3.186e+43	5.39	5.39	3.776e+39	0.0165
7545	diHPCARP_Ib.mppppptpu	5.659e+43	5.74	5.74	3.699e+39	0.0162
7546	diHPCARP_Ib.tmttmppmu	1.085e+44	6.13	6.13	3.695e+39	0.0162
7547	diHPCARP_Ib.mppmptppu	8.995e+42	4.65	4.65	3.681e+39	0.0161
7548	diHPCARP_Ib.tmpmptppu	2.546e+43	5.27	5.27	3.666e+39	0.016
7549	diHPCARP_Ib.tppppptpu	2.996e+44	6.75	6.75	3.604e+39	0.0158
7550	diHPCARP_Ib.ptttmtpmu	1.211e+44	6.21	6.21	3.603e+39	0.0157
7551	diHPCARP_Ib.pppmpttpu	5.088e+43	5.70	5.70	3.588e+39	0.0157
7552	diHPCARP_Ib.ptppppptpu	8.665e+43	6.02	6.02	3.574e+39	0.0156
7553	diHPCARP_Ib.tppmpmpmu	2.525e+43	5.29	5.29	3.563e+39	0.0156
7554	diHPCARP_Ib.tmpmpmtmu	3.198e+43	5.44	5.44	3.495e+39	0.0153
7555	diHPCARP_Ib.ptmtppptpu	6.748e+43	5.89	5.89	3.466e+39	0.0152
7556	diHPCARP_Ib.ptmppttmu	1.595e+44	6.41	6.41	3.408e+39	0.0149
7557	diHPCARP_Ib.tppmptmu	4.070e+43	5.60	5.60	3.405e+39	0.0149
7558	diHPCARP_Ib.pmtmpttmu	1.110e+44	6.20	6.20	3.391e+39	0.0148
7559	diHPCARP_Ib.mmmmtmmmu	3.220e+43	5.47	5.47	3.344e+39	0.0146
7560	diHPCARP_Ib.tmpmpmtmu	8.781e+43	6.07	6.07	3.339e+39	0.0146
7561	diHPCARP_Ib.mppmpttmu	4.917e+43	5.74	5.74	3.260e+39	0.0143
7562	diHPCARP_Ib.mppppmtpu	1.071e+44	6.20	6.20	3.256e+39	0.0142
7563	diHPCARP_Ib.pmtpppppu	1.082e+44	6.21	6.21	3.256e+39	0.0142
7564	diHPCARP_Ib.tmtmmmtmu	2.687e+44	6.75	6.75	3.243e+39	0.0142
7565	diHPCARP_Ib.mppmptpmu	2.606e+43	5.36	5.36	3.237e+39	0.0141
7566	diHPCARP_Ib.pppmmpmtmu	1.630e+43	5.09	5.09	3.183e+39	0.0139
7567	diHPCARP_Ib.tppmpttmu	4.546e+43	5.71	5.71	3.170e+39	0.0139
7568	diHPCARP_Ib.ptttptpmu	1.201e+44	6.29	6.29	3.124e+39	0.0137
7569	diHPCARP_Ib.pppmmtmmu	1.761e+43	5.16	5.16	3.082e+39	0.0135
7570	diHPCARP_Ib.ptppppppu	5.733e+43	5.89	5.89	2.944e+39	0.0129
7571	diHPCARP_Ib.tptmmmpmu	1.840e+44	6.58	6.58	2.939e+39	0.0128
7572	diHPCARP_Ib.mppppptmpu	5.900e+43	5.92	5.92	2.862e+39	0.0125
7573	diHPCARP_Ib.tppmptmmu	2.128e+43	5.32	5.32	2.840e+39	0.0124
7574	diHPCARP_Ib.tmtppmmmu	1.016e+44	6.26	6.26	2.800e+39	0.0122
7575	diHPCARP_Ib.pttmpttpu	2.788e+43	5.49	5.49	2.785e+39	0.0122
7576	diHPCARP_Ib.ppttppmpu	1.405e+44	6.46	6.46	2.743e+39	0.012
7577	diHPCARP_Ib.ptmtpttmu	3.406e+44	7.00	7.00	2.720e+39	0.0119
7578	diHPCARP_Ib.pppptmptmu	9.318e+43	6.24	6.24	2.638e+39	0.0115
7579	diHPCARP_Ib.mmtmppppu	4.977e+43	5.87	5.87	2.615e+39	0.0114
7580	diHPCARP_Ib.tmmtpmmmu	1.093e+44	6.36	6.36	2.563e+39	0.0112
7581	diHPCARP_Ib.tppmpttmu	6.737e+43	6.09	6.09	2.467e+39	0.0108
7582	diHPCARP_Ib.mmmmtmmmu	3.695e+43	5.74	5.74	2.443e+39	0.0107
7583	diHPCARP_Ib.ppppppppu	4.800e+43	5.90	5.90	2.419e+39	0.0106
7584	diHPCARP_Ib.ptmtmttmu	5.170e+43	5.95	5.95	2.409e+39	0.0105
7585	diHPCARP_Ib.mppmpttpu	2.351e+44	6.86	6.86	2.349e+39	0.0103
7586	diHPCARP_Ib.pmtmmmpmu	1.558e+44	6.62	6.62	2.339e+39	0.0102
7587	diHPCARP_Ib.mptppptpu	5.659e+43	6.02	6.02	2.314e+39	0.0101
7588	diHPCARP_Ib.mptmptppu	3.301e+43	5.72	5.72	2.263e+39	0.00989
7589	diHPCARP_Ib.tmttpppmu	8.838e+43	6.31	6.31	2.248e+39	0.00983
7590	diHPCARP_Ib.pmtppmtmu	7.776e+43	6.23	6.23	2.235e+39	0.00977
7591	diHPCARP_Ib.pptpmttpu	3.818e+44	7.19	7.19	2.223e+39	0.00972
7592	diHPCARP_Ib.tppmptmpu	2.938e+43	5.66	5.66	2.195e+39	0.0096
7593	diHPCARP_Ib.tppmpttpu	3.848e+43	5.85	5.85	2.122e+39	0.00928
7594	diHPCARP_Ib.tppppptpu	4.699e+44	7.34	7.34	2.099e+39	0.00918
7595	diHPCARP_Ib.mptmpttmu	1.125e+44	6.51	6.51	2.023e+39	0.00884
7596	diHPCARP_Ib.tppppptpmu	4.433e+44	7.35	7.35	1.961e+39	0.00857
7597	diHPCARP_Ib.pmpmtmmu	7.125e+43	6.27	6.27	1.919e+39	0.00839
7598	diHPCARP_Ib.pppmtmptmu	1.064e+44	6.52	6.52	1.884e+39	0.00823
7599	diHPCARP_Ib.tmtmpttpu	9.617e+43	6.47	6.47	1.872e+39	0.00818
7600	diHPCARP_Ib.tmtppmmmu	1.453e+44	6.72	6.72	1.837e+39	0.00803
7601	diHPCARP_Ib.tppmpmmmu	9.475e+43	6.47	6.47	1.835e+39	0.00802
7602	diHPCARP_Ib.ptptmmtmu	5.880e+43	6.19	6.19	1.820e+39	0.00796
7603	diHPCARP_Ib.tmpmpmmmu	3.375e+43	5.86	5.86	1.803e+39	0.00788
7604	diHPCARP_Ib.pppptppmpu	7.010e+43	6.30	6.30	1.796e+39	0.00785
7605	diHPCARP_Ib.pppmmpmpu	1.025e+44	6.54	6.54	1.769e+39	0.00773
7606	diHPCARP_Ib.tmmtpmpmu	6.055e+43	6.25	6.25	1.690e+39	0.00739
7607	diHPCARP_Ib.tpppmtpmu	6.458e+44	7.66	7.66	1.685e+39	0.00737
7608	diHPCARP_Ib.pmtppmmmu	6.999e+43	6.36	6.36	1.638e+39	0.00716

7609	diHPCARP_Ib.tptpmmtmu	9.360e+43	6.53	6.53	1.636e+39	0.00715
7610	diHPCARP_Ib.mmpmpttpu	3.692e+43	5.99	5.99	1.612e+39	0.00704
7611	diHPCARP_Ib.tptmptmpu	3.746e+44	7.38	7.38	1.569e+39	0.00686
7612	diHPCARP_Ib.ttpppmmmu	9.717e+43	6.61	6.61	1.482e+39	0.00648
7613	diHPCARP_Ib.ttptpttpu	6.201e+43	6.35	6.35	1.465e+39	0.00641
7614	diHPCARP_Ib.mmtmmtpu	5.993e+43	6.33	6.33	1.460e+39	0.00638
7615	diHPCARP_Ib.mmppttpu	4.844e+43	6.21	6.21	1.452e+39	0.00635
7616	diHPCARP_Ib.ptppmpmpu	5.802e+43	6.32	6.32	1.446e+39	0.00632
7617	diHPCARP_Ib.pmpppppmu	4.355e+43	6.15	6.15	1.436e+39	0.00628
7618	diHPCARP_Ib.tptpmmmmu	7.761e+43	6.51	6.51	1.410e+39	0.00616
7619	diHPCARP_Ib.ppmptmpu	2.188e+43	5.76	5.76	1.401e+39	0.00613
7620	diHPCARP_Ib.pmtmpttpu	4.011e+43	6.12	6.12	1.400e+39	0.00612
7621	diHPCARP_Ib.ptptmpppu	9.148e+43	6.61	6.61	1.396e+39	0.0061
7622	diHPCARP_Ib.pptmmtmu	7.210e+43	6.48	6.48	1.383e+39	0.00605
7623	diHPCARP_Ib.mmmmmmtmu	1.618e+44	6.96	6.96	1.378e+39	0.00602
7624	diHPCARP_Ib.pptmmtmu	9.865e+43	6.67	6.67	1.371e+39	0.006
7625	diHPCARP_Ib.tptmptmpu	2.660e+44	7.26	7.26	1.364e+39	0.00596
7626	diHPCARP_Ib.tmmmmmpmu	3.843e+43	6.11	6.11	1.357e+39	0.00593
7627	diHPCARP_Ib.ptppppmpu	1.368e+44	6.87	6.87	1.357e+39	0.00593
7628	diHPCARP_Ib.pptmppppu	9.327e+43	6.66	6.66	1.316e+39	0.00575
7629	diHPCARP_Ib.ppptmtmu	1.259e+44	6.84	6.84	1.313e+39	0.00574
7630	diHPCARP_Ib.pmppttpu	5.020e+43	6.29	6.29	1.307e+39	0.00572
7631	diHPCARP_Ib.tmtmmmmu	2.346e+44	7.22	7.22	1.296e+39	0.00566
7632	diHPCARP_Ib.mptmptmpu	1.388e+44	6.91	6.91	1.295e+39	0.00566
7633	diHPCARP_Ib.mmtmpttpu	8.884e+43	6.64	6.64	1.288e+39	0.00563
7634	diHPCARP_Ib.tptmmtmu	4.062e+44	7.56	7.56	1.273e+39	0.00556
7635	diHPCARP_Ib.pptmmpppu	1.121e+44	6.79	6.79	1.265e+39	0.00553
7636	diHPCARP_Ib.mptmmtmpu	2.514e+44	7.28	7.28	1.242e+39	0.00543
7637	diHPCARP_Ib.tmpmptmpu	2.911e+43	6.01	6.01	1.213e+39	0.0053
7638	diHPCARP_Ib.tptmmtmpu	3.181e+44	7.44	7.44	1.207e+39	0.00528
7639	diHPCARP_Ib.mpptmtpu	7.618e+43	6.61	6.61	1.156e+39	0.00505
7640	diHPCARP_Ib.mmtmpttpu	5.369e+43	6.41	6.41	1.152e+39	0.00503
7641	diHPCARP_Ib.pmpmptmpu	7.736e+43	6.63	6.63	1.150e+39	0.00503
7642	diHPCARP_Ib.mmpppppmu	6.575e+43	6.53	6.53	1.145e+39	0.00501
7643	diHPCARP_Ib.ttptpttpu	2.587e+43	5.98	5.98	1.143e+39	0.00499
7644	diHPCARP_Ib.mmtmpttpu	6.822e+43	6.58	6.58	1.101e+39	0.00481
7645	diHPCARP_Ib.ppmptmpu	1.604e+43	5.72	5.72	1.096e+39	0.00479
7646	diHPCARP_Ib.mptmmtmpu	1.880e+43	5.81	5.81	1.092e+39	0.00477
7647	diHPCARP_Ib.mmpmmmtmu	4.469e+44	7.71	7.71	1.086e+39	0.00475
7648	diHPCARP_Ib.ptmmmpmpu	5.937e+43	6.51	6.51	1.077e+39	0.00471
7649	diHPCARP_Ib.mmpmptmpu	4.774e+43	6.39	6.39	1.057e+39	0.00462
7650	diHPCARP_Ib.mptmpttpu	2.225e+43	5.94	5.94	1.052e+39	0.0046
7651	diHPCARP_Ib.ptmtppppu	4.972e+43	6.42	6.42	1.052e+39	0.0046
7652	diHPCARP_Ib.mtmpttpu	2.933e+43	6.10	6.10	1.050e+39	0.00459
7653	diHPCARP_Ib.mmpmpmpu	1.114e+43	5.53	5.53	1.042e+39	0.00456
7654	diHPCARP_Ib.mmmmtpppu	4.866e+43	6.41	6.41	1.033e+39	0.00452
7655	diHPCARP_Ib.tmmmmmtmu	2.622e+44	7.42	7.42	1.030e+39	0.0045
7656	diHPCARP_Ib.tmttppmmu	2.266e+44	7.34	7.34	1.026e+39	0.00448
7657	diHPCARP_Ib.tttmpttpu	3.921e+44	7.66	7.66	1.022e+39	0.00447
7658	diHPCARP_Ib.ptmmpptpu	2.513e+43	6.03	6.03	1.012e+39	0.00443
7659	diHPCARP_Ib.ttpmppppu	5.271e+43	6.48	6.48	1.003e+39	0.00439
7660	diHPCARP_Ib.mmtmptmpu	1.795e+44	7.21	7.21	1.001e+39	0.00437
7661	diHPCARP_Ib.tmtmpttpu	1.245e+44	7.00	7.00	9.927e+38	0.00434
7662	diHPCARP_Ib.tmtmptmpu	1.514e+45	8.49	8.49	9.914e+38	0.00433
7663	diHPCARP_Ib.mpmmmmtmu	3.320e+43	6.22	6.22	9.805e+38	0.00429
7664	diHPCARP_Ib.tmmmmmtmu	1.071e+44	6.92	6.92	9.745e+38	0.00426
7665	diHPCARP_Ib.ttppttpu	5.575e+44	7.91	7.91	9.687e+38	0.00423
7666	diHPCARP_Ib.ptmtpmpu	9.482e+43	6.86	6.86	9.556e+38	0.00418
7667	diHPCARP_Ib.pptmmtmu	4.812e+44	7.83	7.83	9.518e+38	0.00416
7668	diHPCARP_Ib.pmtmmpu	9.935e+43	6.89	6.89	9.481e+38	0.00414
7669	diHPCARP_Ib.mpmptmpu	1.824e+43	5.88	5.88	9.439e+38	0.00413
7670	diHPCARP_Ib.ttpmpttpu	7.589e+43	6.74	6.74	9.373e+38	0.0041
7671	diHPCARP_Ib.mptmtpu	8.241e+43	6.79	6.79	9.372e+38	0.0041
7672	diHPCARP_Ib.tptmmmmu	1.443e+44	7.12	7.12	9.321e+38	0.00407
7673	diHPCARP_Ib.ptmtpmpu	1.081e+44	6.96	6.96	9.125e+38	0.00399
7674	diHPCARP_Ib.ttpmpttpu	2.724e+43	6.15	6.15	8.948e+38	0.00391
7675	diHPCARP_Ib.ptptptmpu	3.834e+43	6.36	6.36	8.896e+38	0.00389
7676	diHPCARP_Ib.pmttppppu	1.105e+44	7.01	7.01	8.646e+38	0.00378
7677	diHPCARP_Ib.ptptptmu	7.558e+43	6.79	6.79	8.573e+38	0.00375
7678	diHPCARP_Ib.pptpptmpu	2.500e+44	7.51	7.51	8.457e+38	0.0037
7679	diHPCARP_Ib.pppptmpu	1.218e+44	7.08	7.08	8.421e+38	0.00368
7680	diHPCARP_Ib.ttppttpu	1.428e+44	7.19	7.19	8.315e+38	0.00364

7681	diHPCARP_Ib.tmtmptppu	3.893e+44	7.79	7.79	8.228e+38	0.0036
7682	diHPCARP_Ib.pptmmtmpu	3.650e+44	7.76	7.76	8.057e+38	0.00352
7683	diHPCARP_Ib.ppptptpmu	1.015e+44	7.01	7.01	7.946e+38	0.00347
7684	diHPCARP_Ib.ptptmptpu	1.618e+44	7.29	7.29	7.941e+38	0.00347
7685	diHPCARP_Ib.ppppmtmmu	1.816e+44	7.36	7.36	7.940e+38	0.00347
7686	diHPCARP_Ib.tpppmtmmu	1.610e+44	7.30	7.30	7.764e+38	0.00339
7687	diHPCARP_Ib.mpttptppu	1.289e+44	7.17	7.17	7.740e+38	0.00338
7688	diHPCARP_Ib.pmtmptpmu	3.160e+43	6.33	6.33	7.673e+38	0.00335
7689	diHPCARP_Ib.ptmpptpu	4.363e+43	6.54	6.54	7.509e+38	0.00328
7690	diHPCARP_Ib.ttmmtmmu	5.416e+43	6.67	6.67	7.492e+38	0.00328
7691	diHPCARP_Ib.tptmmtppu	4.878e+44	7.99	7.99	7.425e+38	0.00325
7692	diHPCARP_Ib.tttppmpmu	9.092e+43	6.99	6.99	7.399e+38	0.00323
7693	diHPCARP_Ib.pptmptpmu	7.969e+43	6.91	6.91	7.386e+38	0.00323
7694	diHPCARP_Ib.mpppmttmu	4.876e+44	7.99	7.99	7.385e+38	0.00323
7695	diHPCARP_Ib.tptmptppu	3.216e+44	7.75	7.75	7.278e+38	0.00318
7696	diHPCARP_Ib.tttmptpmu	4.157e+43	6.53	6.53	7.242e+38	0.00317
7697	diHPCARP_Ib.pmpmptpu	1.386e+43	5.88	5.88	7.219e+38	0.00316
7698	diHPCARP_Ib.ptmmpmpmu	4.312e+43	6.56	6.56	7.147e+38	0.00312
7699	diHPCARP_Ib.ptppmttmu	5.023e+44	8.03	8.03	7.115e+38	0.00311
7700	diHPCARP_Ib.tpppmtppu	1.931e+44	7.46	7.46	7.110e+38	0.00311
7701	diHPCARP_Ib.mttmptpmu	2.576e+44	7.64	7.64	7.010e+38	0.00306
7702	diHPCARP_Ib.tpppmtpmu	2.004e+44	7.49	7.49	7.009e+38	0.00306
7703	diHPCARP_Ib.tttppmttmu	1.053e+44	7.11	7.11	6.967e+38	0.00305
7704	diHPCARP_Ib.ppppmtmpu	7.326e+44	8.28	8.28	6.833e+38	0.00299
7705	diHPCARP_Ib.pptmptpmu	2.316e+44	7.59	7.59	6.832e+38	0.00299
7706	diHPCARP_Ib.ptmmpmpmu	3.073e+43	6.39	6.39	6.764e+38	0.00296
7707	diHPCARP_Ib.tpppmtmmu	1.765e+44	7.44	7.44	6.708e+38	0.00293
7708	diHPCARP_Ib.mmpmptmpu	2.664e+43	6.31	6.31	6.703e+38	0.00293
7709	diHPCARP_Ib.pmtmmtpmu	2.877e+43	6.37	6.37	6.595e+38	0.00288
7710	diHPCARP_Ib.pptpttmu	1.469e+44	7.36	7.36	6.439e+38	0.00281
7711	diHPCARP_Ib.tpptmmmmu	1.218e+44	7.25	7.25	6.417e+38	0.00281
7712	diHPCARP_Ib.ptmtmptpu	4.004e+43	6.60	6.60	6.276e+38	0.00274
7713	diHPCARP_Ib.mpptptppu	7.158e+43	6.95	6.95	6.168e+38	0.0027
7714	diHPCARP_Ib.mttmmpmpu	2.189e+44	7.63	7.63	6.095e+38	0.00266
7715	diHPCARP_Ib.tmmppmttmu	5.759e+43	6.85	6.85	5.935e+38	0.00259
7716	diHPCARP_Ib.tptmpttmu	2.335e+44	7.69	7.69	5.852e+38	0.00256
7717	diHPCARP_Ib.mttmptppu	1.987e+44	7.61	7.61	5.711e+38	0.0025
7718	diHPCARP_Ib.tptptpmu	3.704e+43	6.61	6.61	5.701e+38	0.00249
7719	diHPCARP_Ib.pptmptpmu	1.898e+44	7.59	7.59	5.658e+38	0.00247
7720	diHPCARP_Ib.tmpmpttmu	6.234e+43	6.92	6.92	5.655e+38	0.00247
7721	diHPCARP_Ib.tmmmpmtpmu	3.110e+43	6.51	6.51	5.651e+38	0.00247
7722	diHPCARP_Ib.mmmmmmtmmu	2.294e+44	7.71	7.71	5.557e+38	0.00243
7723	diHPCARP_Ib.mpppmttmu	6.921e+43	7.00	7.00	5.523e+38	0.00241
7724	diHPCARP_Ib.tmtmmtppu	2.518e+44	7.77	7.77	5.523e+38	0.00241
7725	diHPCARP_Ib.tmpmptmmu	5.317e+43	6.85	6.85	5.396e+38	0.00236
7726	diHPCARP_Ib.mpppmtmpu	6.052e+43	6.94	6.94	5.315e+38	0.00232
7727	diHPCARP_Ib.ttptpttmu	6.671e+43	7.01	7.01	5.262e+38	0.0023
7728	diHPCARP_Ib.ptmpptpmu	1.363e+44	7.43	7.43	5.240e+38	0.00229
7729	diHPCARP_Ib.ttpmptppu	3.654e+43	6.66	6.66	5.170e+38	0.00226
7730	diHPCARP_Ib.ttpmptpmu	1.006e+44	7.26	7.26	5.139e+38	0.00225
7731	diHPCARP_Ib.mmpmmpmpu	8.191e+43	7.14	7.14	5.133e+38	0.00224
7732	diHPCARP_Ib.mptmptmmu	2.224e+44	7.74	7.74	5.124e+38	0.00224
7733	diHPCARP_Ib.tttmpttmu	1.782e+44	7.63	7.63	4.957e+38	0.00217
7734	diHPCARP_Ib.tptmptmmu	3.712e+44	8.07	8.07	4.895e+38	0.00214
7735	diHPCARP_Ib.ptptptppu	4.646e+43	6.83	6.83	4.889e+38	0.00214
7736	diHPCARP_Ib.ppmmttmu	8.891e+43	7.23	7.23	4.815e+38	0.0021
7737	diHPCARP_Ib.ttpmpttmu	5.616e+43	6.96	6.96	4.778e+38	0.00209
7738	diHPCARP_Ib.tmpmpttmu	6.026e+43	7.01	7.01	4.730e+38	0.00207
7739	diHPCARP_Ib.mttmmtmpu	1.824e+44	7.68	7.68	4.659e+38	0.00204
7740	diHPCARP_Ib.mmmmmmtmmu	1.310e+44	7.49	7.49	4.587e+38	0.00201
7741	diHPCARP_Ib.mmtmptpu	1.047e+44	7.36	7.36	4.561e+38	0.00199
7742	diHPCARP_Ib.mptppmtpu	2.531e+44	7.90	7.90	4.484e+38	0.00196
7743	diHPCARP_Ib.tttmmtppu	2.066e+44	7.78	7.78	4.441e+38	0.00194
7744	diHPCARP_Ib.tptpmmmu	1.166e+44	7.44	7.44	4.416e+38	0.00193
7745	diHPCARP_Ib.pppmpttmu	6.668e+43	7.11	7.11	4.382e+38	0.00192
7746	diHPCARP_Ib.tmpmpttmu	5.251e+43	6.97	6.97	4.366e+38	0.00191
7747	diHPCARP_Ib.pptpmttmu	2.292e+44	7.85	7.85	4.365e+38	0.00191
7748	diHPCARP_Ib.ptppppmmu	3.470e+43	6.73	6.73	4.356e+38	0.0019
7749	diHPCARP_Ib.pptptpmu	4.410e+44	8.25	8.25	4.345e+38	0.0019
7750	diHPCARP_Ib.pmpmpttmu	4.459e+43	6.89	6.89	4.297e+38	0.00188
7751	diHPCARP_Ib.tmmmmmttmu	1.412e+44	7.59	7.59	4.179e+38	0.00183
7752	diHPCARP_Ib.tmmmpptppu	1.592e+43	6.29	6.29	4.170e+38	0.00182

7753	diHPCARP_Ib.mptmptpmu	9.075e+44	8.70	8.70	4.146e+38	0.00181
7754	diHPCARP_Ib.pmpptpmu	1.438e+44	7.61	7.61	4.137e+38	0.00181
7755	diHPCARP_Ib.tptpmttptu	2.240e+44	7.87	7.87	4.136e+38	0.00181
7756	diHPCARP_Ib.mpmptpmu	5.509e+43	7.04	7.04	4.121e+38	0.0018
7757	diHPCARP_Ib.tptmmttmu	6.373e+44	8.51	8.51	4.026e+38	0.00176
7758	diHPCARP_Ib.tpmnmtppu	2.827e+43	6.66	6.66	4.004e+38	0.00175
7759	diHPCARP_Ib.pppptpmu	2.600e+44	7.98	7.98	3.980e+38	0.00174
7760	diHPCARP_Ib.tmpmptppu	3.384e+43	6.77	6.77	3.976e+38	0.00174
7761	diHPCARP_Ib.ttmppppmu	2.116e+43	6.49	6.49	3.946e+38	0.00173
7762	diHPCARP_Ib.pmtppmmpu	2.049e+44	7.86	7.86	3.882e+38	0.0017
7763	diHPCARP_Ib.tpptmmtmu	2.147e+44	7.88	7.88	3.876e+38	0.00169
7764	diHPCARP_Ib.mttmmtppu	1.184e+44	7.53	7.53	3.851e+38	0.00168
7765	diHPCARP_Ib.tppppppmu	7.036e+43	7.23	7.23	3.794e+38	0.00166
7766	diHPCARP_Ib.tpmnmpmpu	1.302e+43	6.23	6.23	3.791e+38	0.00166
7767	diHPCARP_Ib.tpppmtpmu	1.793e+44	7.79	7.79	3.782e+38	0.00165
7768	diHPCARP_Ib.mmtptttmu	2.907e+44	8.08	8.08	3.775e+38	0.00165
7769	diHPCARP_Ib.mttmmpmpu	1.587e+44	7.72	7.72	3.767e+38	0.00165
7770	diHPCARP_Ib.mmpmtmtpu	6.760e+43	7.21	7.21	3.751e+38	0.00164
7771	diHPCARP_Ib.tpptpmtmu	2.370e+44	7.97	7.97	3.678e+38	0.00161
7772	diHPCARP_Ib.mmpmmmpmu	6.364e+43	7.19	7.19	3.662e+38	0.0016
7773	diHPCARP_Ib.tmtmptmpu	3.822e+44	8.26	8.26	3.654e+38	0.0016
7774	diHPCARP_Ib.pmmmpmtpu	1.665e+43	6.40	6.40	3.596e+38	0.00157
7775	diHPCARP_Ib.ptppmtppu	2.234e+43	6.59	6.59	3.550e+38	0.00155
7776	diHPCARP_Ib.tpppmttptu	4.093e+43	6.95	6.95	3.549e+38	0.00155
7777	diHPCARP_Ib.tmtpmtppu	2.692e+44	8.08	8.08	3.523e+38	0.00154
7778	diHPCARP_Ib.ppmmtmmtmu	1.140e+44	7.58	7.58	3.455e+38	0.00151
7779	diHPCARP_Ib.ptmtptpmu	7.413e+43	7.33	7.33	3.411e+38	0.00149
7780	diHPCARP_Ib.tmtmmttptu	7.945e+43	7.37	7.37	3.395e+38	0.00148
7781	diHPCARP_Ib.mmtpmmttmu	4.598e+44	8.42	8.42	3.365e+38	0.00147
7782	diHPCARP_Ib.ppmmpmmmu	1.068e+43	6.18	6.18	3.343e+38	0.00146
7783	diHPCARP_Ib.pmpptttmu	6.506e+43	7.27	7.27	3.310e+38	0.00145
7784	diHPCARP_Ib.mppppmtmu	1.398e+44	7.73	7.73	3.293e+38	0.00144
7785	diHPCARP_Ib.ptmpmptpu	4.746e+43	7.09	7.09	3.271e+38	0.00143
7786	diHPCARP_Ib.tpppmtpmu	1.678e+44	7.85	7.85	3.228e+38	0.00141
7787	diHPCARP_Ib.pmmppmmpu	1.720e+43	6.49	6.49	3.223e+38	0.00141
7788	diHPCARP_Ib.mmtmmmpmu	2.504e+44	8.09	8.09	3.194e+38	0.0014
7789	diHPCARP_Ib.tppmpmpu	9.459e+43	7.52	7.52	3.171e+38	0.00139
7790	diHPCARP_Ib.tmtpmtmu	8.678e+43	7.47	7.47	3.145e+38	0.00137
7791	diHPCARP_Ib.pmtppmmpu	2.674e+44	8.14	8.14	3.134e+38	0.00137
7792	diHPCARP_Ib.mpmnmttmu	1.674e+44	7.87	7.87	3.082e+38	0.00135
7793	diHPCARP_Ib.mmtmpmmpu	9.427e+43	7.53	7.53	3.080e+38	0.00135
7794	diHPCARP_Ib.mmpptpppu	7.978e+43	7.43	7.43	3.076e+38	0.00134
7795	diHPCARP_Ib.tmtppptpu	3.563e+44	8.33	8.33	3.039e+38	0.00133
7796	diHPCARP_Ib.tpppmpmu	1.275e+44	7.72	7.72	3.016e+38	0.00132
7797	diHPCARP_Ib.mptpmtmpu	4.569e+43	7.12	7.12	2.993e+38	0.00131
7798	diHPCARP_Ib.pmttmmpu	2.012e+44	8.00	8.00	2.972e+38	0.0013
7799	diHPCARP_Ib.tpptmttptu	7.619e+44	8.81	8.81	2.902e+38	0.00127
7800	diHPCARP_Ib.mpmptpmpu	4.306e+43	7.11	7.11	2.866e+38	0.00125
7801	diHPCARP_Ib.ptppptpmu	1.375e+44	7.80	7.80	2.840e+38	0.00124
7802	diHPCARP_Ib.mtppppmpu	5.774e+44	8.66	8.66	2.832e+38	0.00124
7803	diHPCARP_Ib.tmtmmtpmu	4.478e+44	8.51	8.51	2.828e+38	0.00124
7804	diHPCARP_Ib.pptmmtmmtmu	3.115e+44	8.30	8.30	2.821e+38	0.00123
7805	diHPCARP_Ib.mmtpmmttptu	3.168e+44	8.31	8.31	2.781e+38	0.00122
7806	diHPCARP_Ib.tttmmtmpu	3.101e+44	8.31	8.31	2.758e+38	0.00121
7807	diHPCARP_Ib.ptmtmtpmu	1.603e+44	7.92	7.92	2.733e+38	0.00119
7808	diHPCARP_Ib.tttmptpmu	4.140e+44	8.48	8.48	2.732e+38	0.00119
7809	diHPCARP_Ib.mmtpmmtmu	1.487e+45	9.25	9.25	2.730e+38	0.00119
7810	diHPCARP_Ib.tptpmmmu	1.500e+44	7.89	7.89	2.694e+38	0.00118
7811	diHPCARP_Ib.tmtpmtpmu	5.141e+44	8.62	8.62	2.692e+38	0.00118
7812	diHPCARP_Ib.mtmnmtmpu	7.916e+43	7.51	7.51	2.670e+38	0.00117
7813	diHPCARP_Ib.tpmnmtmpu	4.502e+43	7.18	7.18	2.656e+38	0.00116
7814	diHPCARP_Ib.tmmpnmttptu	2.810e+43	6.90	6.90	2.653e+38	0.00116
7815	diHPCARP_Ib.mptmmtmmtmu	2.633e+44	8.24	8.24	2.621e+38	0.00115
7816	diHPCARP_Ib.ptppppppmu	4.505e+43	7.19	7.19	2.620e+38	0.00115
7817	diHPCARP_Ib.ptpmnmmmu	5.132e+43	7.27	7.27	2.596e+38	0.00113
7818	diHPCARP_Ib.ptptmtpmu	8.422e+43	7.57	7.57	2.558e+38	0.00112
7819	diHPCARP_Ib.tmmppmmpu	8.388e+43	7.57	7.57	2.547e+38	0.00111
7820	diHPCARP_Ib.pmtmmtmpu	3.218e+44	8.39	8.39	2.489e+38	0.00109
7821	diHPCARP_Ib.mtmnmtmpu	6.238e+43	7.41	7.41	2.484e+38	0.00109
7822	diHPCARP_Ib.mmpmtmtpu	1.553e+44	7.97	7.97	2.446e+38	0.00107
7823	diHPCARP_Ib.mptpmttmu	5.593e+44	8.74	8.74	2.395e+38	0.00105
7824	diHPCARP_Ib.tptpmtmmtmu	9.464e+43	7.68	7.68	2.393e+38	0.00105

7825	diHPCARP_Ib.tmtptmtpu	2.270e+44	8.21	8.21	2.362e+38	0.00103
7826	diHPCARP_Ib.mmpmpttmu	3.461e+43	7.10	7.10	2.312e+38	0.00101
7827	diHPCARP_Ib.mmtmpppmu	1.990e+44	8.15	8.15	2.308e+38	0.00101
7828	diHPCARP_Ib.mttmpttmu	9.897e+43	7.74	7.74	2.283e+38	0.000998
7829	diHPCARP_Ib.ptppmptpu	3.929e+44	8.56	8.56	2.274e+38	0.000994
7830	diHPCARP_Ib.tpmmpmpmu	2.441e+43	6.91	6.91	2.256e+38	0.000986
7831	diHPCARP_Ib.ttpptmpu	3.287e+43	7.09	7.09	2.236e+38	0.000977
7832	diHPCARP_Ib.tppppmmu	1.244e+44	7.89	7.89	2.234e+38	0.000977
7833	diHPCARP_Ib.tmpmpttmu	4.525e+43	7.29	7.29	2.207e+38	0.000965
7834	diHPCARP_Ib.tmpmpmpmu	5.779e+43	7.45	7.45	2.179e+38	0.000952
7835	diHPCARP_Ib.mmtmpttmu	6.279e+44	8.87	8.87	2.156e+38	0.000943
7836	diHPCARP_Ib.pmtpttmu	4.409e+44	8.66	8.66	2.155e+38	0.000942
7837	diHPCARP_Ib.mmtmptpmu	1.465e+44	8.01	8.01	2.154e+38	0.000942
7838	diHPCARP_Ib.pmpmpmpu	1.811e+43	6.79	6.79	2.055e+38	0.000898
7839	diHPCARP_Ib.ttmpttmu	1.748e+44	8.15	8.15	2.017e+38	0.000882
7840	diHPCARP_Ib.tpmptmpu	2.250e+43	6.94	6.94	1.994e+38	0.000872
7841	diHPCARP_Ib.mmtmpttmu	2.181e+44	8.30	8.30	1.954e+38	0.000854
7842	diHPCARP_Ib.tttpttmu	2.026e+44	8.26	8.26	1.945e+38	0.00085
7843	diHPCARP_Ib.tmmpttmu	3.705e+44	8.62	8.62	1.941e+38	0.000849
7844	diHPCARP_Ib.tppmpmpmu	2.773e+43	7.09	7.09	1.905e+38	0.000833
7845	diHPCARP_Ib.pptmpttmu	3.220e+44	8.55	8.55	1.902e+38	0.000832
7846	diHPCARP_Ib.ptppptpu	1.891e+44	8.23	8.23	1.902e+38	0.000832
7847	diHPCARP_Ib.mmtmmpmu	6.976e+43	7.64	7.64	1.899e+38	0.00083
7848	diHPCARP_Ib.mmtmmpmpu	9.927e+43	7.85	7.85	1.882e+38	0.000823
7849	diHPCARP_Ib.tmpmpmpmu	7.067e+43	7.66	7.66	1.874e+38	0.000819
7850	diHPCARP_Ib.tmtmppppu	1.691e+44	8.18	8.18	1.873e+38	0.000819
7851	diHPCARP_Ib.tpptmpttmu	6.852e+44	9.01	9.01	1.863e+38	0.000814
7852	diHPCARP_Ib.mtmmpptpu	7.830e+43	7.72	7.72	1.848e+38	0.000808
7853	diHPCARP_Ib.tttmptpmu	2.606e+44	8.44	8.44	1.845e+38	0.000807
7854	diHPCARP_Ib.tppmmpttmu	1.055e+44	7.91	7.91	1.835e+38	0.000802
7855	diHPCARP_Ib.tmtmpttmu	5.539e+44	8.90	8.90	1.832e+38	0.000801
7856	diHPCARP_Ib.pppmpttmu	3.334e+44	8.60	8.60	1.827e+38	0.000798
7857	diHPCARP_Ib.tmmpttmu	3.313e+44	8.59	8.59	1.826e+38	0.000798
7858	diHPCARP_Ib.tttmpttmu	3.719e+44	8.67	8.67	1.806e+38	0.00079
7859	diHPCARP_Ib.mpppttmu	1.077e+44	7.93	7.93	1.804e+38	0.000788
7860	diHPCARP_Ib.pmtpttmu	2.307e+44	8.39	8.39	1.789e+38	0.000782
7861	diHPCARP_Ib.pmptmpmu	5.097e+43	7.49	7.49	1.773e+38	0.000775
7862	diHPCARP_Ib.mmppttmu	7.523e+43	7.73	7.73	1.765e+38	0.000772
7863	diHPCARP_Ib.tptpmtpu	8.879e+44	9.21	9.21	1.745e+38	0.000763
7864	diHPCARP_Ib.mmmmmmmmu	2.025e+44	8.33	8.33	1.718e+38	0.000751
7865	diHPCARP_Ib.tmtmpttmu	2.709e+44	8.51	8.51	1.716e+38	0.00075
7866	diHPCARP_Ib.mmpmpmpmu	5.294e+43	7.54	7.54	1.707e+38	0.000746
7867	diHPCARP_Ib.mtmpttmu	7.280e+43	7.73	7.73	1.703e+38	0.000744
7868	diHPCARP_Ib.mttpttmu	9.957e+43	7.92	7.92	1.698e+38	0.000742
7869	diHPCARP_Ib.mptmpttmu	5.141e+43	7.52	7.52	1.696e+38	0.000741
7870	diHPCARP_Ib.mttpttmu	1.640e+44	8.22	8.22	1.694e+38	0.000741
7871	diHPCARP_Ib.ttmmppttmu	2.840e+43	7.17	7.17	1.685e+38	0.000737
7872	diHPCARP_Ib.mtptpttmu	2.620e+43	7.13	7.13	1.679e+38	0.000734
7873	diHPCARP_Ib.pttmppppu	5.351e+43	7.56	7.56	1.678e+38	0.000733
7874	diHPCARP_Ib.mmpmptpmu	3.104e+43	7.24	7.24	1.655e+38	0.000724
7875	diHPCARP_Ib.mmmmttmu	3.647e+44	8.71	8.71	1.651e+38	0.000722
7876	diHPCARP_Ib.pptmpttmu	9.057e+43	7.88	7.88	1.647e+38	0.00072
7877	diHPCARP_Ib.mttpttmu	9.853e+43	7.93	7.93	1.642e+38	0.000718
7878	diHPCARP_Ib.ttpmpttmu	2.574e+44	8.51	8.51	1.636e+38	0.000715
7879	diHPCARP_Ib.mptpmttmu	1.038e+44	7.97	7.97	1.615e+38	0.000706
7880	diHPCARP_Ib.pmptppppu	1.806e+43	6.94	6.94	1.600e+38	0.0007
7881	diHPCARP_Ib.tmppppttmu	1.374e+44	8.15	8.15	1.598e+38	0.000699
7882	diHPCARP_Ib.mmtppmpmu	2.617e+44	8.55	8.55	1.539e+38	0.000673
7883	diHPCARP_Ib.tptmpttmu	1.227e+44	8.10	8.10	1.530e+38	0.000669
7884	diHPCARP_Ib.mtptpttmu	5.426e+43	7.62	7.62	1.514e+38	0.000662
7885	diHPCARP_Ib.tttpttmu	2.522e+44	8.54	8.54	1.505e+38	0.000658
7886	diHPCARP_Ib.ptmmpmpmu	6.077e+43	7.70	7.70	1.502e+38	0.000657
7887	diHPCARP_Ib.mtmpttmu	4.508e+43	7.52	7.52	1.494e+38	0.000653
7888	diHPCARP_Ib.mpppmttmu	1.924e+44	8.40	8.40	1.471e+38	0.000643
7889	diHPCARP_Ib.mtptpttmu	2.616e+43	7.21	7.21	1.466e+38	0.000641
7890	diHPCARP_Ib.ttmmpmpmu	1.437e+44	8.23	8.23	1.462e+38	0.000639
7891	diHPCARP_Ib.pptmpttmu	5.830e+43	7.69	7.69	1.452e+38	0.000635
7892	diHPCARP_Ib.mmpmpmpmu	4.271e+43	7.51	7.51	1.442e+38	0.00063
7893	diHPCARP_Ib.mpppmttmu	1.227e+44	8.14	8.14	1.431e+38	0.000625
7894	diHPCARP_Ib.ttmmppttmu	2.214e+44	8.50	8.50	1.419e+38	0.00062
7895	diHPCARP_Ib.tptpmttmu	2.409e+44	8.55	8.55	1.416e+38	0.000619
7896	diHPCARP_Ib.pptpmttmu	3.327e+44	8.75	8.75	1.412e+38	0.000617

7897	diHPCARP_Ib.ppmtptpmu	8.514e+43	7.94	7.94	1.401e+38	0.000612
7898	diHPCARP_Ib.mpttmtmpu	1.939e+44	8.44	8.44	1.386e+38	0.000606
7899	diHPCARP_Ib.pttpmptpu	1.412e+44	8.26	8.26	1.348e+38	0.000589
7900	diHPCARP_Ib.tpmptpmu	4.158e+43	7.55	7.55	1.311e+38	0.000573
7901	diHPCARP_Ib.tptmmpmu	1.173e+44	8.17	8.17	1.301e+38	0.000569
7902	diHPCARP_Ib.mmmppmtmu	4.974e+43	7.67	7.67	1.288e+38	0.000563
7903	diHPCARP_Ib.pptmttptu	3.400e+44	8.82	8.82	1.283e+38	0.000561
7904	diHPCARP_Ib.tptpmtpmu	1.202e+44	8.20	8.20	1.271e+38	0.000555
7905	diHPCARP_Ib.tmtmmpppu	7.886e+43	7.95	7.95	1.266e+38	0.000554
7906	diHPCARP_Ib.tptpmmmpu	5.540e+43	7.74	7.74	1.265e+38	0.000553
7907	diHPCARP_Ib.tpttmmmpu	1.363e+44	8.28	8.28	1.263e+38	0.000552
7908	diHPCARP_Ib.ppppmtppu	1.609e+44	8.38	8.38	1.258e+38	0.00055
7909	diHPCARP_Ib.pmpmtmpu	2.703e+44	8.70	8.70	1.245e+38	0.000544
7910	diHPCARP_Ib.mmtppppmu	1.282e+44	8.26	8.26	1.242e+38	0.000543
7911	diHPCARP_Ib.mmtpmtpmu	9.538e+43	8.08	8.08	1.234e+38	0.00054
7912	diHPCARP_Ib.ttmmttptu	1.531e+44	8.37	8.37	1.232e+38	0.000538
7913	diHPCARP_Ib.tmpmptpmu	4.084e+43	7.58	7.58	1.228e+38	0.000537
7914	diHPCARP_Ib.mmtmmtmmu	5.292e+44	9.11	9.11	1.221e+38	0.000534
7915	diHPCARP_Ib.ptptmmpu	1.550e+44	8.38	8.38	1.219e+38	0.000533
7916	diHPCARP_Ib.pptpmtppu	2.179e+44	8.59	8.59	1.209e+38	0.000528
7917	diHPCARP_Ib.pmpptmmpu	6.298e+43	7.85	7.85	1.203e+38	0.000526
7918	diHPCARP_Ib.mmpmptmmu	2.831e+43	7.38	7.38	1.190e+38	0.00052
7919	diHPCARP_Ib.pttmmmpu	3.275e+43	7.47	7.47	1.185e+38	0.000518
7920	diHPCARP_Ib.tpptptmmu	3.937e+44	8.95	8.95	1.182e+38	0.000517
7921	diHPCARP_Ib.tmtpptpmu	5.191e+44	9.12	9.12	1.181e+38	0.000516
7922	diHPCARP_Ib.pptmtmpu	1.054e+44	8.17	8.17	1.176e+38	0.000514
7923	diHPCARP_Ib.tptpmtpmu	1.529e+44	8.40	8.40	1.170e+38	0.000512
7924	diHPCARP_Ib.pptpmtmmu	7.240e+43	7.95	7.95	1.164e+38	0.000509
7925	diHPCARP_Ib.ptptmpmpu	1.637e+44	8.44	8.44	1.161e+38	0.000507
7926	diHPCARP_Ib.tmmtmmppu	2.697e+43	7.37	7.37	1.156e+38	0.000505
7927	diHPCARP_Ib.mmmtmmppu	3.738e+43	7.57	7.57	1.152e+38	0.000504
7928	diHPCARP_Ib.mpmmtmpu	7.953e+43	8.02	8.02	1.149e+38	0.000502
7929	diHPCARP_Ib.pppmtmpu	2.006e+43	7.21	7.21	1.122e+38	0.00049
7930	diHPCARP_Ib.tpptpttmu	7.764e+44	9.39	9.39	1.119e+38	0.000489
7931	diHPCARP_Ib.mtpmptpmu	2.497e+43	7.34	7.34	1.114e+38	0.000487
7932	diHPCARP_Ib.pptmtmpu	1.565e+44	8.44	8.44	1.105e+38	0.000483
7933	diHPCARP_Ib.mtpmpttpu	4.414e+43	7.69	7.69	1.103e+38	0.000482
7934	diHPCARP_Ib.tmtmpttpu	6.474e+43	7.92	7.92	1.098e+38	0.00048
7935	diHPCARP_Ib.mtppmmpu	2.225e+43	7.29	7.29	1.090e+38	0.000477
7936	diHPCARP_Ib.ptmpmmppu	2.238e+43	7.80	7.80	1.083e+38	0.000473
7937	diHPCARP_Ib.tttptmpu	2.485e+44	8.73	8.73	1.080e+38	0.000472
7938	diHPCARP_Ib.tmtmmtmu	2.889e+44	8.83	8.83	1.076e+38	0.00047
7939	diHPCARP_Ib.ptmtpptpu	2.252e+44	8.68	8.68	1.072e+38	0.000469
7940	diHPCARP_Ib.ptmppmmpu	6.511e+43	7.95	7.95	1.052e+38	0.00046
7941	diHPCARP_Ib.mmmppmmpu	4.616e+43	7.75	7.75	1.048e+38	0.000458
7942	diHPCARP_Ib.ttpmmttptu	6.287e+43	7.93	7.93	1.047e+38	0.000458
7943	diHPCARP_Ib.pptmmtppu	8.272e+44	9.47	9.47	1.040e+38	0.000455
7944	diHPCARP_Ib.tmmppmmpu	2.103e+43	7.29	7.29	1.030e+38	0.00045
7945	diHPCARP_Ib.tmtpmtmpu	2.144e+44	8.68	8.68	1.027e+38	0.000449
7946	diHPCARP_Ib.mpmmttptu	2.214e+44	8.70	8.70	1.025e+38	0.000448
7947	diHPCARP_Ib.ppptpttpu	3.528e+44	8.98	8.98	1.018e+38	0.000445
7948	diHPCARP_Ib.mmpmtpppu	4.789e+43	7.79	7.79	1.018e+38	0.000445
7949	diHPCARP_Ib.mptmmtpmu	4.963e+44	9.19	9.19	1.005e+38	0.000439
7950	diHPCARP_Ib.tmttmtppu	3.920e+44	9.05	9.05	1.002e+38	0.000438
7951	diHPCARP_Ib.tpttmtmmu	3.071e+44	8.91	8.91	9.903e+37	0.000433
7952	diHPCARP_Ib.mpppmttptu	1.218e+44	8.36	8.36	9.899e+37	0.000433
7953	diHPCARP_Ib.ttpptmpu	1.645e+44	8.54	8.54	9.862e+37	0.000431
7954	diHPCARP_Ib.tttptptmu	4.590e+44	9.16	9.16	9.781e+37	0.000428
7955	diHPCARP_Ib.mmmppmmpu	4.618e+43	7.79	7.79	9.747e+37	0.000426
7956	diHPCARP_Ib.pptmtmmu	1.597e+44	8.53	8.53	9.731e+37	0.000425
7957	diHPCARP_Ib.pmpptmpu	2.468e+43	7.43	7.43	9.481e+37	0.000414
7958	diHPCARP_Ib.tmtmtmpu	8.402e+43	8.17	8.17	9.440e+37	0.000413
7959	diHPCARP_Ib.tpttmtpmu	3.019e+44	8.93	8.93	9.370e+37	0.00041
7960	diHPCARP_Ib.ttmmttmmu	2.791e+44	8.89	8.89	9.363e+37	0.000409
7961	diHPCARP_Ib.ptmmmtpmu	3.920e+43	7.72	7.72	9.289e+37	0.000406
7962	diHPCARP_Ib.mmtppmmpu	1.152e+44	8.37	8.37	9.160e+37	0.0004
7963	diHPCARP_Ib.pmpmmpmu	2.541e+43	7.48	7.48	9.066e+37	0.000396
7964	diHPCARP_Ib.tmmtpmtmu	2.962e+44	8.95	8.95	9.010e+37	0.000394
7965	diHPCARP_Ib.ppppmtmpu	2.575e+43	7.50	7.50	8.897e+37	0.000389
7966	diHPCARP_Ib.pptmttptu	1.004e+45	9.68	9.68	8.892e+37	0.000389
7967	diHPCARP_Ib.tpptmtmmu	2.342e+44	8.81	8.81	8.876e+37	0.000388
7968	diHPCARP_Ib.mptpmtmmu	8.944e+43	8.25	8.25	8.810e+37	0.000385

7969	diHPCARP_Ib.ttmtmpmpmu	7.094e+43	8.11	8.11	8.799e+37	0.000385
7970	diHPCARP_Ib.mmptpttpu	1.599e+44	8.60	8.60	8.757e+37	0.000383
7971	diHPCARP_Ib.mpptmtmpu	1.098e+44	8.38	8.38	8.692e+37	0.00038
7972	diHPCARP_Ib.tptpmtmpu	1.844e+44	8.69	8.69	8.666e+37	0.000379
7973	diHPCARP_Ib.tmmppmmpu	7.019e+43	8.12	8.12	8.594e+37	0.000376
7974	diHPCARP_Ib.ppmmpmpu	3.463e+43	7.70	7.70	8.561e+37	0.000374
7975	diHPCARP_Ib.mtmppppmu	7.388e+43	8.15	8.15	8.556e+37	0.000374
7976	diHPCARP_Ib.mmptmtmpu	7.920e+43	8.19	8.19	8.536e+37	0.000373
7977	diHPCARP_Ib.mpttptmpu	2.021e+44	8.75	8.75	8.519e+37	0.000372
7978	diHPCARP_Ib.mmptpttpu	8.556e+43	8.24	8.24	8.479e+37	0.000371
7979	diHPCARP_Ib.mmmmtmtmu	2.446e+44	8.88	8.88	8.305e+37	0.000363
7980	diHPCARP_Ib.pptpmmmpu	2.993e+43	7.63	7.63	8.258e+37	0.000361
7981	diHPCARP_Ib.mttptmpu	5.549e+43	8.00	8.00	8.251e+37	0.000361
7982	diHPCARP_Ib.pmpmpmpu	8.231e+42	6.87	6.87	8.185e+37	0.000358
7983	diHPCARP_Ib.mpmmmtpu	1.686e+43	7.30	7.30	8.063e+37	0.000352
7984	diHPCARP_Ib.tmtmtmpu	3.676e+44	9.14	9.14	8.015e+37	0.00035
7985	diHPCARP_Ib.mtmpttpu	1.906e+44	8.76	8.76	7.909e+37	0.000346
7986	diHPCARP_Ib.ttmpptpu	3.695e+44	9.16	9.16	7.904e+37	0.000346
7987	diHPCARP_Ib.mmmptmtmu	3.830e+44	9.18	9.18	7.861e+37	0.000344
7988	diHPCARP_Ib.mmtppmpu	1.423e+44	8.59	8.59	7.852e+37	0.000343
7989	diHPCARP_Ib.tmmmtmtmu	1.028e+44	8.40	8.40	7.811e+37	0.000341
7990	diHPCARP_Ib.tppmmtpu	1.909e+44	8.77	8.77	7.788e+37	0.00034
7991	diHPCARP_Ib.ppptmpu	6.561e+43	8.14	8.14	7.767e+37	0.00034
7992	diHPCARP_Ib.mmtptmtmu	2.176e+44	8.85	8.85	7.735e+37	0.000338
7993	diHPCARP_Ib.tttptmpu	1.167e+44	8.49	8.49	7.576e+37	0.000331
7994	diHPCARP_Ib.mtppmmmpu	3.107e+43	7.71	7.71	7.549e+37	0.00033
7995	diHPCARP_Ib.tmmppmmpu	8.805e+43	8.33	8.33	7.545e+37	0.00033
7996	diHPCARP_Ib.mtptmtmpu	1.085e+44	8.46	8.46	7.468e+37	0.000326
7997	diHPCARP_Ib.tmtppppu	1.027e+44	8.44	8.44	7.341e+37	0.000321
7998	diHPCARP_Ib.pmttmtmpu	9.001e+44	9.75	9.75	7.131e+37	0.000312
7999	diHPCARP_Ib.tmpmpppu	3.167e+43	7.76	7.76	7.082e+37	0.00031
8000	diHPCARP_Ib.mtptmtmpu	3.046e+43	7.74	7.74	7.032e+37	0.000307
8001	diHPCARP_Ib.ppptmtmu	1.965e+44	8.85	8.85	7.002e+37	0.000306
8002	diHPCARP_Ib.tttptmtmu	2.945e+44	9.10	9.10	6.944e+37	0.000304
8003	diHPCARP_Ib.pmpptmtmu	3.327e+43	7.80	7.80	6.942e+37	0.000303
8004	diHPCARP_Ib.tmtmtmtmu	4.701e+44	9.38	9.38	6.926e+37	0.000303
8005	diHPCARP_Ib.pmtptmpu	2.889e+44	9.11	9.11	6.724e+37	0.000294
8006	diHPCARP_Ib.mtppptmpu	1.201e+44	8.58	8.58	6.710e+37	0.000293
8007	diHPCARP_Ib.ptpmpptmu	4.512e+43	8.00	8.00	6.667e+37	0.000291
8008	diHPCARP_Ib.mtppptmtmu	2.573e+44	9.05	9.05	6.596e+37	0.000288
8009	diHPCARP_Ib.ttmppmpu	2.060e+44	8.92	8.92	6.596e+37	0.000288
8010	diHPCARP_Ib.tpttmtmpu	2.654e+44	9.07	9.07	6.583e+37	0.000288
8011	diHPCARP_Ib.mmttmmmpu	3.614e+44	9.26	9.26	6.464e+37	0.000283
8012	diHPCARP_Ib.mmttmmmpu	7.578e+44	9.70	9.70	6.462e+37	0.000283
8013	diHPCARP_Ib.mmpmpmtmu	8.590e+43	8.41	8.41	6.403e+37	0.00028
8014	diHPCARP_Ib.mtppptmpu	1.169e+44	8.60	8.60	6.375e+37	0.000279
8015	diHPCARP_Ib.tpptmmmpu	1.563e+44	8.77	8.77	6.372e+37	0.000279
8016	diHPCARP_Ib.tmttmtmpu	5.919e+44	9.57	9.57	6.360e+37	0.000278
8017	diHPCARP_Ib.pmpptmpu	2.877e+43	7.77	7.77	6.286e+37	0.000275
8018	diHPCARP_Ib.tpptmtmpu	2.100e+44	8.96	8.96	6.281e+37	0.000275
8019	diHPCARP_Ib.ttmppmmpu	5.004e+43	8.10	8.10	6.273e+37	0.000274
8020	diHPCARP_Ib.mmpppmtmu	1.312e+44	8.68	8.68	6.232e+37	0.000272
8021	diHPCARP_Ib.tpttmtmu	8.526e+44	9.80	9.80	6.206e+37	0.000271
8022	diHPCARP_Ib.tpptpttpu	5.096e+44	9.50	9.50	6.149e+37	0.000269
8023	diHPCARP_Ib.mtmppptmu	6.259e+43	8.25	8.25	6.148e+37	0.000269
8024	diHPCARP_Ib.tptptmpu	1.901e+44	8.91	8.91	6.145e+37	0.000269
8025	diHPCARP_Ib.mmpmpmtmu	1.645e+43	7.46	7.46	6.081e+37	0.000266
8026	diHPCARP_Ib.mtppptmpu	1.314e+44	8.70	8.70	6.072e+37	0.000265
8027	diHPCARP_Ib.mtptptmpu	2.150e+43	7.62	7.62	6.060e+37	0.000265
8028	diHPCARP_Ib.mttmmtpu	2.446e+44	9.07	9.07	6.042e+37	0.000264
8029	diHPCARP_Ib.tptptmpu	1.417e+44	8.75	8.75	6.027e+37	0.000263
8030	diHPCARP_Ib.tptptmpu	2.808e+44	9.17	9.17	5.911e+37	0.000258
8031	diHPCARP_Ib.pmtptmpu	1.015e+44	8.56	8.56	5.883e+37	0.000257
8032	diHPCARP_Ib.ttmptmpu	1.220e+44	8.68	8.68	5.811e+37	0.000254
8033	diHPCARP_Ib.tmmptmpu	1.569e+43	7.46	7.46	5.754e+37	0.000252
8034	diHPCARP_Ib.tmttmtmpu	4.745e+44	9.50	9.50	5.744e+37	0.000251
8035	diHPCARP_Ib.pmttmtmu	3.876e+44	9.38	9.38	5.732e+37	0.000251
8036	diHPCARP_Ib.tmtptmpu	2.340e+44	9.08	9.08	5.731e+37	0.000251
8037	diHPCARP_Ib.tptptmtmu	3.743e+44	9.36	9.36	5.640e+37	0.000247
8038	diHPCARP_Ib.mptptmpu	1.051e+44	8.61	8.61	5.633e+37	0.000246
8039	diHPCARP_Ib.mmpmtmpu	1.127e+44	8.66	8.66	5.580e+37	0.000244
8040	diHPCARP_Ib.pptptmpu	9.946e+43	8.58	8.58	5.567e+37	0.000243

8041	diHPCARP_Ib.mmmtpptpmu	3.421e+44	9.33	9.33	5.502e+37	0.000241
8042	diHPCARP_Ib.ttmptmtmu	4.220e+43	8.08	8.08	5.494e+37	0.00024
8043	diHPCARP_Ib.ttptmttptu	3.631e+44	9.37	9.37	5.422e+37	0.000237
8044	diHPCARP_Ib.ttmtpmmmu	1.007e+44	8.61	8.61	5.408e+37	0.000236
8045	diHPCARP_Ib.ttptmttptu	2.008e+44	9.03	9.03	5.301e+37	0.000232
8046	diHPCARP_Ib.mtttmtmpmu	1.983e+44	9.02	9.02	5.286e+37	0.000231
8047	diHPCARP_Ib.ptptmtptmu	1.494e+44	8.86	8.86	5.251e+37	0.00023
8048	diHPCARP_Ib.mpmmpmtptu	2.499e+43	7.79	7.79	5.251e+37	0.00023
8049	diHPCARP_Ib.tptmttptpu	3.443e+44	9.37	9.37	5.143e+37	0.000225
8050	diHPCARP_Ib.ptppptmtmu	1.163e+44	8.72	8.72	5.135e+37	0.000224
8051	diHPCARP_Ib.tpttptmtmu	1.530e+45	10.26	10.26	5.120e+37	0.000224
8052	diHPCARP_Ib.ttmtmttptu	4.083e+43	8.10	8.10	5.100e+37	0.000223
8053	diHPCARP_Ib.mmmmpmtmu	1.709e+44	8.96	8.96	5.050e+37	0.000221
8054	diHPCARP_Ib.ttpptmtmu	2.642e+44	9.22	9.22	5.047e+37	0.000221
8055	diHPCARP_Ib.ttttmttptu	3.057e+44	9.31	9.31	5.031e+37	0.00022
8056	diHPCARP_Ib.tpptmtptmu	3.985e+44	9.47	9.47	5.022e+37	0.00022
8057	diHPCARP_Ib.pppmpptmu	1.452e+43	7.50	7.50	5.010e+37	0.000219
8058	diHPCARP_Ib.tttpttptmu	2.977e+44	9.30	9.30	4.988e+37	0.000218
8059	diHPCARP_Ib.tpptmttptu	3.905e+44	9.46	9.46	4.984e+37	0.000218
8060	diHPCARP_Ib.tmmtpmtmu	2.528e+44	9.21	9.21	4.957e+37	0.000217
8061	diHPCARP_Ib.ptpmpptmu	4.729e+43	8.22	8.22	4.887e+37	0.000214
8062	diHPCARP_Ib.pmtptmtptu	1.882e+44	9.04	9.04	4.875e+37	0.000213
8063	diHPCARP_Ib.mmpptppmpu	1.088e+44	8.72	8.72	4.856e+37	0.000212
8064	diHPCARP_Ib.mptpmttptu	1.697e+44	9.00	9.00	4.746e+37	0.000207
8065	diHPCARP_Ib.mpppmmmmu	1.574e+44	8.95	8.95	4.743e+37	0.000207
8066	diHPCARP_Ib.tpptpmpmu	1.448e+44	8.90	8.90	4.741e+37	0.000207
8067	diHPCARP_Ib.tmpptppmu	2.391e+43	7.83	7.83	4.710e+37	0.000206
8068	diHPCARP_Ib.tmtptmtptu	8.950e+44	9.99	9.99	4.694e+37	0.000205
8069	diHPCARP_Ib.mtttpttptu	1.666e+44	9.00	9.00	4.608e+37	0.000201
8070	diHPCARP_Ib.mmtptpmpmu	3.728e+44	9.49	9.49	4.586e+37	0.0002
8071	diHPCARP_Ib.mtttmttptu	1.555e+44	8.97	8.97	4.580e+37	0.0002
8072	diHPCARP_Ib.pmpptmtmu	1.510e+44	8.95	8.95	4.571e+37	0.0002
8073	diHPCARP_Ib.ptmpptppmu	3.243e+43	8.04	8.04	4.519e+37	0.000198
8074	diHPCARP_Ib.mtppmtptmu	6.063e+43	8.41	8.41	4.519e+37	0.000198
8075	diHPCARP_Ib.mmpmtmpmpu	1.121e+44	8.78	8.78	4.500e+37	0.000197
8076	diHPCARP_Ib.tmttpttptu	3.697e+44	9.49	9.49	4.480e+37	0.000196
8077	diHPCARP_Ib.tmtpttptmu	2.712e+44	9.31	9.31	4.478e+37	0.000196
8078	diHPCARP_Ib.pmpptppptmu	9.869e+43	8.71	8.71	4.445e+37	0.000194
8079	diHPCARP_Ib.ptpmpmpmu	1.525e+44	8.97	8.97	4.430e+37	0.000194
8080	diHPCARP_Ib.tmtmpmpmu	7.622e+44	9.93	9.93	4.412e+37	0.000193
8081	diHPCARP_Ib.ptptmmtmu	7.748e+44	9.95	9.95	4.400e+37	0.000192
8082	diHPCARP_Ib.ppttpttptu	5.910e+44	9.79	9.79	4.378e+37	0.000191
8083	diHPCARP_Ib.ttmtpttptu	4.345e+44	9.61	9.61	4.352e+37	0.00019
8084	diHPCARP_Ib.mtptpttmtu	3.991e+43	8.19	8.19	4.325e+37	0.000189
8085	diHPCARP_Ib.tpptptptmu	4.697e+44	9.66	9.66	4.311e+37	0.000188
8086	diHPCARP_Ib.pppmmmpptu	1.291e+43	7.52	7.52	4.288e+37	0.000187
8087	diHPCARP_Ib.mmmmpmmpmu	1.242e+44	8.88	8.88	4.245e+37	0.000186
8088	diHPCARP_Ib.tmtptmttmtu	2.801e+44	9.37	9.37	4.208e+37	0.000184
8089	diHPCARP_Ib.mmttmttptu	3.649e+44	9.53	9.53	4.180e+37	0.000183
8090	diHPCARP_Ib.tpptpttptu	3.059e+44	9.43	9.43	4.150e+37	0.000181
8091	diHPCARP_Ib.tpptpttptu	6.781e+44	9.91	9.91	4.062e+37	0.000178
8092	diHPCARP_Ib.ppptmttptu	3.818e+44	9.58	9.58	4.036e+37	0.000176
8093	diHPCARP_Ib.pmmmttptu	1.737e+44	9.11	9.11	3.988e+37	0.000174
8094	diHPCARP_Ib.mmtmmpmmpu	5.037e+44	9.75	9.75	3.981e+37	0.000174
8095	diHPCARP_Ib.mtpmmpptmu	4.781e+43	8.35	8.35	3.963e+37	0.000173
8096	diHPCARP_Ib.ptpmpmtmu	2.126e+44	9.24	9.24	3.963e+37	0.000173
8097	diHPCARP_Ib.mtttmttptu	1.983e+44	9.20	9.20	3.960e+37	0.000173
8098	diHPCARP_Ib.tpttptpmpu	1.552e+44	9.05	9.05	3.941e+37	0.000172
8099	diHPCARP_Ib.tttmpppmpu	8.065e+43	8.67	8.67	3.878e+37	0.00017
8100	diHPCARP_Ib.tpttptpmpu	3.326e+44	9.52	9.52	3.869e+37	0.000169
8101	diHPCARP_Ib.ptptmttmtu	6.025e+44	9.87	9.87	3.863e+37	0.000169
8102	diHPCARP_Ib.tppmmmpmu	1.608e+44	9.09	9.09	3.829e+37	0.000167
8103	diHPCARP_Ib.mtttpttptu	1.447e+44	9.03	9.03	3.810e+37	0.000167
8104	diHPCARP_Ib.mppmttmtmu	1.265e+45	10.33	10.33	3.792e+37	0.000166
8105	diHPCARP_Ib.mmttmtpppu	1.814e+44	9.18	9.18	3.748e+37	0.000164
8106	diHPCARP_Ib.ppttppmpmu	1.859e+44	9.20	9.20	3.722e+37	0.000163
8107	diHPCARP_Ib.tmtpttmtmu	7.079e+44	9.99	9.99	3.713e+37	0.000162
8108	diHPCARP_Ib.ttmmttmtmu	2.376e+44	9.35	9.35	3.685e+37	0.000161
8109	diHPCARP_Ib.mmmtpmpmu	1.832e+44	9.19	9.19	3.679e+37	0.000161
8110	diHPCARP_Ib.pptpttmtmu	1.378e+44	9.02	9.02	3.675e+37	0.000161
8111	diHPCARP_Ib.tpttmttptu	6.475e+44	9.95	9.95	3.672e+37	0.000161
8112	diHPCARP_Ib.ttmppptmu	6.659e+43	8.60	8.60	3.633e+37	0.000159

8113	diHPCARP_Ib.mttmtpu	1.405e+44	9.05	9.05	3.620e+37	0.000158
8114	diHPCARP_Ib.tmttptpmu	7.687e+44	10.06	10.06	3.595e+37	0.000157
8115	diHPCARP_Ib.ttmppptpu	7.495e+43	8.68	8.68	3.556e+37	0.000155
8116	diHPCARP_Ib.tmmmttmu	4.837e+44	9.80	9.80	3.529e+37	0.000154
8117	diHPCARP_Ib.pptmtmpu	2.128e+44	9.32	9.32	3.444e+37	0.000151
8118	diHPCARP_Ib.pmpmmtmu	4.253e+43	8.36	8.36	3.432e+37	0.00015
8119	diHPCARP_Ib.tmtmppppu	7.632e+43	8.71	8.71	3.431e+37	0.00015
8120	diHPCARP_Ib.tmmtpptpmu	4.057e+44	9.72	9.72	3.393e+37	0.000148
8121	diHPCARP_Ib.mpptmtmmu	2.053e+44	9.31	9.31	3.364e+37	0.000147
8122	diHPCARP_Ib.mmpmpmmmu	6.865e+43	8.67	8.67	3.321e+37	0.000145
8123	diHPCARP_Ib.tmmptpmu	1.717e+43	7.85	7.85	3.302e+37	0.000144
8124	diHPCARP_Ib.tmmppttpu	1.430e+44	9.12	9.12	3.223e+37	0.000141
8125	diHPCARP_Ib.tmmmtmpu	2.829e+44	9.53	9.53	3.218e+37	0.000141
8126	diHPCARP_Ib.tmpptmpu	2.361e+44	9.43	9.43	3.203e+37	0.00014
8127	diHPCARP_Ib.tmpptpmu	2.353e+44	9.43	9.43	3.200e+37	0.00014
8128	diHPCARP_Ib.tmpppmpu	4.807e+43	8.48	8.48	3.191e+37	0.00014
8129	diHPCARP_Ib.mtmtmttu	2.078e+44	9.36	9.36	3.160e+37	0.000138
8130	diHPCARP_Ib.mmtmtmmu	5.832e+44	9.98	9.98	3.125e+37	0.000137
8131	diHPCARP_Ib.ttmmpmtmu	1.639e+44	9.23	9.23	3.089e+37	0.000135
8132	diHPCARP_Ib.mmtptpmu	4.600e+44	9.85	9.85	3.087e+37	0.000135
8133	diHPCARP_Ib.ptmmpppu	2.776e+43	8.18	8.18	3.047e+37	0.000133
8134	diHPCARP_Ib.tttmptpmu	1.549e+44	9.21	9.21	3.023e+37	0.000132
8135	diHPCARP_Ib.mptmtmmu	2.042e+44	9.38	9.38	2.995e+37	0.000131
8136	diHPCARP_Ib.mmtptmpu	3.455e+44	9.70	9.70	2.961e+37	0.000129
8137	diHPCARP_Ib.tmmppttmu	7.126e+43	8.76	8.76	2.958e+37	0.000129
8138	diHPCARP_Ib.tpttptpu	6.285e+44	10.08	10.08	2.840e+37	0.000124
8139	diHPCARP_Ib.tmmmtmpu	3.502e+44	9.74	9.74	2.815e+37	0.000123
8140	diHPCARP_Ib.tttptpmu	3.345e+44	9.71	9.71	2.804e+37	0.000123
8141	diHPCARP_Ib.ppppmtmu	1.590e+44	9.28	9.28	2.767e+37	0.000121
8142	diHPCARP_Ib.tttmtmpu	3.508e+44	9.75	9.75	2.763e+37	0.000121
8143	diHPCARP_Ib.tppmmtmu	2.492e+44	9.56	9.56	2.713e+37	0.000119
8144	diHPCARP_Ib.mmpptpmu	1.249e+44	9.15	9.15	2.695e+37	0.000118
8145	diHPCARP_Ib.pmttptmpu	7.436e+44	10.21	10.21	2.693e+37	0.000118
8146	diHPCARP_Ib.mttmptmpu	9.390e+43	8.98	8.98	2.680e+37	0.000117
8147	diHPCARP_Ib.pttppmpu	9.543e+43	9.00	9.00	2.660e+37	0.000116
8148	diHPCARP_Ib.pttppppu	7.603e+43	8.86	8.86	2.659e+37	0.000116
8149	diHPCARP_Ib.mtmppmtmu	6.766e+43	8.80	8.80	2.621e+37	0.000115
8150	diHPCARP_Ib.ptptppmpu	4.598e+44	9.95	9.95	2.608e+37	0.000114
8151	diHPCARP_Ib.ptptppppu	8.488e+43	8.94	8.94	2.587e+37	0.000113
8152	diHPCARP_Ib.ttptmtmu	4.590e+44	9.96	9.96	2.568e+37	0.000112
8153	diHPCARP_Ib.ppttptmmu	2.903e+44	9.69	9.69	2.551e+37	0.000112
8154	diHPCARP_Ib.pptmmpu	6.719e+43	8.82	8.82	2.542e+37	0.000111
8155	diHPCARP_Ib.pppmptpu	1.824e+43	8.04	8.04	2.538e+37	0.000111
8156	diHPCARP_Ib.mptmmpu	9.001e+43	8.99	8.99	2.529e+37	0.000111
8157	diHPCARP_Ib.ptpmpmpu	6.532e+43	8.80	8.80	2.526e+37	0.00011
8158	diHPCARP_Ib.tmtptmpu	1.318e+45	10.60	10.60	2.499e+37	0.000109
8159	diHPCARP_Ib.mmtppmmu	3.819e+44	9.86	9.86	2.498e+37	0.000109
8160	diHPCARP_Ib.mmpmtmmu	7.580e+43	8.92	8.92	2.425e+37	0.000106
8161	diHPCARP_Ib.mppptpmu	3.289e+44	9.79	9.79	2.425e+37	0.000106
8162	diHPCARP_Ib.pptmtmmu	1.641e+44	9.38	9.38	2.422e+37	0.000106
8163	diHPCARP_Ib.tmmpmttu	5.559e+43	8.74	8.74	2.380e+37	0.000104
8164	diHPCARP_Ib.mmtmpppmu	1.583e+44	9.37	9.37	2.368e+37	0.000104
8165	diHPCARP_Ib.tmtmtmpu	9.286e+43	9.06	9.06	2.349e+37	0.000103
8166	diHPCARP_Ib.pmpmpmmu	6.330e+43	8.84	8.84	2.295e+37	0.0001
8167	diHPCARP_Ib.mmtppppu	3.028e+44	9.78	9.78	2.276e+37	9.95e-05
8168	diHPCARP_Ib.mptpptpmu	4.744e+44	10.05	10.05	2.258e+37	9.87e-05
8169	diHPCARP_Ib.tttmtmpu	4.098e+44	9.97	9.97	2.242e+37	9.8e-05
8170	diHPCARP_Ib.ptpmmmtmu	1.036e+44	9.16	9.16	2.213e+37	9.67e-05
8171	diHPCARP_Ib.pttppppu	1.823e+44	9.50	9.50	2.201e+37	9.62e-05
8172	diHPCARP_Ib.mtpmpmpmu	4.402e+43	8.66	8.66	2.179e+37	9.53e-05
8173	diHPCARP_Ib.pmpmtmmu	3.834e+44	9.96	9.96	2.138e+37	9.35e-05
8174	diHPCARP_Ib.tmtmmpmpu	3.833e+44	9.96	9.96	2.131e+37	9.32e-05
8175	diHPCARP_Ib.tppmpttu	4.755e+43	8.72	8.72	2.129e+37	9.31e-05
8176	diHPCARP_Ib.tttmptpmu	1.099e+44	9.22	9.22	2.114e+37	9.24e-05
8177	diHPCARP_Ib.pmpmpmmu	4.751e+43	8.73	8.73	2.085e+37	9.11e-05
8178	diHPCARP_Ib.tmpmptpu	3.013e+43	8.47	8.47	2.037e+37	8.9e-05
8179	diHPCARP_Ib.ttttptpu	2.434e+44	9.72	9.72	2.035e+37	8.9e-05
8180	diHPCARP_Ib.tmmpptpmu	2.071e+44	9.62	9.62	2.027e+37	8.86e-05
8181	diHPCARP_Ib.tmttptmpu	3.664e+44	9.97	9.97	2.008e+37	8.78e-05
8182	diHPCARP_Ib.ppttptmpu	3.876e+44	10.00	10.00	2.007e+37	8.77e-05
8183	diHPCARP_Ib.tmpmptpmu	5.745e+43	8.87	8.87	2.001e+37	8.75e-05
8184	diHPCARP_Ib.tmtmtmmu	5.349e+44	10.22	10.22	1.914e+37	8.37e-05

8185	diHPCARP_Ib.mmttptmnu	6.242e+44	10.33	10.33	1.869e+37	8.17e-05
8186	diHPCARP_Ib.mmtpppmnu	5.351e+44	10.24	10.24	1.869e+37	8.17e-05
8187	diHPCARP_Ib.mptmpmppy	7.675e+43	9.09	9.09	1.818e+37	7.95e-05
8188	diHPCARP_Ib.tpmtptmpu	1.099e+44	9.31	9.31	1.815e+37	7.93e-05
8189	diHPCARP_Ib.tmnttptpu	2.064e+44	9.69	9.69	1.810e+37	7.91e-05
8190	diHPCARP_Ib.ttttptmpu	3.385e+44	9.98	9.98	1.803e+37	7.88e-05
8191	diHPCARP_Ib.mmpmntppu	4.601e+43	8.80	8.80	1.797e+37	7.86e-05
8192	diHPCARP_Ib.mmmtpmmnu	3.344e+44	10.00	10.00	1.746e+37	7.63e-05
8193	diHPCARP_Ib.pmpptppmu	1.509e+43	8.15	8.15	1.746e+37	7.63e-05
8194	diHPCARP_Ib.ttttmtmnu	4.114e+44	10.12	10.12	1.732e+37	7.57e-05
8195	diHPCARP_Ib.mtmpppppu	4.154e+43	8.76	8.76	1.716e+37	7.5e-05
8196	diHPCARP_Ib.ptttmpppu	1.160e+44	9.38	9.38	1.707e+37	7.46e-05
8197	diHPCARP_Ib.mppmttptu	1.584e+44	9.57	9.57	1.701e+37	7.44e-05
8198	diHPCARP_Ib.ttptmtmpu	2.242e+44	9.78	9.78	1.695e+37	7.41e-05
8199	diHPCARP_Ib.mptmpmtpu	7.232e+43	9.10	9.10	1.688e+37	7.38e-05
8200	diHPCARP_Ib.mptpmtmpu	2.295e+44	9.80	9.80	1.665e+37	7.28e-05
8201	diHPCARP_Ib.mmtmmtpmu	7.115e+44	10.48	10.48	1.661e+37	7.26e-05
8202	diHPCARP_Ib.mtmmtttmu	2.568e+44	9.87	9.87	1.655e+37	7.23e-05
8203	diHPCARP_Ib.tmppmppy	4.879e+43	8.89	8.89	1.631e+37	7.13e-05
8204	diHPCARP_Ib.ttmmtmnu	7.171e+44	10.49	10.49	1.623e+37	7.1e-05
8205	diHPCARP_Ib.tttptttmu	6.852e+44	10.47	10.47	1.618e+37	7.07e-05
8206	diHPCARP_Ib.pmpppmtpu	8.452e+43	9.23	9.23	1.590e+37	6.95e-05
8207	diHPCARP_Ib.ttpmpmpu	4.846e+43	8.91	8.91	1.572e+37	6.87e-05
8208	diHPCARP_Ib.ttmmtptpu	5.868e+43	9.02	9.02	1.567e+37	6.85e-05
8209	diHPCARP_Ib.mmttpppmu	1.350e+44	9.54	9.54	1.518e+37	6.64e-05
8210	diHPCARP_Ib.tmntmtmnu	4.590e+44	10.27	10.27	1.517e+37	6.63e-05
8211	diHPCARP_Ib.mppppmppy	5.389e+43	9.00	9.00	1.488e+37	6.5e-05
8212	diHPCARP_Ib.pmttptmnu	4.717e+44	10.30	10.30	1.486e+37	6.49e-05
8213	diHPCARP_Ib.pmpppmmpu	1.621e+44	9.66	9.66	1.482e+37	6.48e-05
8214	diHPCARP_Ib.mtmmtttmu	1.030e+44	9.40	9.40	1.470e+37	6.43e-05
8215	diHPCARP_Ib.mmmtmmpmu	1.472e+44	9.61	9.61	1.460e+37	6.38e-05
8216	diHPCARP_Ib.ttttptpmu	5.043e+44	10.36	10.36	1.435e+37	6.27e-05
8217	diHPCARP_Ib.mpmmpptmu	1.354e+43	8.20	8.20	1.429e+37	6.25e-05
8218	diHPCARP_Ib.tmmpmtttmu	6.535e+43	9.14	9.14	1.427e+37	6.24e-05
8219	diHPCARP_Ib.mmttptmpu	5.261e+44	10.39	10.39	1.418e+37	6.2e-05
8220	diHPCARP_Ib.mmmmmmpmu	6.709e+43	9.16	9.16	1.415e+37	6.19e-05
8221	diHPCARP_Ib.mtmmttppu	3.551e+43	8.79	8.79	1.399e+37	6.12e-05
8222	diHPCARP_Ib.ttpmmpmnu	4.981e+43	9.00	9.00	1.383e+37	6.04e-05
8223	diHPCARP_Ib.tmpmtmpu	2.928e+44	10.09	10.09	1.306e+37	5.71e-05
8224	diHPCARP_Ib.ttttptmnu	4.630e+44	10.37	10.37	1.302e+37	5.69e-05
8225	diHPCARP_Ib.mpttmtmpu	5.792e+44	10.50	10.50	1.297e+37	5.67e-05
8226	diHPCARP_Ib.pptpptmnu	2.336e+44	9.97	9.97	1.270e+37	5.55e-05
8227	diHPCARP_Ib.mtpmpttmu	6.665e+43	9.23	9.23	1.259e+37	5.5e-05
8228	diHPCARP_Ib.tmmpmtmpu	6.034e+43	9.17	9.17	1.259e+37	5.5e-05
8229	diHPCARP_Ib.ttmpppppu	5.144e+43	9.08	9.08	1.254e+37	5.48e-05
8230	diHPCARP_Ib.pmttmtmpu	1.990e+44	9.89	9.89	1.240e+37	5.42e-05
8231	diHPCARP_Ib.tppmntppu	1.448e+44	9.70	9.70	1.239e+37	5.42e-05
8232	diHPCARP_Ib.tmpmpptpu	4.865e+43	9.06	9.06	1.228e+37	5.37e-05
8233	diHPCARP_Ib.tpmmnttptu	1.979e+44	9.90	9.90	1.224e+37	5.35e-05
8234	diHPCARP_Ib.ttmppttptu	2.471e+44	10.03	10.03	1.214e+37	5.31e-05
8235	diHPCARP_Ib.tmpppptmu	6.815e+43	9.27	9.27	1.213e+37	5.3e-05
8236	diHPCARP_Ib.tpmtptttptu	3.652e+44	10.27	10.27	1.207e+37	5.28e-05
8237	diHPCARP_Ib.mtpmmtmmpu	2.170e+45	11.33	11.33	1.207e+37	5.28e-05
8238	diHPCARP_Ib.mtpmmttptu	5.550e+43	9.16	9.16	1.177e+37	5.15e-05
8239	diHPCARP_Ib.ttpmpttmu	6.170e+43	9.23	9.23	1.165e+37	5.09e-05
8240	diHPCARP_Ib.mpttptmnu	2.388e+44	10.05	10.05	1.149e+37	5.02e-05
8241	diHPCARP_Ib.tmttptmnu	6.890e+44	10.69	10.69	1.132e+37	4.95e-05
8242	diHPCARP_Ib.mtmtppppu	1.677e+44	9.85	9.85	1.111e+37	4.86e-05
8243	diHPCARP_Ib.mptmnmnu	7.023e+44	10.71	10.71	1.104e+37	4.83e-05
8244	diHPCARP_Ib.pmnttpttptu	2.205e+44	10.02	10.02	1.100e+37	4.81e-05
8245	diHPCARP_Ib.tmntmpppu	1.888e+43	8.56	8.56	1.089e+37	4.76e-05
8246	diHPCARP_Ib.mtpmptmpu	3.616e+43	8.95	8.95	1.085e+37	4.74e-05
8247	diHPCARP_Ib.tmpppttptu	2.432e+44	10.10	10.10	1.072e+37	4.69e-05
8248	diHPCARP_Ib.mmttmmpmu	9.982e+44	10.96	10.96	1.040e+37	4.55e-05
8249	diHPCARP_Ib.tppmntpmu	2.274e+44	10.08	10.08	1.034e+37	4.52e-05
8250	diHPCARP_Ib.tpmtptmnu	1.301e+44	9.75	9.75	1.032e+37	4.51e-05
8251	diHPCARP_Ib.mtppppppu	7.080e+43	9.38	9.38	1.031e+37	4.51e-05
8252	diHPCARP_Ib.mmttmnmnu	8.332e+44	10.86	10.86	1.016e+37	4.44e-05
8253	diHPCARP_Ib.tpmtptttmu	5.902e+44	10.66	10.66	1.015e+37	4.44e-05
8254	diHPCARP_Ib.mtttpttptu	3.388e+44	10.33	10.33	1.015e+37	4.44e-05
8255	diHPCARP_Ib.mtttmtptpu	3.339e+44	10.33	10.33	1.004e+37	4.39e-05
8256	diHPCARP_Ib.tmttppppu	1.116e+44	9.67	9.67	1.002e+37	4.38e-05

8257	diHPCARP_Ib.mmmppmtmu	1.092e+44	9.68	9.68	9.707e+36	4.24e-05
8258	diHPCARP_Ib.tptmtmpu	2.249e+44	10.12	10.12	9.592e+36	4.19e-05
8259	diHPCARP_Ib.pmpppmmmu	1.558e+44	9.91	9.91	9.470e+36	4.14e-05
8260	diHPCARP_Ib.mtmmpmtmu	5.845e+44	10.71	10.71	9.233e+36	4.04e-05
8261	diHPCARP_Ib.mmmpptpmu	1.636e+44	9.95	9.95	9.173e+36	4.01e-05
8262	diHPCARP_Ib.tmmmmpppu	3.984e+44	10.49	10.49	9.136e+36	3.99e-05
8263	diHPCARP_Ib.mmpmmtmpu	4.628e+43	9.22	9.22	8.911e+36	3.9e-05
8264	diHPCARP_Ib.mmpppmtmu	9.273e+43	9.64	9.64	8.796e+36	3.85e-05
8265	diHPCARP_Ib.tmpppttmu	1.399e+44	9.90	9.90	8.593e+36	3.76e-05
8266	diHPCARP_Ib.mmpppttmu	1.460e+44	9.93	9.93	8.545e+36	3.74e-05
8267	diHPCARP_Ib.ppptmtppu	2.072e+44	10.14	10.14	8.498e+36	3.71e-05
8268	diHPCARP_Ib.mpppttpu	1.797e+44	10.06	10.06	8.468e+36	3.7e-05
8269	diHPCARP_Ib.mmmppttmu	1.795e+44	10.06	10.06	8.444e+36	3.69e-05
8270	diHPCARP_Ib.tpmtppmmu	1.088e+44	9.76	9.76	8.428e+36	3.68e-05
8271	diHPCARP_Ib.tpmmtmpu	5.643e+43	9.37	9.37	8.401e+36	3.67e-05
8272	diHPCARP_Ib.tmppptpu	7.985e+43	9.58	9.58	8.321e+36	3.64e-05
8273	diHPCARP_Ib.tmmttppu	2.843e+44	10.35	10.35	8.153e+36	3.56e-05
8274	diHPCARP_Ib.tpmmtttmu	2.103e+44	10.18	10.18	8.020e+36	3.51e-05
8275	diHPCARP_Ib.tmpmppmpu	5.205e+43	9.36	9.36	7.863e+36	3.44e-05
8276	diHPCARP_Ib.mtttmttpu	3.567e+44	10.51	10.51	7.819e+36	3.42e-05
8277	diHPCARP_Ib.mttmptmpu	2.558e+44	10.32	10.32	7.818e+36	3.42e-05
8278	diHPCARP_Ib.mppmtmpu	2.729e+44	10.36	10.36	7.777e+36	3.4e-05
8279	diHPCARP_Ib.mptmpmmu	3.782e+44	10.56	10.56	7.715e+36	3.37e-05
8280	diHPCARP_Ib.tmpmmmpmu	3.065e+43	9.06	9.06	7.665e+36	3.35e-05
8281	diHPCARP_Ib.ttmppmpu	1.660e+44	10.07	10.07	7.614e+36	3.33e-05
8282	diHPCARP_Ib.tmmpptmu	5.659e+43	9.44	9.44	7.557e+36	3.3e-05
8283	diHPCARP_Ib.mptmpmmpu	3.578e+44	10.54	10.54	7.547e+36	3.3e-05
8284	diHPCARP_Ib.mppmmttmu	3.415e+44	10.52	10.52	7.459e+36	3.26e-05
8285	diHPCARP_Ib.tttmpmmu	1.776e+44	10.13	10.13	7.456e+36	3.26e-05
8286	diHPCARP_Ib.mppppmtmu	2.597e+44	10.36	10.36	7.315e+36	3.2e-05
8287	diHPCARP_Ib.mpttmttmu	9.172e+44	11.12	11.12	7.274e+36	3.18e-05
8288	diHPCARP_Ib.tmmpmttmu	7.612e+43	9.64	9.64	7.252e+36	3.17e-05
8289	diHPCARP_Ib.mppptttmu	7.591e+43	9.64	9.64	7.238e+36	3.16e-05
8290	diHPCARP_Ib.ptptmtppu	1.498e+44	10.05	10.05	7.095e+36	3.1e-05
8291	diHPCARP_Ib.pttmtmpu	1.997e+44	10.23	10.23	7.068e+36	3.09e-05
8292	diHPCARP_Ib.mtpppptpu	9.864e+43	9.82	9.82	6.912e+36	3.02e-05
8293	diHPCARP_Ib.ttmmptpmu	1.147e+44	9.92	9.92	6.834e+36	2.99e-05
8294	diHPCARP_Ib.pptmptppu	1.427e+44	10.06	10.06	6.681e+36	2.92e-05
8295	diHPCARP_Ib.ptmpmmtmu	5.400e+43	9.49	9.49	6.644e+36	2.9e-05
8296	diHPCARP_Ib.pmpmtppu	8.574e+42	8.40	8.40	6.546e+36	2.86e-05
8297	diHPCARP_Ib.ppptptppu	4.292e+44	10.74	10.74	6.471e+36	2.83e-05
8298	diHPCARP_Ib.tmttppppu	1.100e+44	9.93	9.93	6.452e+36	2.82e-05
8299	diHPCARP_Ib.pptmmttmu	4.014e+44	10.72	10.72	6.262e+36	2.74e-05
8300	diHPCARP_Ib.mmppptpmu	1.013e+44	9.90	9.90	6.238e+36	2.73e-05
8301	diHPCARP_Ib.tmmpptpmu	3.527e+43	9.27	9.27	6.216e+36	2.72e-05
8302	diHPCARP_Ib.pptmpttmu	1.422e+44	10.10	10.10	6.207e+36	2.71e-05
8303	diHPCARP_Ib.mmmppmtpu	7.585e+43	9.73	9.73	6.179e+36	2.7e-05
8304	diHPCARP_Ib.ptptmttpu	2.724e+44	10.49	10.49	6.168e+36	2.7e-05
8305	diHPCARP_Ib.pptmpmmpu	9.285e+43	9.85	9.85	6.165e+36	2.69e-05
8306	diHPCARP_Ib.mptmmmmmpu	3.400e+44	10.63	10.63	6.141e+36	2.68e-05
8307	diHPCARP_Ib.mtptmpppu	1.339e+44	10.08	10.08	6.086e+36	2.66e-05
8308	diHPCARP_Ib.tmpppmtpu	3.815e+44	10.70	10.70	6.083e+36	2.66e-05
8309	diHPCARP_Ib.mtpmpmppu	7.313e+44	11.09	11.09	6.077e+36	2.66e-05
8310	diHPCARP_Ib.pmpmmtmu	5.516e+43	9.56	9.56	6.039e+36	2.64e-05
8311	diHPCARP_Ib.pptpttpu	1.414e+45	11.49	11.49	6.012e+36	2.63e-05
8312	diHPCARP_Ib.mppppmmmu	3.441e+44	10.65	10.65	5.990e+36	2.62e-05
8313	diHPCARP_Ib.pptpmmtmu	2.429e+44	10.45	10.45	5.953e+36	2.6e-05
8314	diHPCARP_Ib.ttmppppmu	4.528e+43	9.45	9.45	5.930e+36	2.59e-05
8315	diHPCARP_Ib.ttpmppppmu	5.799e+43	9.60	9.60	5.888e+36	2.57e-05
8316	diHPCARP_Ib.ttmtpmtmu	1.105e+45	11.36	11.36	5.864e+36	2.56e-05
8317	diHPCARP_Ib.pmpmmtpmu	1.797e+43	8.91	8.91	5.814e+36	2.54e-05
8318	diHPCARP_Ib.mttmmtmpu	2.062e+44	10.37	10.37	5.770e+36	2.52e-05
8319	diHPCARP_Ib.tpppptpu	2.944e+44	10.58	10.58	5.743e+36	2.51e-05
8320	diHPCARP_Ib.pmttptmpu	1.973e+44	10.35	10.35	5.736e+36	2.51e-05
8321	diHPCARP_Ib.tmpptmpu	1.909e+43	8.96	8.96	5.711e+36	2.5e-05
8322	diHPCARP_Ib.mtmppppmu	5.604e+43	9.60	9.60	5.706e+36	2.49e-05
8323	diHPCARP_Ib.tmtppppmu	2.666e+44	10.53	10.53	5.694e+36	2.49e-05
8324	diHPCARP_Ib.tmpppmtmu	1.110e+44	10.01	10.01	5.660e+36	2.47e-05
8325	diHPCARP_Ib.tmpppmtmu	9.065e+43	9.89	9.89	5.657e+36	2.47e-05
8326	diHPCARP_Ib.ttmtpmmpu	4.208e+44	10.81	10.81	5.613e+36	2.45e-05
8327	diHPCARP_Ib.pptmmttmu	1.671e+44	10.27	10.27	5.507e+36	2.41e-05
8328	diHPCARP_Ib.pptmmmmmu	1.137e+45	11.42	11.42	5.453e+36	2.38e-05

8329	diHPCARP_Ib.mpptptpmu	5.048e+43	9.57	9.57	5.350e+36	2.34e-05
8330	diHPCARP_Ib.mmmppmtmu	2.815e+44	10.60	10.60	5.316e+36	2.32e-05
8331	diHPCARP_Ib.pppmpmpmu	3.293e+43	9.33	9.33	5.289e+36	2.31e-05
8332	diHPCARP_Ib.tppppppmu	1.433e+44	10.21	10.21	5.255e+36	2.3e-05
8333	diHPCARP_Ib.mmpmpptmu	1.169e+44	10.09	10.09	5.193e+36	2.27e-05
8334	diHPCARP_Ib.tpmnmtmu	6.494e+43	9.74	9.74	5.171e+36	2.26e-05
8335	diHPCARP_Ib.mtptmptpu	1.370e+44	10.19	10.19	5.159e+36	2.26e-05
8336	diHPCARP_Ib.ttmppppmu	1.414e+44	10.21	10.21	5.158e+36	2.25e-05
8337	diHPCARP_Ib.ttmmpmpmu	1.285e+44	10.15	10.15	5.153e+36	2.25e-05
8338	diHPCARP_Ib.mtptmtmpu	1.653e+44	10.32	10.32	5.045e+36	2.21e-05
8339	diHPCARP_Ib.mppmpmpmu	5.454e+43	9.66	9.66	5.045e+36	2.21e-05
8340	diHPCARP_Ib.tmmmtmpmu	3.797e+44	10.81	10.81	5.033e+36	2.2e-05
8341	diHPCARP_Ib.pmpptptmu	1.689e+44	10.36	10.36	4.832e+36	2.11e-05
8342	diHPCARP_Ib.ttttmppmu	2.125e+44	10.51	10.51	4.657e+36	2.04e-05
8343	diHPCARP_Ib.mtptmtppu	3.364e+44	10.81	10.81	4.484e+36	1.96e-05
8344	diHPCARP_Ib.pmpmttmu	1.345e+44	10.27	10.27	4.415e+36	1.93e-05
8345	diHPCARP_Ib.mptppppmu	5.643e+43	9.77	9.77	4.292e+36	1.88e-05
8346	diHPCARP_Ib.tmpmmttmu	2.488e+43	9.28	9.28	4.289e+36	1.88e-05
8347	diHPCARP_Ib.tmtppmpmu	2.682e+44	10.70	10.70	4.280e+36	1.87e-05
8348	diHPCARP_Ib.mtptmttmu	2.466e+44	10.66	10.66	4.255e+36	1.86e-05
8349	diHPCARP_Ib.ttpptppmu	3.306e+44	10.83	10.83	4.231e+36	1.85e-05
8350	diHPCARP_Ib.ptpmmppmu	5.174e+43	9.74	9.74	4.186e+36	1.83e-05
8351	diHPCARP_Ib.pmpmtmmmu	3.052e+44	10.80	10.80	4.147e+36	1.81e-05
8352	diHPCARP_Ib.mtmppptmu	7.139e+43	9.94	9.94	4.086e+36	1.79e-05
8353	diHPCARP_Ib.ttmppppmu	5.086e+43	9.75	9.75	4.034e+36	1.76e-05
8354	diHPCARP_Ib.mtptmmpmu	1.093e+44	10.20	10.20	4.029e+36	1.76e-05
8355	diHPCARP_Ib.mmmtpppmu	1.607e+44	10.44	10.44	4.013e+36	1.75e-05
8356	diHPCARP_Ib.tmtptptpu	2.433e+44	10.69	10.69	3.945e+36	1.72e-05
8357	diHPCARP_Ib.ptptpmpmu	7.417e+44	11.36	11.36	3.938e+36	1.72e-05
8358	diHPCARP_Ib.mmttppmmu	4.728e+44	11.09	11.09	3.925e+36	1.72e-05
8359	diHPCARP_Ib.ttmppppmu	4.921e+43	9.75	9.75	3.904e+36	1.71e-05
8360	diHPCARP_Ib.mmmmmppmu	9.061e+43	10.12	10.12	3.853e+36	1.68e-05
8361	diHPCARP_Ib.pppmmmmmu	1.955e+43	9.21	9.21	3.818e+36	1.67e-05
8362	diHPCARP_Ib.mtppppmpu	7.600e+43	10.03	10.03	3.732e+36	1.63e-05
8363	diHPCARP_Ib.ttpmttmu	3.221e+44	10.90	10.90	3.718e+36	1.63e-05
8364	diHPCARP_Ib.ttpmpppmu	7.767e+43	10.06	10.06	3.640e+36	1.59e-05
8365	diHPCARP_Ib.pppmmtppu	3.551e+44	10.97	10.97	3.627e+36	1.59e-05
8366	diHPCARP_Ib.pmttptpmu	2.789e+44	10.83	10.83	3.594e+36	1.57e-05
8367	diHPCARP_Ib.mpttptpmu	6.283e+44	11.32	11.32	3.578e+36	1.56e-05
8368	diHPCARP_Ib.mtptmttmu	2.354e+44	10.74	10.74	3.554e+36	1.55e-05
8369	diHPCARP_Ib.tmpppmmpu	5.375e+44	11.23	11.23	3.541e+36	1.55e-05
8370	diHPCARP_Ib.mtmmmmmmu	1.744e+44	10.57	10.57	3.465e+36	1.51e-05
8371	diHPCARP_Ib.tmmppptpu	8.881e+43	10.17	10.17	3.463e+36	1.51e-05
8372	diHPCARP_Ib.ptptmtmpu	4.197e+44	11.10	11.10	3.414e+36	1.49e-05
8373	diHPCARP_Ib.ppmptmtpu	4.096e+44	11.11	11.11	3.305e+36	1.44e-05
8374	diHPCARP_Ib.mtmmpptmu	1.278e+44	10.42	10.42	3.305e+36	1.44e-05
8375	diHPCARP_Ib.mtppmtpmu	2.453e+43	9.44	9.44	3.272e+36	1.43e-05
8376	diHPCARP_Ib.mtmmmppmu	6.193e+43	9.99	9.99	3.242e+36	1.42e-05
8377	diHPCARP_Ib.tmttmmpmu	7.025e+44	11.45	11.45	3.221e+36	1.41e-05
8378	diHPCARP_Ib.tpmmpmpmu	2.105e+43	9.36	9.36	3.201e+36	1.4e-05
8379	diHPCARP_Ib.ttpmpptpu	5.912e+43	9.99	9.99	3.146e+36	1.38e-05
8380	diHPCARP_Ib.mptmttmu	3.477e+44	11.05	11.05	3.094e+36	1.35e-05
8381	diHPCARP_Ib.mppppmpmu	4.855e+44	11.26	11.26	3.062e+36	1.34e-05
8382	diHPCARP_Ib.ttmmpmpmu	4.114e+43	9.79	9.79	3.031e+36	1.33e-05
8383	diHPCARP_Ib.mttmpmtmu	2.383e+44	10.86	10.86	2.925e+36	1.28e-05
8384	diHPCARP_Ib.ttpmmmtmu	4.953e+43	9.92	9.92	2.916e+36	1.27e-05
8385	diHPCARP_Ib.ttmtpptpu	2.655e+44	10.93	10.93	2.879e+36	1.26e-05
8386	diHPCARP_Ib.ptpmmmpmu	9.019e+43	10.30	10.30	2.845e+36	1.24e-05
8387	diHPCARP_Ib.mmmppmmmu	1.070e+44	10.40	10.40	2.835e+36	1.24e-05
8388	diHPCARP_Ib.tpmmpmtpu	3.353e+43	9.72	9.72	2.780e+36	1.22e-05
8389	diHPCARP_Ib.mmpptptmu	4.757e+44	11.32	11.32	2.690e+36	1.18e-05
8390	diHPCARP_Ib.mtptmtmpu	9.694e+43	10.39	10.39	2.624e+36	1.15e-05
8391	diHPCARP_Ib.pmmmttmu	5.986e+43	10.10	10.10	2.615e+36	1.14e-05
8392	diHPCARP_Ib.mptpmmtpu	6.436e+44	11.52	11.52	2.607e+36	1.14e-05
8393	diHPCARP_Ib.tmpmmmtmu	5.040e+43	10.01	10.01	2.585e+36	1.13e-05
8394	diHPCARP_Ib.ttpmtmtmu	7.573e+44	11.62	11.62	2.577e+36	1.13e-05
8395	diHPCARP_Ib.tptmpmtpu	6.249e+43	10.15	10.15	2.518e+36	1.1e-05
8396	diHPCARP_Ib.tmmmmtpmu	7.542e+43	10.27	10.27	2.509e+36	1.1e-05
8397	diHPCARP_Ib.tmmmmtpmu	1.617e+44	10.73	10.73	2.479e+36	1.08e-05
8398	diHPCARP_Ib.pppppmmmu	8.059e+43	10.32	10.32	2.432e+36	1.06e-05
8399	diHPCARP_Ib.pmpmtmtmu	2.363e+44	10.97	10.97	2.429e+36	1.06e-05
8400	diHPCARP_Ib.tmmmmmtmu	1.748e+44	10.79	10.79	2.429e+36	1.06e-05

8401	diHPCARP_Ib.tmpptppu	2.566e+44	11.02	11.02	2.395e+36	1.05e-05
8402	diHPCARP_Ib.mtmmppmu	1.710e+44	10.80	10.80	2.330e+36	1.02e-05
8403	diHPCARP_Ib.tmpmttptu	5.365e+44	11.48	11.48	2.327e+36	1.02e-05
8404	diHPCARP_Ib.ttppppmu	1.601e+44	10.76	10.76	2.324e+36	1.02e-05
8405	diHPCARP_Ib.tpmptttmu	1.652e+44	10.78	10.78	2.305e+36	1.01e-05
8406	diHPCARP_Ib.tmpptppmu	4.344e+43	9.99	9.99	2.292e+36	1e-05
8407	diHPCARP_Ib.mtmmptmtu	1.732e+44	10.82	10.82	2.263e+36	9.89e-06
8408	diHPCARP_Ib.ttpmppppu	5.993e+43	10.19	10.19	2.249e+36	9.83e-06
8409	diHPCARP_Ib.mptpmmpu	4.636e+43	10.04	10.04	2.245e+36	9.81e-06
8410	diHPCARP_Ib.mpmmpmmu	3.154e+43	9.85	9.85	2.117e+36	9.26e-06
8411	diHPCARP_Ib.tptmptmtu	1.315e+44	10.71	10.71	2.057e+36	8.99e-06
8412	diHPCARP_Ib.mtmtmtpmu	1.122e+44	10.63	10.63	2.030e+36	8.88e-06
8413	diHPCARP_Ib.mmpmntttmu	5.665e+43	10.22	10.22	2.022e+36	8.84e-06
8414	diHPCARP_Ib.mpttppmpu	2.794e+44	11.18	11.18	2.018e+36	8.82e-06
8415	diHPCARP_Ib.mtptptmtu	4.702e+43	10.12	10.12	2.011e+36	8.79e-06
8416	diHPCARP_Ib.pmmptttpu	2.293e+43	9.69	9.69	1.997e+36	8.73e-06
8417	diHPCARP_Ib.mpmmpmpu	1.062e+43	9.25	9.25	1.939e+36	8.48e-06
8418	diHPCARP_Ib.tmpmtttmu	3.220e+44	11.28	11.28	1.938e+36	8.47e-06
8419	diHPCARP_Ib.mppppmmpu	1.074e+44	10.63	10.63	1.935e+36	8.46e-06
8420	diHPCARP_Ib.mtmmmtmtu	2.345e+44	11.10	11.10	1.933e+36	8.45e-06
8421	diHPCARP_Ib.pttppmpu	1.354e+44	10.78	10.78	1.912e+36	8.36e-06
8422	diHPCARP_Ib.ptmmpmmpu	1.282e+44	10.75	10.75	1.887e+36	8.25e-06
8423	diHPCARP_Ib.mtmmptmtu	8.759e+43	10.53	10.53	1.879e+36	8.21e-06
8424	diHPCARP_Ib.tppppmtptu	2.281e+44	11.10	11.10	1.873e+36	8.19e-06
8425	diHPCARP_Ib.mptmptmtu	3.910e+43	10.05	10.05	1.852e+36	8.1e-06
8426	diHPCARP_Ib.pptmmtmu	3.376e+44	11.34	11.34	1.843e+36	8.06e-06
8427	diHPCARP_Ib.mtptmptmu	1.538e+44	10.88	10.88	1.822e+36	7.97e-06
8428	diHPCARP_Ib.pmntmtmtu	4.843e+43	10.23	10.23	1.721e+36	7.52e-06
8429	diHPCARP_Ib.mtptmmtptu	3.859e+44	11.48	11.48	1.664e+36	7.27e-06
8430	diHPCARP_Ib.pptptmtmu	3.530e+44	11.44	11.44	1.632e+36	7.13e-06
8431	diHPCARP_Ib.mtmmptmtu	1.312e+44	10.85	10.85	1.629e+36	7.12e-06
8432	diHPCARP_Ib.pmpmmpmmpu	1.755e+43	9.66	9.66	1.607e+36	7.03e-06
8433	diHPCARP_Ib.mtmtmtpmu	5.220e+43	10.31	10.31	1.602e+36	7e-06
8434	diHPCARP_Ib.tmpmmpmmpu	4.781e+43	10.27	10.27	1.565e+36	6.84e-06
8435	diHPCARP_Ib.pmpptttptu	4.202e+43	10.20	10.20	1.558e+36	6.81e-06
8436	diHPCARP_Ib.mtmtmmtmu	3.021e+44	11.38	11.38	1.540e+36	6.73e-06
8437	diHPCARP_Ib.mtptptpmu	2.215e+44	11.20	11.20	1.526e+36	6.67e-06
8438	diHPCARP_Ib.tpmmmmmmu	3.166e+43	10.05	10.05	1.506e+36	6.58e-06
8439	diHPCARP_Ib.tmpmtptmu	1.364e+44	10.93	10.93	1.487e+36	6.5e-06
8440	diHPCARP_Ib.mtmtptttmu	3.447e+44	11.49	11.49	1.467e+36	6.41e-06
8441	diHPCARP_Ib.tmpmttppu	2.090e+44	11.19	11.19	1.462e+36	6.39e-06
8442	diHPCARP_Ib.pmmptmtmu	9.343e+43	10.72	10.72	1.462e+36	6.39e-06
8443	diHPCARP_Ib.ttmpmntmtu	3.793e+43	10.18	10.18	1.461e+36	6.39e-06
8444	diHPCARP_Ib.tmpmntmtmu	2.034e+43	9.81	9.81	1.445e+36	6.32e-06
8445	diHPCARP_Ib.mpttmmppu	9.775e+43	10.76	10.76	1.411e+36	6.17e-06
8446	diHPCARP_Ib.tmtpppppu	9.942e+43	10.78	10.78	1.403e+36	6.13e-06
8447	diHPCARP_Ib.mptptttptu	2.040e+44	11.21	11.21	1.392e+36	6.08e-06
8448	diHPCARP_Ib.mtmtmmtmu	2.955e+44	11.44	11.44	1.374e+36	6.01e-06
8449	diHPCARP_Ib.tmpmtmtptu	2.339e+44	11.30	11.30	1.374e+36	6.01e-06
8450	diHPCARP_Ib.mtppmtmtmu	5.415e+43	10.44	10.44	1.336e+36	5.84e-06
8451	diHPCARP_Ib.tmpmptmtu	6.692e+43	10.57	10.57	1.330e+36	5.82e-06
8452	diHPCARP_Ib.tpmpttppu	2.489e+44	11.36	11.36	1.318e+36	5.76e-06
8453	diHPCARP_Ib.tmpptttptu	7.235e+44	12.00	12.00	1.302e+36	5.69e-06
8454	diHPCARP_Ib.tpmmttptmu	2.247e+43	9.96	9.96	1.237e+36	5.41e-06
8455	diHPCARP_Ib.ttttmmmpu	2.096e+44	11.30	11.30	1.234e+36	5.4e-06
8456	diHPCARP_Ib.ppmptttptu	2.128e+44	11.31	11.31	1.224e+36	5.35e-06
8457	diHPCARP_Ib.ttpppmpu	2.678e+44	11.45	11.45	1.212e+36	5.3e-06
8458	diHPCARP_Ib.mmpmtmtpmu	2.460e+44	11.41	11.41	1.198e+36	5.24e-06
8459	diHPCARP_Ib.tmpppmpu	5.035e+44	11.85	11.85	1.181e+36	5.16e-06
8460	diHPCARP_Ib.mpmptmtpu	1.377e+44	11.08	11.08	1.178e+36	5.15e-06
8461	diHPCARP_Ib.mtptmppmu	6.246e+43	10.62	10.62	1.146e+36	5.01e-06
8462	diHPCARP_Ib.pmpptmtpu	3.985e+43	10.36	10.36	1.133e+36	4.95e-06
8463	diHPCARP_Ib.mmpmtmtmu	1.203e+44	11.02	11.02	1.129e+36	4.94e-06
8464	diHPCARP_Ib.tpmmmmmmu	5.703e+43	10.59	10.59	1.092e+36	4.77e-06
8465	diHPCARP_Ib.tmppttptmu	1.722e+44	11.27	11.27	1.070e+36	4.68e-06
8466	diHPCARP_Ib.tmpmtmtmu	2.099e+44	11.39	11.39	1.067e+36	4.66e-06
8467	diHPCARP_Ib.mpttmmmpu	6.334e+44	12.05	12.05	1.062e+36	4.64e-06
8468	diHPCARP_Ib.mmpmtmtmu	2.145e+44	11.40	11.40	1.055e+36	4.61e-06
8469	diHPCARP_Ib.tptmptptu	2.460e+44	11.49	11.49	1.055e+36	4.61e-06
8470	diHPCARP_Ib.tmtpttptmu	4.939e+44	11.91	11.91	1.045e+36	4.57e-06
8471	diHPCARP_Ib.mptpmmpu	1.906e+44	11.35	11.35	1.033e+36	4.52e-06
8472	diHPCARP_Ib.mptpmmtmu	2.181e+44	11.44	11.44	1.003e+36	4.38e-06

8473	diHPCARP_Ib.tmpppptpu	2.020e+44	11.43	11.43	9.518e+35	4.16e-06
8474	diHPCARP_Ib.mptppmmpu	1.799e+44	11.38	11.38	9.257e+35	4.05e-06
8475	diHPCARP_Ib.tmpmmttptu	5.794e+43	10.72	10.72	9.017e+35	3.94e-06
8476	diHPCARP_Ib.mmppppptmu	3.130e+44	11.73	11.73	8.951e+35	3.91e-06
8477	diHPCARP_Ib.tmttppmpu	3.146e+44	11.74	11.74	8.860e+35	3.87e-06
8478	diHPCARP_Ib.tmmmpmtptu	1.387e+44	11.25	11.25	8.858e+35	3.87e-06
8479	diHPCARP_Ib.ttpmtpppu	1.616e+44	11.34	11.34	8.827e+35	3.86e-06
8480	diHPCARP_Ib.ppmmmmpmu	1.352e+43	9.86	9.86	8.803e+35	3.85e-06
8481	diHPCARP_Ib.pmpptmtmu	2.897e+44	11.72	11.72	8.457e+35	3.7e-06
8482	diHPCARP_Ib.tmpptttmu	3.587e+44	11.84	11.84	8.445e+35	3.69e-06
8483	diHPCARP_Ib.tptmppmpu	2.345e+44	11.59	11.59	8.407e+35	3.68e-06
8484	diHPCARP_Ib.mttppppmu	2.871e+44	11.72	11.72	8.320e+35	3.64e-06
8485	diHPCARP_Ib.tpmmmmtmu	5.198e+43	10.71	10.71	8.229e+35	3.6e-06
8486	diHPCARP_Ib.tmpptmtmu	6.399e+43	10.85	10.85	8.048e+35	3.52e-06
8487	diHPCARP_Ib.tmppttptmu	6.451e+44	12.23	12.23	7.998e+35	3.5e-06
8488	diHPCARP_Ib.tppppppmu	1.668e+44	11.43	11.43	7.890e+35	3.45e-06
8489	diHPCARP_Ib.mmpptppmu	1.984e+45	12.94	12.94	7.404e+35	3.24e-06
8490	diHPCARP_Ib.tpmtptpmu	3.046e+44	11.83	11.83	7.396e+35	3.23e-06
8491	diHPCARP_Ib.pmmptmtmu	2.346e+43	10.30	10.30	7.392e+35	3.23e-06
8492	diHPCARP_Ib.pptmtmmmu	9.897e+43	11.16	11.16	7.390e+35	3.23e-06
8493	diHPCARP_Ib.tmmppmpu	6.974e+43	10.95	10.95	7.347e+35	3.21e-06
8494	diHPCARP_Ib.pptptpmu	1.771e+44	11.51	11.51	7.246e+35	3.17e-06
8495	diHPCARP_Ib.mtmtppptmu	1.590e+44	11.45	11.45	7.230e+35	3.16e-06
8496	diHPCARP_Ib.mtppmmpmu	4.848e+43	10.76	10.76	7.052e+35	3.08e-06
8497	diHPCARP_Ib.pptpmmmu	1.255e+44	11.33	11.33	7.017e+35	3.07e-06
8498	diHPCARP_Ib.mmpmmtmmu	3.867e+43	10.64	10.64	6.878e+35	3.01e-06
8499	diHPCARP_Ib.mtttmtptmu	2.545e+44	11.77	11.77	6.817e+35	2.98e-06
8500	diHPCARP_Ib.mptpmmpmu	1.046e+44	11.24	11.24	6.761e+35	2.96e-06
8501	diHPCARP_Ib.tmmmpmmpu	4.051e+43	10.70	10.70	6.523e+35	2.85e-06
8502	diHPCARP_Ib.mttppmmpmu	1.499e+44	11.49	11.49	6.415e+35	2.8e-06
8503	diHPCARP_Ib.tmpmtmtptu	7.227e+44	12.43	12.43	6.375e+35	2.79e-06
8504	diHPCARP_Ib.pptmmpmmu	9.999e+43	11.26	11.26	6.254e+35	2.73e-06
8505	diHPCARP_Ib.tpmmmmpmu	3.146e+43	10.58	10.58	6.192e+35	2.71e-06
8506	diHPCARP_Ib.ttmppppmu	2.105e+44	11.71	11.71	6.170e+35	2.7e-06
8507	diHPCARP_Ib.ttmtpppmu	1.228e+44	11.39	11.39	6.145e+35	2.69e-06
8508	diHPCARP_Ib.mppppptmu	1.305e+44	11.46	11.46	5.822e+35	2.55e-06
8509	diHPCARP_Ib.ttmmpppmu	6.531e+43	11.06	11.06	5.725e+35	2.5e-06
8510	diHPCARP_Ib.mpttmmmpmu	3.508e+44	12.07	12.07	5.677e+35	2.48e-06
8511	diHPCARP_Ib.tmpmmttptu	9.766e+43	11.31	11.31	5.598e+35	2.45e-06
8512	diHPCARP_Ib.pmpppptmu	6.792e+43	11.10	11.10	5.568e+35	2.43e-06
8513	diHPCARP_Ib.mtmppppmu	5.389e+43	10.97	10.97	5.529e+35	2.42e-06
8514	diHPCARP_Ib.pptpmpmmu	2.521e+43	10.54	10.54	5.311e+35	2.32e-06
8515	diHPCARP_Ib.tttppppmu	1.647e+44	11.66	11.66	5.302e+35	2.32e-06
8516	diHPCARP_Ib.mmmppppmu	7.951e+43	11.25	11.25	5.072e+35	2.22e-06
8517	diHPCARP_Ib.mmmppppmu	3.015e+43	10.67	10.67	5.053e+35	2.21e-06
8518	diHPCARP_Ib.tmmptmtptu	6.431e+44	12.53	12.53	4.821e+35	2.11e-06
8519	diHPCARP_Ib.pmmmttptu	4.061e+43	10.88	10.88	4.795e+35	2.1e-06
8520	diHPCARP_Ib.mmmmppppmu	3.503e+43	10.80	10.80	4.746e+35	2.07e-06
8521	diHPCARP_Ib.tpmmttptu	6.108e+43	11.13	11.13	4.743e+35	2.07e-06
8522	diHPCARP_Ib.ttpmtppmu	2.834e+44	12.07	12.07	4.551e+35	1.99e-06
8523	diHPCARP_Ib.mpmmmmtptu	1.545e+44	11.73	11.73	4.432e+35	1.94e-06
8524	diHPCARP_Ib.mtttppppmu	2.073e+44	11.92	11.92	4.324e+35	1.89e-06
8525	diHPCARP_Ib.pmmtpptmu	2.613e+43	10.69	10.69	4.299e+35	1.88e-06
8526	diHPCARP_Ib.mtmtpppmu	1.074e+44	11.54	11.54	4.192e+35	1.83e-06
8527	diHPCARP_Ib.ttpmmpmmu	2.815e+43	10.75	10.75	4.177e+35	1.83e-06
8528	diHPCARP_Ib.pptpmmmmu	8.510e+43	11.42	11.42	4.101e+35	1.79e-06
8529	diHPCARP_Ib.mtpmmpmmu	8.772e+43	11.44	11.44	4.095e+35	1.79e-06
8530	diHPCARP_Ib.tmpmpptpu	1.924e+44	11.96	11.96	3.701e+35	1.62e-06
8531	diHPCARP_Ib.tptmmpppu	5.769e+44	12.68	12.68	3.358e+35	1.47e-06
8532	diHPCARP_Ib.mmpmmtptmu	4.310e+43	11.13	11.13	3.338e+35	1.46e-06
8533	diHPCARP_Ib.mppmtmmpu	5.968e+43	11.33	11.33	3.319e+35	1.45e-06
8534	diHPCARP_Ib.mtmppppmu	4.344e+43	11.15	11.15	3.298e+35	1.44e-06
8535	diHPCARP_Ib.ppmmpmmpu	5.799e+42	9.96	9.96	3.197e+35	1.4e-06
8536	diHPCARP_Ib.mtmtpmtmu	5.378e+44	12.67	12.67	3.194e+35	1.4e-06
8537	diHPCARP_Ib.pptpmtppu	1.250e+44	11.80	11.80	3.167e+35	1.38e-06
8538	diHPCARP_Ib.tppppppmu	1.732e+44	12.00	12.00	3.165e+35	1.38e-06
8539	diHPCARP_Ib.mppptmmpu	6.664e+43	11.43	11.43	3.146e+35	1.38e-06
8540	diHPCARP_Ib.mpmtpmmpu	1.677e+44	12.01	12.01	3.008e+35	1.31e-06
8541	diHPCARP_Ib.mppptmtmu	7.395e+43	11.52	11.52	2.996e+35	1.31e-06
8542	diHPCARP_Ib.mtpmmpmmu	2.114e+45	13.57	13.57	2.760e+35	1.21e-06
8543	diHPCARP_Ib.mtttptptmu	2.128e+44	12.20	12.20	2.756e+35	1.2e-06
8544	diHPCARP_Ib.mpttpmmpu	4.030e+44	12.60	12.60	2.669e+35	1.17e-06

8545	diHPCARP_Ib.tmpmmpptpu	1.188e+44	11.90	11.90	2.551e+35	1.12e-06
8546	diHPCARP_Ib.tptmnmumu	2.807e+44	12.43	12.43	2.476e+35	1.08e-06
8547	diHPCARP_Ib.ppptmnmumu	1.168e+44	11.91	11.91	2.468e+35	1.08e-06
8548	diHPCARP_Ib.tptpppppu	2.367e+44	12.33	12.33	2.453e+35	1.07e-06
8549	diHPCARP_Ib.tmmtpppmu	4.927e+44	12.79	12.79	2.358e+35	1.03e-06
8550	diHPCARP_Ib.mpmnmnmumu	3.280e+43	11.18	11.18	2.357e+35	1.03e-06
8551	diHPCARP_Ib.ttmpmmpmu	2.310e+43	10.97	10.97	2.338e+35	1.02e-06
8552	diHPCARP_Ib.mpttpmumu	5.394e+44	12.86	12.86	2.296e+35	1e-06
8553	diHPCARP_Ib.mtpppppmu	7.952e+43	11.72	11.72	2.287e+35	1e-06
8554	diHPCARP_Ib.tptmppppu	3.049e+44	12.55	12.55	2.214e+35	9.68e-07
8555	diHPCARP_Ib.mtttpppmu	1.764e+44	12.23	12.23	2.181e+35	9.53e-07
8556	diHPCARP_Ib.mtmppmtmu	9.357e+43	11.88	11.88	2.085e+35	9.11e-07
8557	diHPCARP_Ib.pppppmumu	3.812e+43	11.35	11.35	2.053e+35	8.98e-07
8558	diHPCARP_Ib.mppptmnmumu	1.945e+44	12.36	12.36	1.921e+35	8.4e-07
8559	diHPCARP_Ib.mppptmnmumu	3.176e+44	12.67	12.67	1.886e+35	8.24e-07
8560	diHPCARP_Ib.tpmmpmpmu	2.479e+43	11.16	11.16	1.850e+35	8.09e-07
8561	diHPCARP_Ib.pptmnmumu	3.083e+44	12.66	12.66	1.841e+35	8.05e-07
8562	diHPCARP_Ib.ppttpmumu	1.352e+44	12.18	12.18	1.806e+35	7.89e-07
8563	diHPCARP_Ib.mtttmtmumu	3.172e+44	12.69	12.69	1.800e+35	7.87e-07
8564	diHPCARP_Ib.ppmnmmtmu	3.523e+43	11.38	11.38	1.796e+35	7.85e-07
8565	diHPCARP_Ib.mppptpmumu	5.160e+44	12.99	12.99	1.770e+35	7.74e-07
8566	diHPCARP_Ib.mppptppmu	1.236e+44	12.14	12.14	1.758e+35	7.69e-07
8567	diHPCARP_Ib.mtptmmpmu	1.875e+44	12.40	12.40	1.734e+35	7.58e-07
8568	diHPCARP_Ib.tptpmmtmu	1.951e+44	12.43	12.43	1.727e+35	7.55e-07
8569	diHPCARP_Ib.mpmtpmtmu	5.873e+43	11.74	11.74	1.638e+35	7.16e-07
8570	diHPCARP_Ib.tmmmmpppu	5.189e+43	11.72	11.72	1.513e+35	6.61e-07
8571	diHPCARP_Ib.tptmpmpmu	1.520e+44	12.37	12.37	1.489e+35	6.51e-07
8572	diHPCARP_Ib.ttmnmtpmu	6.951e+43	11.91	11.91	1.476e+35	6.45e-07
8573	diHPCARP_Ib.mtttptmumu	3.538e+44	12.93	12.93	1.346e+35	5.88e-07
8574	diHPCARP_Ib.mtmnmppmu	9.151e+43	12.14	12.14	1.308e+35	5.72e-07
8575	diHPCARP_Ib.mtttptmumu	1.777e+44	12.55	12.55	1.283e+35	5.61e-07
8576	diHPCARP_Ib.ttmpptmpu	4.530e+43	11.74	11.74	1.279e+35	5.59e-07
8577	diHPCARP_Ib.tpmppptmu	2.204e+44	12.68	12.68	1.277e+35	5.58e-07
8578	diHPCARP_Ib.tmmtppppu	1.512e+44	12.46	12.46	1.276e+35	5.58e-07
8579	diHPCARP_Ib.mtmtpmpmu	1.262e+44	12.35	12.35	1.270e+35	5.55e-07
8580	diHPCARP_Ib.pmpptmnmumu	1.112e+44	12.28	12.28	1.268e+35	5.54e-07
8581	diHPCARP_Ib.tpmtpmpmu	8.735e+43	12.14	12.14	1.260e+35	5.51e-07
8582	diHPCARP_Ib.tmmmmpppu	4.476e+43	11.75	11.75	1.234e+35	5.4e-07
8583	diHPCARP_Ib.mpmmtmtmu	5.566e+43	11.89	11.89	1.211e+35	5.3e-07
8584	diHPCARP_Ib.pnmmpmtmu	3.257e+43	11.62	11.62	1.114e+35	4.87e-07
8585	diHPCARP_Ib.mptmnmumu	4.524e+44	13.19	13.19	1.107e+35	4.84e-07
8586	diHPCARP_Ib.mtppppptmu	2.244e+44	12.79	12.79	1.086e+35	4.75e-07
8587	diHPCARP_Ib.mtttmpmumu	3.873e+44	13.12	13.12	1.066e+35	4.66e-07
8588	diHPCARP_Ib.mppptmnmumu	1.423e+44	12.54	12.54	1.050e+35	4.59e-07
8589	diHPCARP_Ib.mtptmptmu	4.295e+44	13.20	13.20	1.037e+35	4.53e-07
8590	diHPCARP_Ib.ppmtpmmpu	4.119e+44	13.21	13.21	9.801e+34	4.28e-07
8591	diHPCARP_Ib.ttmppppmu	2.492e+43	11.57	11.57	9.280e+34	4.06e-07
8592	diHPCARP_Ib.tptmmtmu	5.563e+44	13.44	13.44	9.078e+34	3.97e-07
8593	diHPCARP_Ib.mtttppmumu	3.632e+44	13.20	13.20	8.864e+34	3.87e-07
8594	diHPCARP_Ib.mppptmmtmu	3.292e+44	13.17	13.17	8.402e+34	3.67e-07
8595	diHPCARP_Ib.mppptmnmumu	6.471e+44	13.64	13.64	7.478e+34	3.27e-07
8596	diHPCARP_Ib.mtpppppmu	2.780e+44	13.16	13.16	7.195e+34	3.15e-07
8597	diHPCARP_Ib.tptmmpmu	2.301e+44	13.06	13.06	7.086e+34	3.1e-07
8598	diHPCARP_Ib.mtptpppmu	4.572e+44	13.49	13.49	6.864e+34	3e-07
8599	diHPCARP_Ib.tptppppmu	1.616e+44	12.92	12.92	6.286e+34	2.75e-07
8600	diHPCARP_Ib.mpmmtmtpmu	3.427e+43	12.01	12.01	6.067e+34	2.65e-07
8601	diHPCARP_Ib.tppptmnmumu	3.056e+44	13.33	13.33	5.969e+34	2.61e-07
8602	diHPCARP_Ib.mpmnmmtmu	2.919e+44	13.31	13.31	5.876e+34	2.57e-07
8603	diHPCARP_Ib.mpmtpmtmu	5.131e+44	13.65	13.65	5.800e+34	2.54e-07
8604	diHPCARP_Ib.tppmnmtpu	6.865e+43	12.46	12.46	5.714e+34	2.5e-07
8605	diHPCARP_Ib.mpmnmmpmu	1.938e+44	13.09	13.09	5.626e+34	2.46e-07
8606	diHPCARP_Ib.tpmtpmtpu	5.824e+44	13.79	13.79	5.234e+34	2.29e-07
8607	diHPCARP_Ib.mtptmmpmu	3.130e+44	13.42	13.42	5.196e+34	2.27e-07
8608	diHPCARP_Ib.tppptmmpmu	5.924e+44	13.84	13.84	4.936e+34	2.16e-07
8609	diHPCARP_Ib.tpmmpmtmu	4.130e+43	12.28	12.28	4.661e+34	2.04e-07
8610	diHPCARP_Ib.mppmnmmpmu	7.093e+44	13.99	13.99	4.552e+34	1.99e-07
8611	diHPCARP_Ib.mpmnmmtmu	2.723e+43	12.15	12.15	3.862e+34	1.69e-07
8612	diHPCARP_Ib.mpmmtmtpu	1.808e+44	13.29	13.29	3.785e+34	1.65e-07
8613	diHPCARP_Ib.tpmnmmpmu	3.265e+43	12.37	12.37	3.201e+34	1.4e-07
8614	diHPCARP_Ib.mpmmtmmpmu	1.607e+44	13.33	13.33	3.144e+34	1.37e-07
8615	diHPCARP_Ib.tmmppptmu	4.418e+43	12.58	12.58	3.010e+34	1.32e-07
8616	diHPCARP_Ib.tptppppmu	2.875e+44	13.85	13.85	2.326e+34	1.02e-07

8617	diHPCARP_Ib.mpptmmtpu	1.871e+44	13.65	13.65	2.129e+34	9.31e-08
8618	diHPCARP_Ib.tpptmmtpu	3.958e+44	14.13	14.13	2.027e+34	8.86e-08
8619	diHPCARP_Ib.tpptmpppu	3.561e+44	14.07	14.07	2.013e+34	8.8e-08
8620	diHPCARP_Ib.mppmmmtmu	5.815e+43	13.02	13.02	1.904e+34	8.32e-08
8621	diHPCARP_Ib.tpptppmpu	4.496e+44	14.24	14.24	1.903e+34	8.32e-08
8622	diHPCARP_Ib.mpmmpmpmu	2.101e+43	12.46	12.46	1.747e+34	7.64e-08
8623	diHPCARP_Ib.tppmmmpmu	6.320e+43	13.20	13.20	1.529e+34	6.68e-08
8624	diHPCARP_Ib.tpttmpppu	2.883e+44	14.11	14.11	1.523e+34	6.66e-08
8625	diHPCARP_Ib.tptmppppu	1.126e+44	13.57	13.57	1.455e+34	6.36e-08
8626	diHPCARP_Ib.mmpmmmpmu	3.929e+43	12.96	12.96	1.414e+34	6.18e-08
8627	diHPCARP_Ib.mtmppmpmu	1.189e+44	13.66	13.66	1.341e+34	5.86e-08
8628	diHPCARP_Ib.mpptmmtpu	1.823e+44	13.97	13.97	1.205e+34	5.27e-08
8629	diHPCARP_Ib.tmpmmpppu	5.362e+43	13.32	13.32	1.057e+34	4.62e-08
8630	diHPCARP_Ib.mtmmtmtpu	1.289e+44	13.89	13.89	9.868e+33	4.31e-08
8631	diHPCARP_Ib.tppmmpppu	5.235e+43	13.47	13.47	8.072e+33	3.53e-08
8632	diHPCARP_Ib.tpttmpppu	5.836e+44	14.92	14.92	7.872e+33	3.44e-08
8633	diHPCARP_Ib.mmpmmppmu	3.489e+43	13.32	13.32	6.860e+33	3e-08
8634	diHPCARP_Ib.tpmppmtpu	4.486e+43	13.60	13.60	5.559e+33	2.43e-08
8635	diHPCARP_Ib.tpptppppu	3.586e+44	14.88	14.88	5.210e+33	2.28e-08
8636	diHPCARP_Ib.mpmtpmpu	1.986e+44	14.58	14.58	4.717e+33	2.06e-08
8637	diHPCARP_Ib.mmpmmmtmu	1.059e+44	14.23	14.23	4.585e+33	2e-08
8638	diHPCARP_Ib.tpmppmmpu	3.270e+43	13.73	13.73	3.250e+33	1.42e-08
8639	diHPCARP_Ib.mpmmmpppu	3.464e+43	13.81	13.81	3.011e+33	1.32e-08
8640	diHPCARP_Ib.tpmppmpppu	1.722e+43	13.50	13.50	2.529e+33	1.11e-08
8641	diHPCARP_Ib.mpmmtmmtmu	6.099e+43	14.38	14.38	2.041e+33	8.92e-09
8642	diHPCARP_Ib.mmpmmmmmu	8.010e+43	14.56	14.56	1.977e+33	8.64e-09
8643	diHPCARP_Ib.tpmtmmpu	1.252e+44	15.01	15.01	1.455e+33	6.36e-09
8644	diHPCARP_Ib.tpmtpmtpu	1.622e+44	15.33	15.33	1.103e+33	4.82e-09
8645	diHPCARP_Ib.tpmmmmtpu	9.776e+43	15.05	15.05	1.059e+33	4.63e-09
8646	diHPCARP_Ib.tmmppmmpu	3.623e+43	14.49	14.49	1.013e+33	4.43e-09
8647	diHPCARP_Ib.tpmmmmpu	6.816e+43	14.97	14.97	8.505e+32	3.72e-09
8648	diHPCARP_Ib.mpmmtmmtmu	6.498e+43	14.95	14.95	8.326e+32	3.64e-09
8649	diHPCARP_Ib.pmmptppu	3.005e+43	14.81	14.81	4.922e+32	2.15e-09
8650	diHPCARP_Ib.mpmtpmtmu	5.500e+44	16.84	16.84	2.967e+32	1.3e-09
8651	diHPCARP_Ib.tpmtppppu	1.500e+44	16.40	16.40	1.705e+32	7.45e-10
8652	diHPCARP_Ib.mpmmtmmpu	2.599e+43	15.41	15.41	1.556e+32	6.8e-10
8653	diHPCARP_Ib.tpmppmppu	6.140e+43	15.96	15.96	1.439e+32	6.29e-10
8654	diHPCARP_Ib.tpmmmppu	1.179e+44	18.27	18.27	5.766e+30	2.52e-11
8655	Total				2.288e+43	100

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8657
8658
8659 (2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-Ic)
8660

8661
8662 Population analysis at 300K. Vibrational scaling: 0.971.
8663 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
8664 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
8665 %: contribution to the population (with current data set assumed 100%)
8666

Compound	Qtot	Erel	Erel2	n*Q*MB	%
8667					
8668	diHPCARP_Ic.tmtmppppu	3.289e+43	0.00	0.00	3.289e+43 42.5
8669	diHPCARP_Ic.pmtpppppu	1.624e+43	0.44	0.44	7.805e+42 10.1
8670	diHPCARP_Ic.pttpmtppu	1.484e+43	0.63	0.63	5.158e+42 6.67
8671	diHPCARP_Ic.pmmmpmtmu	1.241e+43	0.58	0.58	4.663e+42 6.03
8672	diHPCARP_Ic.ptmmmttmu	1.931e+43	0.88	0.88	4.432e+42 5.73
8673	diHPCARP_Ic.tmmmmmtmu	1.935e+43	0.92	0.92	4.117e+42 5.33
8674	diHPCARP_Ic.pptpmtppu	1.270e+43	1.20	1.20	1.707e+42 2.21
8675	diHPCARP_Ic.pppppmpmu	2.653e+43	1.94	1.94	1.026e+42 1.33
8676	diHPCARP_Ic.pttmmttmu	7.023e+43	2.70	2.70	7.612e+41 0.985
8677	diHPCARP_Ic.ptppmtmmu	4.772e+43	2.54	2.54	6.765e+41 0.875
8678	diHPCARP_Ic.pmmmpmppu	2.132e+43	2.08	2.08	6.556e+41 0.848
8679	diHPCARP_Ic.pttmmtmpu	4.368e+43	2.55	2.55	6.108e+41 0.79
8680	diHPCARP_Ic.tmtppptpu	1.576e+43	1.98	1.98	5.676e+41 0.734
8681	diHPCARP_Ic.tpppmmpmu	5.010e+43	2.79	2.79	4.641e+41 0.6
8682	diHPCARP_Ic.pptppmtmu	5.907e+43	3.02	3.02	3.735e+41 0.483
8683	diHPCARP_Ic.pptppmppu	2.215e+43	2.44	2.44	3.718e+41 0.481
8684	diHPCARP_Ic.ptttmttmu	1.220e+44	3.48	3.48	3.576e+41 0.463
8685	diHPCARP_Ic.tpppmppmu	3.508e+43	2.77	2.77	3.346e+41 0.433
8686	diHPCARP_Ic.tptmmppmu	3.937e+43	2.87	2.87	3.185e+41 0.412
8687	diHPCARP_Ic.ppmmttmu	3.511e+43	2.85	2.85	2.946e+41 0.381
8688	diHPCARP_Ic.mtmmpmttmu	1.699e+43	2.42	2.42	2.913e+41 0.377

8689	diHPCARP_Ic.pmpmntpmu	4.365e+43	2.99	2.99	2.892e+41	0.374
8690	diHPCARP_Ic.pppppmmpu	1.542e+43	2.37	2.37	2.891e+41	0.374
8691	diHPCARP_Ic.ptttmtmpu	8.017e+43	3.36	3.36	2.859e+41	0.37
8692	diHPCARP_Ic.ppppmpmpu	3.112e+43	2.81	2.81	2.779e+41	0.359
8693	diHPCARP_Ic.pttpmtmmu	6.218e+43	3.27	3.27	2.580e+41	0.334
8694	diHPCARP_Ic.mptpptppu	1.102e+43	2.25	2.25	2.542e+41	0.329
8695	diHPCARP_Ic.tmtmmpppu	3.768e+43	2.99	2.99	2.480e+41	0.321
8696	diHPCARP_Ic.tmmmmpppu	2.586e+43	2.81	2.81	2.320e+41	0.3
8697	diHPCARP_Ic.mmtppmpu	3.436e+43	2.98	2.98	2.313e+41	0.299
8698	diHPCARP_Ic.pppmttppu	6.966e+43	3.42	3.42	2.244e+41	0.29
8699	diHPCARP_Ic.ptmtmtmpu	7.487e+43	3.48	3.48	2.184e+41	0.283
8700	diHPCARP_Ic.ptmmmtmpu	4.034e+43	3.14	3.14	2.074e+41	0.268
8701	diHPCARP_Ic.ppptmpmpu	3.613e+43	3.11	3.11	1.975e+41	0.255
8702	diHPCARP_Ic.pttpmtmpu	4.709e+43	3.29	3.29	1.874e+41	0.242
8703	diHPCARP_Ic.tmtmtmpu	7.961e+44	4.98	4.98	1.868e+41	0.242
8704	diHPCARP_Ic.pmtmppppu	3.748e+43	3.18	3.18	1.814e+41	0.235
8705	diHPCARP_Ic.pttmntpmu	3.348e+43	3.12	3.12	1.796e+41	0.232
8706	diHPCARP_Ic.pttmntppu	1.146e+44	3.87	3.87	1.729e+41	0.224
8707	diHPCARP_Ic.pmpptmpu	1.537e+43	2.75	2.75	1.538e+41	0.199
8708	diHPCARP_Ic.pptmpmtmu	4.159e+43	3.35	3.35	1.510e+41	0.195
8709	diHPCARP_Ic.tmtmpppu	2.158e+44	4.34	4.34	1.482e+41	0.192
8710	diHPCARP_Ic.pptmpmpmu	7.577e+43	3.81	3.81	1.270e+41	0.164
8711	diHPCARP_Ic.mmtmptpmu	2.124e+43	3.10	3.10	1.168e+41	0.151
8712	diHPCARP_Ic.ptmmntppu	2.651e+43	3.24	3.24	1.164e+41	0.151
8713	diHPCARP_Ic.mmpptpmu	2.177e+43	3.14	3.14	1.132e+41	0.146
8714	diHPCARP_Ic.tptmmpmpu	2.104e+43	3.16	3.16	1.057e+41	0.137
8715	diHPCARP_Ic.pptmntppu	3.224e+43	3.41	3.41	1.051e+41	0.136
8716	diHPCARP_Ic.mmmmmntmu	7.433e+43	3.99	3.99	9.290e+40	0.12
8717	diHPCARP_Ic.pptmpmpu	7.930e+43	4.03	4.03	9.166e+40	0.119
8718	diHPCARP_Ic.tmtpppppu	2.898e+43	3.43	3.43	9.138e+40	0.118
8719	diHPCARP_Ic.pppppptmu	7.709e+43	4.03	4.03	8.955e+40	0.116
8720	diHPCARP_Ic.ppmnttppu	5.483e+43	3.84	3.84	8.732e+40	0.113
8721	diHPCARP_Ic.pptmpmpmu	1.133e+44	4.29	4.29	8.464e+40	0.109
8722	diHPCARP_Ic.mmtmppppu	7.389e+43	4.09	4.09	7.757e+40	0.1
8723	diHPCARP_Ic.ppptmpmpu	1.698e+43	3.22	3.22	7.669e+40	0.0992
8724	diHPCARP_Ic.tptpmtppu	3.647e+43	3.68	3.68	7.577e+40	0.098
8725	diHPCARP_Ic.pmtpptppu	4.275e+43	3.81	3.81	7.129e+40	0.0922
8726	diHPCARP_Ic.pttpmtmpu	3.026e+43	3.72	3.72	5.860e+40	0.0758
8727	diHPCARP_Ic.pmntppppu	4.897e+43	4.02	4.02	5.808e+40	0.0751
8728	diHPCARP_Ic.pmttppppu	1.297e+44	4.61	4.61	5.721e+40	0.074
8729	diHPCARP_Ic.ptttmtmpu	4.597e+43	3.99	3.99	5.717e+40	0.074
8730	diHPCARP_Ic.tpptmmpmu	5.569e+43	4.10	4.10	5.700e+40	0.0737
8731	diHPCARP_Ic.tpptmpmpu	1.036e+44	4.48	4.48	5.639e+40	0.0729
8732	diHPCARP_Ic.tmtmmpppu	4.154e+43	3.94	3.94	5.563e+40	0.072
8733	diHPCARP_Ic.pmntpmtmu	1.214e+44	4.59	4.59	5.526e+40	0.0715
8734	diHPCARP_Ic.pmtppmtmu	5.167e+43	4.09	4.09	5.443e+40	0.0704
8735	diHPCARP_Ic.pttmnttmu	1.429e+44	4.72	4.72	5.184e+40	0.0671
8736	diHPCARP_Ic.tmtpptppu	4.952e+43	4.14	4.14	4.735e+40	0.0613
8737	diHPCARP_Ic.pmpmtmpmu	3.178e+43	3.90	3.90	4.565e+40	0.0591
8738	diHPCARP_Ic.tmtmmmmmu	1.927e+44	4.99	4.99	4.475e+40	0.0579
8739	diHPCARP_Ic.ppmntmpu	7.115e+42	3.07	3.07	4.135e+40	0.0535
8740	diHPCARP_Ic.tptmmpmpu	1.085e+44	4.70	4.70	4.113e+40	0.0532
8741	diHPCARP_Ic.tmtmmntmu	7.750e+43	4.50	4.50	4.067e+40	0.0526
8742	diHPCARP_Ic.tmtmmpu	6.601e+43	4.42	4.42	3.993e+40	0.0517
8743	diHPCARP_Ic.tmmmpmtmu	4.315e+43	4.20	4.20	3.766e+40	0.0487
8744	diHPCARP_Ic.pptmpmpu	3.145e+43	4.02	4.02	3.733e+40	0.0483
8745	diHPCARP_Ic.ppptmttppu	6.705e+43	4.47	4.47	3.701e+40	0.0479
8746	diHPCARP_Ic.pppppptpu	1.019e+44	4.73	4.73	3.630e+40	0.047
8747	diHPCARP_Ic.pppmmpmpu	3.513e+43	4.13	4.13	3.434e+40	0.0444
8748	diHPCARP_Ic.tmmmmntmu	9.862e+43	4.75	4.75	3.393e+40	0.0439
8749	diHPCARP_Ic.tptpmtmu	8.075e+43	4.64	4.64	3.384e+40	0.0438
8750	diHPCARP_Ic.mmtmpttmu	4.305e+43	4.27	4.27	3.343e+40	0.0433
8751	diHPCARP_Ic.pptmpmpu	1.514e+44	5.04	5.04	3.206e+40	0.0415
8752	diHPCARP_Ic.pmntpmtpu	1.847e+44	5.16	5.16	3.200e+40	0.0414
8753	diHPCARP_Ic.pptmmpmpu	4.473e+43	4.32	4.32	3.194e+40	0.0413
8754	diHPCARP_Ic.ptmmntmmu	8.249e+43	4.72	4.72	2.984e+40	0.0386
8755	diHPCARP_Ic.tppppptmu	1.144e+44	4.92	4.92	2.961e+40	0.0383
8756	diHPCARP_Ic.pmtmpmtmu	5.136e+43	4.46	4.46	2.904e+40	0.0376
8757	diHPCARP_Ic.pptppmpmu	4.460e+44	5.75	5.75	2.887e+40	0.0373
8758	diHPCARP_Ic.pppmttppu	3.080e+43	4.16	4.16	2.869e+40	0.0371
8759	diHPCARP_Ic.mmtpmtppu	2.143e+43	3.95	3.95	2.858e+40	0.037
8760	diHPCARP_Ic.pmtmmntmu	4.522e+43	4.40	4.40	2.840e+40	0.0367

8761	diHPCARP_Ic.ptppppmpu	3.604e+43	4.30	4.30	2.648e+40	0.0342
8762	diHPCARP_Ic.tmtmtmtmu	1.347e+44	5.09	5.09	2.638e+40	0.0341
8763	diHPCARP_Ic.ptppmpmpu	1.409e+43	3.75	3.75	2.619e+40	0.0339
8764	diHPCARP_Ic.pptpmmppu	3.585e+43	4.31	4.31	2.596e+40	0.0336
8765	diHPCARP_Ic.mmmtmtmpu	1.018e+44	4.93	4.93	2.593e+40	0.0335
8766	diHPCARP_Ic.pmmppmpu	4.448e+43	4.45	4.45	2.542e+40	0.0329
8767	diHPCARP_Ic.pppmmmtpu	3.132e+43	4.26	4.26	2.460e+40	0.0318
8768	diHPCARP_Ic.tptpptppu	3.874e+43	4.39	4.39	2.458e+40	0.0318
8769	diHPCARP_Ic.tpppmmpu	2.466e+43	4.13	4.13	2.430e+40	0.0314
8770	diHPCARP_Ic.pptpmtmu	5.220e+43	4.58	4.58	2.391e+40	0.0309
8771	diHPCARP_Ic.ptmtmtmu	9.860e+43	4.97	4.97	2.350e+40	0.0304
8772	diHPCARP_Ic.pmpmmtpu	6.367e+43	4.74	4.74	2.229e+40	0.0288
8773	diHPCARP_Ic.ptttmtmu	1.192e+44	5.12	5.12	2.221e+40	0.0287
8774	diHPCARP_Ic.pptmpptpu	1.043e+44	5.07	5.07	2.101e+40	0.0272
8775	diHPCARP_Ic.tptmpmpu	4.676e+43	4.60	4.60	2.084e+40	0.027
8776	diHPCARP_Ic.pmttmtmu	8.627e+43	4.98	4.98	2.048e+40	0.0265
8777	diHPCARP_Ic.pmtmtmtmu	8.478e+43	4.98	4.98	2.006e+40	0.026
8778	diHPCARP_Ic.pmmmpmtpu	5.250e+43	4.69	4.69	1.996e+40	0.0258
8779	diHPCARP_Ic.ppppmtpu	5.602e+43	4.74	4.74	1.986e+40	0.0257
8780	diHPCARP_Ic.pppppmpu	4.958e+43	4.66	4.66	1.982e+40	0.0256
8781	diHPCARP_Ic.mmmmmmtmu	5.451e+43	4.73	4.73	1.944e+40	0.0251
8782	diHPCARP_Ic.mmpptptpu	3.328e+43	4.45	4.45	1.898e+40	0.0245
8783	diHPCARP_Ic.pmtmpmmu	4.385e+43	4.64	4.64	1.835e+40	0.0237
8784	diHPCARP_Ic.pppmmmpu	1.473e+43	4.00	4.00	1.789e+40	0.0231
8785	diHPCARP_Ic.tmtmtmtmu	1.114e+44	5.21	5.21	1.778e+40	0.023
8786	diHPCARP_Ic.tptmmtmtmu	6.794e+43	4.92	4.92	1.774e+40	0.0229
8787	diHPCARP_Ic.tmtpmtppu	6.726e+43	4.93	4.93	1.709e+40	0.0221
8788	diHPCARP_Ic.tptmmpmpu	1.061e+44	5.24	5.24	1.619e+40	0.0209
8789	diHPCARP_Ic.tpppmmtmu	1.318e+44	5.40	5.40	1.540e+40	0.0199
8790	diHPCARP_Ic.ptmtmtmpu	5.222e+43	4.85	4.85	1.529e+40	0.0198
8791	diHPCARP_Ic.tmtmpmpu	1.767e+44	5.60	5.60	1.468e+40	0.019
8792	diHPCARP_Ic.ptptppmpu	1.525e+44	5.52	5.52	1.450e+40	0.0188
8793	diHPCARP_Ic.tptmmmmu	1.341e+44	5.45	5.45	1.431e+40	0.0185
8794	diHPCARP_Ic.mtmtmtmu	1.709e+44	5.61	5.61	1.388e+40	0.018
8795	diHPCARP_Ic.pptmtppu	3.793e+43	4.73	4.73	1.350e+40	0.0175
8796	diHPCARP_Ic.ptpmpmpu	2.008e+43	4.36	4.36	1.332e+40	0.0172
8797	diHPCARP_Ic.tmtptmpu	6.479e+43	5.07	5.07	1.323e+40	0.0171
8798	diHPCARP_Ic.mppmpttmu	2.596e+43	4.52	4.52	1.316e+40	0.017
8799	diHPCARP_Ic.mmtmpptpu	3.200e+43	4.66	4.66	1.299e+40	0.0168
8800	diHPCARP_Ic.ptmtppmpu	1.160e+44	5.42	5.42	1.297e+40	0.0168
8801	diHPCARP_Ic.mmpmptmu	4.350e+43	4.84	4.84	1.292e+40	0.0167
8802	diHPCARP_Ic.pptppmpu	1.317e+44	5.51	5.51	1.280e+40	0.0166
8803	diHPCARP_Ic.pmtmmtppu	2.983e+43	4.62	4.62	1.277e+40	0.0165
8804	diHPCARP_Ic.tmtppmmu	1.739e+44	5.68	5.68	1.270e+40	0.0164
8805	diHPCARP_Ic.pmtmmttptu	3.270e+43	4.69	4.69	1.256e+40	0.0162
8806	diHPCARP_Ic.tmtmmtmu	2.822e+44	5.98	5.98	1.240e+40	0.016
8807	diHPCARP_Ic.pppmptmpu	1.375e+43	4.18	4.18	1.234e+40	0.016
8808	diHPCARP_Ic.tmtmmttptu	2.419e+44	5.90	5.90	1.220e+40	0.0158
8809	diHPCARP_Ic.ptpmmtmu	1.583e+43	4.29	4.29	1.193e+40	0.0154
8810	diHPCARP_Ic.tmttptmpu	8.422e+43	5.30	5.30	1.169e+40	0.0151
8811	diHPCARP_Ic.tptmmtppu	2.971e+44	6.05	6.05	1.158e+40	0.015
8812	diHPCARP_Ic.pppmmttptu	5.428e+43	5.04	5.04	1.156e+40	0.015
8813	diHPCARP_Ic.ptmtmtppu	2.882e+43	4.66	4.66	1.153e+40	0.0149
8814	diHPCARP_Ic.pppmpttptu	3.213e+43	4.73	4.73	1.152e+40	0.0149
8815	diHPCARP_Ic.mmmtmtmpu	4.058e+43	4.87	4.87	1.151e+40	0.0149
8816	diHPCARP_Ic.ppppmtmu	4.864e+43	4.98	4.98	1.143e+40	0.0148
8817	diHPCARP_Ic.tmmmpmtmu	3.641e+43	4.81	4.81	1.142e+40	0.0148
8818	diHPCARP_Ic.tptmmtptu	1.818e+44	5.77	5.77	1.141e+40	0.0148
8819	diHPCARP_Ic.ptppmpmpu	1.222e+43	4.16	4.16	1.136e+40	0.0147
8820	diHPCARP_Ic.ppmmtmtmpu	3.471e+43	4.78	4.78	1.135e+40	0.0147
8821	diHPCARP_Ic.ptmtmttmu	4.776e+43	4.98	4.98	1.124e+40	0.0145
8822	diHPCARP_Ic.ppttppmpu	1.875e+44	5.81	5.81	1.100e+40	0.0142
8823	diHPCARP_Ic.pptpmpmpu	9.795e+43	5.43	5.43	1.088e+40	0.0141
8824	diHPCARP_Ic.pptmmtmtmu	7.812e+43	5.30	5.30	1.078e+40	0.0139
8825	diHPCARP_Ic.pppmpptmu	1.154e+44	5.53	5.53	1.074e+40	0.0139
8826	diHPCARP_Ic.tmmppmpmpu	6.666e+43	5.22	5.22	1.048e+40	0.0136
8827	diHPCARP_Ic.tptpmpmpu	3.461e+43	4.83	4.83	1.046e+40	0.0135
8828	diHPCARP_Ic.tpppmmtptu	1.629e+44	5.77	5.77	1.020e+40	0.0132
8829	diHPCARP_Ic.tmmmpmtmu	3.193e+43	4.80	4.80	1.018e+40	0.0132
8830	diHPCARP_Ic.ptptmtmpu	2.700e+43	4.73	4.73	9.616e+39	0.0124
8831	diHPCARP_Ic.tpptptmpu	1.355e+44	5.70	5.70	9.591e+39	0.0124
8832	diHPCARP_Ic.ppppmtmpu	4.550e+43	5.05	5.05	9.570e+39	0.0124

8833	diHPCARP_Ic.ppppptpmu	4.331e+43	5.05	5.05	9.133e+39	0.0118
8834	diHPCARP_Ic.ppptptpmu	1.202e+44	5.68	5.68	8.793e+39	0.0114
8835	diHPCARP_Ic.mttmptppu	5.463e+43	5.22	5.22	8.653e+39	0.0112
8836	diHPCARP_Ic.pmntpmmmu	1.125e+44	5.65	5.65	8.580e+39	0.0111
8837	diHPCARP_Ic.mpmtptmpu	6.472e+43	5.33	5.33	8.485e+39	0.011
8838	diHPCARP_Ic.pmmppmtmu	2.058e+43	4.67	4.67	8.177e+39	0.0106
8839	diHPCARP_Ic.mmpppptpmu	3.581e+43	5.00	5.00	8.117e+39	0.0105
8840	diHPCARP_Ic.tmmptmmu	2.567e+43	4.83	4.83	7.767e+39	0.01
8841	diHPCARP_Ic.pptmpmpu	8.207e+43	5.55	5.55	7.413e+39	0.00959
8842	diHPCARP_Ic.ttmpttmu	3.346e+43	5.02	5.02	7.406e+39	0.00958
8843	diHPCARP_Ic.pptmpttpu	9.318e+43	5.63	5.63	7.403e+39	0.00958
8844	diHPCARP_Ic.mptmptpmu	5.672e+43	5.34	5.34	7.358e+39	0.00952
8845	diHPCARP_Ic.mptmptppu	2.996e+43	4.96	4.96	7.263e+39	0.00939
8846	diHPCARP_Ic.tmmmmmtmu	6.910e+43	5.48	5.48	7.025e+39	0.00909
8847	diHPCARP_Ic.ptppmtmpu	6.196e+43	5.42	5.42	6.950e+39	0.00899
8848	diHPCARP_Ic.pptmmttmu	6.366e+43	5.45	5.45	6.821e+39	0.00882
8849	diHPCARP_Ic.pptpmpmpu	5.106e+43	5.36	5.36	6.346e+39	0.00821
8850	diHPCARP_Ic.mmtmptmpu	2.205e+43	4.87	4.87	6.262e+39	0.0081
8851	diHPCARP_Ic.pmtppttmu	4.251e+44	6.65	6.65	6.123e+39	0.00792
8852	diHPCARP_Ic.pmntptpmu	4.820e+43	5.36	5.36	5.968e+39	0.00772
8853	diHPCARP_Ic.ppptmtpu	3.530e+43	5.18	5.18	5.960e+39	0.00771
8854	diHPCARP_Ic.pmmmpmmmu	5.730e+43	5.47	5.47	5.958e+39	0.00771
8855	diHPCARP_Ic.tpptmmmpu	2.976e+43	5.08	5.08	5.893e+39	0.00762
8856	diHPCARP_Ic.pmttppmmmu	2.508e+44	6.36	6.36	5.881e+39	0.00761
8857	diHPCARP_Ic.ttpmpmpu	3.397e+43	5.17	5.17	5.798e+39	0.0075
8858	diHPCARP_Ic.mmtmppmmu	4.068e+43	5.29	5.29	5.722e+39	0.0074
8859	diHPCARP_Ic.mmpmmptpu	7.173e+43	5.63	5.63	5.711e+39	0.00739
8860	diHPCARP_Ic.tptmptpmu	2.892e+44	6.47	6.47	5.596e+39	0.00724
8861	diHPCARP_Ic.ptmptmpu	1.713e+44	6.18	6.18	5.407e+39	0.00699
8862	diHPCARP_Ic.pmmptmu	1.279e+43	4.63	4.63	5.396e+39	0.00698
8863	diHPCARP_Ic.mpmmpmtmu	1.442e+43	4.71	4.71	5.375e+39	0.00695
8864	diHPCARP_Ic.mpppmtpmu	7.923e+43	5.72	5.72	5.370e+39	0.00695
8865	diHPCARP_Ic.tpptmmtmu	4.821e+44	6.80	6.80	5.364e+39	0.00694
8866	diHPCARP_Ic.mptmptmmu	5.354e+43	5.49	5.49	5.363e+39	0.00694
8867	diHPCARP_Ic.ppmmtppu	1.856e+43	4.87	4.87	5.295e+39	0.00685
8868	diHPCARP_Ic.mmmmmmtmpu	2.709e+43	5.09	5.09	5.263e+39	0.00681
8869	diHPCARP_Ic.tmmmmmtmpu	4.537e+43	5.40	5.40	5.248e+39	0.00679
8870	diHPCARP_Ic.pptpmmtpu	5.498e+43	5.53	5.53	5.168e+39	0.00668
8871	diHPCARP_Ic.mppppptpmu	3.372e+43	5.24	5.24	5.108e+39	0.00661
8872	diHPCARP_Ic.tppppppmu	4.364e+43	5.40	5.40	5.050e+39	0.00653
8873	diHPCARP_Ic.tptmmpmpu	1.273e+44	6.05	6.05	4.942e+39	0.00639
8874	diHPCARP_Ic.tmpmpmpu	9.693e+43	5.92	5.92	4.745e+39	0.00614
8875	diHPCARP_Ic.mmppppppu	9.817e+43	5.93	5.93	4.704e+39	0.00608
8876	diHPCARP_Ic.ttpmmpmpu	1.806e+44	6.30	6.30	4.624e+39	0.00598
8877	diHPCARP_Ic.tmmmpmtmpu	3.788e+43	5.38	5.38	4.578e+39	0.00592
8878	diHPCARP_Ic.pptmmttmu	9.263e+43	5.91	5.91	4.556e+39	0.00589
8879	diHPCARP_Ic.pptppmpu	6.885e+43	5.74	5.74	4.533e+39	0.00586
8880	diHPCARP_Ic.ptmptmpu	8.025e+43	5.83	5.83	4.531e+39	0.00586
8881	diHPCARP_Ic.pmtmmttmu	5.274e+44	6.95	6.95	4.527e+39	0.00586
8882	diHPCARP_Ic.tptmptppu	2.620e+44	6.54	6.54	4.522e+39	0.00585
8883	diHPCARP_Ic.tmttptpmu	4.325e+44	6.86	6.86	4.386e+39	0.00567
8884	diHPCARP_Ic.ptmmtmpmu	1.955e+43	5.01	5.01	4.360e+39	0.00564
8885	diHPCARP_Ic.ppmppmpmu	1.179e+43	4.71	4.71	4.350e+39	0.00563
8886	diHPCARP_Ic.ppptppmpu	1.425e+44	6.20	6.20	4.330e+39	0.0056
8887	diHPCARP_Ic.mmtmmtpmu	2.922e+44	6.64	6.64	4.255e+39	0.0055
8888	diHPCARP_Ic.mmtmpttpu	1.116e+44	6.07	6.07	4.215e+39	0.00545
8889	diHPCARP_Ic.tmmmmmmmu	1.619e+44	6.32	6.32	4.044e+39	0.00523
8890	diHPCARP_Ic.pmtmmtmmu	3.115e+43	5.34	5.34	4.013e+39	0.00519
8891	diHPCARP_Ic.tttptppu	3.671e+43	5.44	5.44	4.009e+39	0.00519
8892	diHPCARP_Ic.mmtmpmtmu	4.845e+44	6.98	6.98	3.997e+39	0.00517
8893	diHPCARP_Ic.ptmmpptmu	1.379e+43	4.86	4.86	3.966e+39	0.00513
8894	diHPCARP_Ic.tmpptpmu	3.273e+44	6.75	6.75	3.955e+39	0.00512
8895	diHPCARP_Ic.pmttptppu	1.429e+45	7.64	7.64	3.880e+39	0.00502
8896	diHPCARP_Ic.ppmptmpu	9.668e+43	6.04	6.04	3.824e+39	0.00495
8897	diHPCARP_Ic.ppptpttpu	1.386e+44	6.26	6.26	3.798e+39	0.00491
8898	diHPCARP_Ic.tptmpppmu	8.298e+43	5.97	5.97	3.714e+39	0.0048
8899	diHPCARP_Ic.pmpmmtmpu	1.209e+43	4.82	4.82	3.708e+39	0.0048
8900	diHPCARP_Ic.ptttptmpu	1.754e+44	6.42	6.42	3.692e+39	0.00478
8901	diHPCARP_Ic.tptmmtmpu	1.242e+44	6.23	6.23	3.620e+39	0.00468
8902	diHPCARP_Ic.tpppttpu	3.388e+44	6.83	6.83	3.583e+39	0.00463
8903	diHPCARP_Ic.mmtmmmpmu	2.040e+44	6.53	6.53	3.583e+39	0.00463
8904	diHPCARP_Ic.tpmmmmtmu	1.944e+43	5.13	5.13	3.580e+39	0.00463

8905	diHPCARP_Ic.tpppptomu	5.691e+44	7.14	7.14	3.570e+39	0.00462
8906	diHPCARP_Ic.mtttptppu	1.403e+44	6.31	6.31	3.527e+39	0.00456
8907	diHPCARP_Ic.ptppmmmpu	9.621e+43	6.11	6.11	3.407e+39	0.00441
8908	diHPCARP_Ic.mmtmmpppu	1.505e+44	6.38	6.38	3.406e+39	0.00441
8909	diHPCARP_Ic.tptmtmtmu	1.030e+44	6.16	6.16	3.343e+39	0.00432
8910	diHPCARP_Ic.pptmtmtmu	4.444e+43	5.66	5.66	3.322e+39	0.0043
8911	diHPCARP_Ic.mmpptomu	7.253e+43	5.96	5.96	3.310e+39	0.00428
8912	diHPCARP_Ic.tmmppmpu	1.991e+43	5.19	5.19	3.308e+39	0.00428
8913	diHPCARP_Ic.mptmptmu	2.496e+43	5.33	5.33	3.262e+39	0.00422
8914	diHPCARP_Ic.mttmptmu	8.933e+43	6.10	6.10	3.213e+39	0.00416
8915	diHPCARP_Ic.tmtmmmtmu	1.007e+44	6.17	6.17	3.206e+39	0.00415
8916	diHPCARP_Ic.pppppmpu	6.020e+43	5.87	5.87	3.182e+39	0.00412
8917	diHPCARP_Ic.tpppmtmu	3.255e+44	6.89	6.89	3.106e+39	0.00402
8918	diHPCARP_Ic.mttptmtmu	8.316e+43	6.08	6.08	3.102e+39	0.00401
8919	diHPCARP_Ic.tpmptpmu	4.607e+43	5.73	5.73	3.076e+39	0.00398
8920	diHPCARP_Ic.tpttmmmu	2.938e+44	6.84	6.84	3.055e+39	0.00395
8921	diHPCARP_Ic.ptmmpmpu	2.210e+43	5.30	5.30	3.039e+39	0.00393
8922	diHPCARP_Ic.tmtmptmu	5.709e+43	5.88	5.88	2.950e+39	0.00382
8923	diHPCARP_Ic.tptmmtmu	2.122e+44	6.68	6.68	2.901e+39	0.00375
8924	diHPCARP_Ic.mtmmpmpu	2.704e+43	5.46	5.46	2.833e+39	0.00367
8925	diHPCARP_Ic.tmmtmmmu	1.524e+44	6.50	6.50	2.803e+39	0.00363
8926	diHPCARP_Ic.tpmmtmtmu	4.866e+43	5.82	5.82	2.789e+39	0.00361
8927	diHPCARP_Ic.ttpmmpmu	1.442e+43	5.10	5.10	2.781e+39	0.0036
8928	diHPCARP_Ic.tmpmmtmu	2.013e+43	5.30	5.30	2.775e+39	0.00359
8929	diHPCARP_Ic.pptmtmtmu	1.240e+44	6.39	6.39	2.757e+39	0.00357
8930	diHPCARP_Ic.pmpmtmtmu	4.880e+43	5.85	5.85	2.691e+39	0.00348
8931	diHPCARP_Ic.mpmmpmtmu	1.439e+43	5.12	5.12	2.664e+39	0.00345
8932	diHPCARP_Ic.ptmpmpmpu	1.740e+43	5.24	5.24	2.663e+39	0.00344
8933	diHPCARP_Ic.mtttptmtmu	1.290e+44	6.44	6.44	2.636e+39	0.00341
8934	diHPCARP_Ic.pptmtmtmu	5.723e+43	5.95	5.95	2.629e+39	0.0034
8935	diHPCARP_Ic.pptmmtmu	6.952e+43	6.07	6.07	2.613e+39	0.00338
8936	diHPCARP_Ic.tttmmtmu	9.275e+43	6.25	6.25	2.597e+39	0.00336
8937	diHPCARP_Ic.ttpmmpmpu	2.159e+43	5.38	5.38	2.593e+39	0.00335
8938	diHPCARP_Ic.mpttptmtmu	1.263e+44	6.44	6.44	2.572e+39	0.00333
8939	diHPCARP_Ic.ptmmpmtmu	7.404e+43	6.14	6.14	2.506e+39	0.00324
8940	diHPCARP_Ic.ptmpmpmpu	4.200e+43	5.81	5.81	2.470e+39	0.00319
8941	diHPCARP_Ic.mpppmtmu	2.752e+43	5.59	5.59	2.336e+39	0.00302
8942	diHPCARP_Ic.tmpmptmu	1.143e+44	6.44	6.44	2.334e+39	0.00302
8943	diHPCARP_Ic.ptppmtmu	1.937e+43	5.39	5.39	2.292e+39	0.00297
8944	diHPCARP_Ic.tpttmmppu	1.759e+44	6.72	6.72	2.237e+39	0.00289
8945	diHPCARP_Ic.tttmptmu	7.871e+43	6.24	6.24	2.231e+39	0.00289
8946	diHPCARP_Ic.tmmtmtmu	2.314e+45	8.26	8.26	2.230e+39	0.00288
8947	diHPCARP_Ic.mpmptptmu	2.271e+43	5.50	5.50	2.226e+39	0.00288
8948	diHPCARP_Ic.mmpppppmu	5.861e+43	6.07	6.07	2.209e+39	0.00286
8949	diHPCARP_Ic.ptmtptmu	1.560e+44	6.67	6.67	2.155e+39	0.00279
8950	diHPCARP_Ic.tptmmtmu	1.807e+44	6.77	6.77	2.117e+39	0.00274
8951	diHPCARP_Ic.mmmmmmpu	6.147e+43	6.13	6.13	2.114e+39	0.00273
8952	diHPCARP_Ic.pptppmpu	8.819e+43	6.35	6.35	2.090e+39	0.0027
8953	diHPCARP_Ic.mpppmtmu	5.070e+43	6.02	6.02	2.084e+39	0.0027
8954	diHPCARP_Ic.tmtmppppu	8.316e+43	6.32	6.32	2.058e+39	0.00266
8955	diHPCARP_Ic.tppmmmtmu	1.422e+44	6.66	6.66	2.014e+39	0.00261
8956	diHPCARP_Ic.tpppmtmu	4.782e+44	7.38	7.38	2.006e+39	0.0026
8957	diHPCARP_Ic.ppttpmpu	1.543e+44	6.71	6.71	2.002e+39	0.00259
8958	diHPCARP_Ic.ppttptmu	3.036e+43	5.74	5.74	1.991e+39	0.00258
8959	diHPCARP_Ic.tpmmpmtmu	6.923e+43	6.24	6.24	1.959e+39	0.00253
8960	diHPCARP_Ic.mtttptmu	1.183e+44	6.56	6.56	1.953e+39	0.00253
8961	diHPCARP_Ic.tmmptmu	2.940e+43	5.74	5.74	1.927e+39	0.00249
8962	diHPCARP_Ic.mmpmtmu	3.160e+43	5.79	5.79	1.913e+39	0.00248
8963	diHPCARP_Ic.mptmmtmu	1.775e+44	6.82	6.82	1.908e+39	0.00247
8964	diHPCARP_Ic.mptmptmu	3.425e+43	5.86	5.86	1.843e+39	0.00238
8965	diHPCARP_Ic.tptmpmpu	8.173e+43	6.39	6.39	1.822e+39	0.00236
8966	diHPCARP_Ic.pmtmptmu	4.096e+44	7.36	7.36	1.791e+39	0.00232
8967	diHPCARP_Ic.tmpppmpu	1.483e+44	6.75	6.75	1.782e+39	0.00231
8968	diHPCARP_Ic.pptppmpu	2.888e+43	5.79	5.79	1.744e+39	0.00226
8969	diHPCARP_Ic.pptmtmtmu	8.144e+43	6.41	6.41	1.744e+39	0.00226
8970	diHPCARP_Ic.pmtmptmu	6.728e+43	6.30	6.30	1.744e+39	0.00226
8971	diHPCARP_Ic.tmtmmpmu	1.142e+44	6.61	6.61	1.743e+39	0.00225
8972	diHPCARP_Ic.mpppmtmu	3.413e+43	5.91	5.91	1.677e+39	0.00217
8973	diHPCARP_Ic.tptmptmu	1.932e+44	6.96	6.96	1.645e+39	0.00213
8974	diHPCARP_Ic.pmpmtmu	1.377e+43	5.39	5.39	1.625e+39	0.0021
8975	diHPCARP_Ic.tpttmmmpu	1.362e+44	6.76	6.76	1.608e+39	0.00208
8976	diHPCARP_Ic.tpttptmu	7.356e+44	7.77	7.77	1.600e+39	0.00207

8977	diHPCARP_Ic.pttpptmpu	9.915e+43	6.60	6.60	1.540e+39	0.00199
8978	diHPCARP_Ic.pptmmmpu	1.191e+44	6.71	6.71	1.535e+39	0.00199
8979	diHPCARP_Ic.pppmpmpu	9.417e+42	5.20	5.20	1.524e+39	0.00197
8980	diHPCARP_Ic.mmmptmpu	1.351e+43	5.42	5.42	1.510e+39	0.00195
8981	diHPCARP_Ic.pppmptmpu	6.264e+43	6.34	6.34	1.506e+39	0.00195
8982	diHPCARP_Ic.tpttmtppu	3.504e+44	7.38	7.38	1.473e+39	0.00191
8983	diHPCARP_Ic.tmmptmpu	2.291e+43	5.78	5.78	1.410e+39	0.00182
8984	diHPCARP_Ic.mpptptmpu	3.457e+43	6.03	6.03	1.403e+39	0.00182
8985	diHPCARP_Ic.mtmtptppu	2.245e+44	7.15	7.15	1.395e+39	0.0018
8986	diHPCARP_Ic.mptpmtmu	6.731e+43	6.43	6.43	1.382e+39	0.00179
8987	diHPCARP_Ic.mmppttpu	1.414e+44	6.88	6.88	1.377e+39	0.00178
8988	diHPCARP_Ic.ptppptpu	9.007e+43	6.61	6.61	1.374e+39	0.00178
8989	diHPCARP_Ic.tmtmmtpu	1.787e+44	7.03	7.03	1.348e+39	0.00174
8990	diHPCARP_Ic.mmttmtmpu	5.243e+44	7.69	7.69	1.321e+39	0.00171
8991	diHPCARP_Ic.ppppttpu	4.316e+44	7.57	7.57	1.309e+39	0.00169
8992	diHPCARP_Ic.mpttptppu	4.114e+43	6.18	6.18	1.305e+39	0.00169
8993	diHPCARP_Ic.tppptppu	1.882e+44	7.08	7.08	1.298e+39	0.00168
8994	diHPCARP_Ic.mttmptmpu	3.796e+43	6.13	6.13	1.296e+39	0.00168
8995	diHPCARP_Ic.mpttptmpu	7.660e+43	6.56	6.56	1.284e+39	0.00166
8996	diHPCARP_Ic.ptmtptmpu	2.588e+44	7.29	7.29	1.272e+39	0.00165
8997	diHPCARP_Ic.tptmmtppu	2.774e+44	7.33	7.33	1.264e+39	0.00164
8998	diHPCARP_Ic.tppmmmpu	8.887e+43	6.66	6.66	1.254e+39	0.00162
8999	diHPCARP_Ic.mmtptmtmu	1.916e+44	7.12	7.12	1.250e+39	0.00162
9000	diHPCARP_Ic.pmpptmpu	6.975e+43	6.52	6.52	1.245e+39	0.00161
9001	diHPCARP_Ic.mmpmptmpu	3.134e+43	6.05	6.05	1.229e+39	0.00159
9002	diHPCARP_Ic.ppttmttppu	1.750e+44	7.08	7.08	1.214e+39	0.00157
9003	diHPCARP_Ic.tmmptppu	5.170e+43	6.36	6.36	1.209e+39	0.00156
9004	diHPCARP_Ic.mppmtmpu	6.216e+43	6.48	6.48	1.191e+39	0.00154
9005	diHPCARP_Ic.mmttmpppu	2.456e+44	7.30	7.30	1.180e+39	0.00153
9006	diHPCARP_Ic.tmtmmtmpu	7.499e+43	6.59	6.59	1.177e+39	0.00152
9007	diHPCARP_Ic.tmtpttpu	1.289e+44	6.92	6.92	1.177e+39	0.00152
9008	diHPCARP_Ic.tmpptmpu	5.123e+44	7.74	7.74	1.168e+39	0.00151
9009	diHPCARP_Ic.tmtmptppu	1.060e+44	6.81	6.81	1.161e+39	0.0015
9010	diHPCARP_Ic.pmpmttppu	4.810e+43	6.34	6.34	1.160e+39	0.0015
9011	diHPCARP_Ic.mptmpppu	2.032e+43	5.83	5.83	1.154e+39	0.00149
9012	diHPCARP_Ic.tmtppptmu	3.405e+44	7.52	7.52	1.123e+39	0.00145
9013	diHPCARP_Ic.mmtmmtmu	4.198e+44	7.65	7.65	1.123e+39	0.00145
9014	diHPCARP_Ic.tppmmpmpu	2.305e+43	5.92	5.92	1.114e+39	0.00144
9015	diHPCARP_Ic.mpppttpu	7.969e+43	6.67	6.67	1.105e+39	0.00143
9016	diHPCARP_Ic.pptmptmu	1.345e+44	6.98	6.98	1.099e+39	0.00142
9017	diHPCARP_Ic.mppppptmu	1.359e+44	6.99	6.99	1.098e+39	0.00142
9018	diHPCARP_Ic.ppttpttppu	1.416e+44	7.02	7.02	1.094e+39	0.00142
9019	diHPCARP_Ic.tppmtppu	2.242e+44	7.31	7.31	1.053e+39	0.00136
9020	diHPCARP_Ic.pmpmtmtmu	1.377e+44	7.02	7.02	1.053e+39	0.00136
9021	diHPCARP_Ic.tptmpttmu	1.598e+44	7.12	7.12	1.040e+39	0.00135
9022	diHPCARP_Ic.ppttmtmpu	1.197e+44	6.95	6.95	1.027e+39	0.00133
9023	diHPCARP_Ic.tppmptpu	1.087e+44	6.90	6.90	1.026e+39	0.00133
9024	diHPCARP_Ic.ptpmmmpu	1.770e+43	5.82	5.82	1.022e+39	0.00132
9025	diHPCARP_Ic.mmttppppu	3.467e+44	7.61	7.61	9.990e+38	0.00129
9026	diHPCARP_Ic.pptpptppu	3.016e+43	6.16	6.16	9.850e+38	0.00127
9027	diHPCARP_Ic.tppmmpmu	3.770e+44	7.67	7.67	9.798e+38	0.00127
9028	diHPCARP_Ic.tmtmpttmu	3.377e+44	7.60	7.60	9.763e+38	0.00126
9029	diHPCARP_Ic.mppptmpu	3.203e+43	6.20	6.20	9.735e+38	0.00126
9030	diHPCARP_Ic.pmtmpttmu	1.077e+44	6.92	6.92	9.729e+38	0.00126
9031	diHPCARP_Ic.ppmmtmpu	1.085e+44	6.93	6.93	9.689e+38	0.00125
9032	diHPCARP_Ic.tttmmmpu	4.947e+43	6.48	6.48	9.366e+38	0.00121
9033	diHPCARP_Ic.pmpmptpu	3.661e+43	6.31	6.31	9.298e+38	0.0012
9034	diHPCARP_Ic.pmpptmpu	7.781e+42	5.39	5.39	9.208e+38	0.00119
9035	diHPCARP_Ic.ppmmmmpu	6.077e+42	5.25	5.25	9.138e+38	0.00118
9036	diHPCARP_Ic.ttttptmpu	1.682e+44	7.23	7.23	9.136e+38	0.00118
9037	diHPCARP_Ic.ppttpttppu	1.734e+44	7.25	7.25	9.111e+38	0.00118
9038	diHPCARP_Ic.tppmpttppu	4.101e+44	7.76	7.76	9.044e+38	0.00117
9039	diHPCARP_Ic.mppppptpu	8.406e+43	6.82	6.82	9.027e+38	0.00117
9040	diHPCARP_Ic.pttmptmpu	6.355e+43	6.66	6.66	8.993e+38	0.00116
9041	diHPCARP_Ic.ppmmttppu	2.672e+43	6.14	6.14	8.927e+38	0.00115
9042	diHPCARP_Ic.ptttppmpu	6.449e+43	6.70	6.70	8.494e+38	0.0011
9043	diHPCARP_Ic.tppmptmu	1.606e+44	7.25	7.25	8.472e+38	0.0011
9044	diHPCARP_Ic.mmtmmtmpu	5.364e+43	6.60	6.60	8.411e+38	0.00109
9045	diHPCARP_Ic.ppmmttmmu	1.360e+43	5.78	5.78	8.387e+38	0.00108
9046	diHPCARP_Ic.tppmpppu	4.877e+43	6.55	6.55	8.270e+38	0.00107
9047	diHPCARP_Ic.tttmmptmu	2.139e+43	6.06	6.06	8.263e+38	0.00107
9048	diHPCARP_Ic.tppptppmu	1.366e+44	7.17	7.17	8.166e+38	0.00106

9049	diHPCARP_Ic.pptmmtpmu	5.094e+43	6.59	6.59	8.058e+38	0.00104
9050	diHPCARP_Ic.pppppmmmu	7.410e+43	6.82	6.82	7.913e+38	0.00102
9051	diHPCARP_Ic.tmttptmpu	1.050e+44	7.05	7.05	7.676e+38	0.000993
9052	diHPCARP_Ic.mpttptmpu	5.710e+43	6.69	6.69	7.656e+38	0.00099
9053	diHPCARP_Ic.mtmtpttmu	4.647e+43	6.57	6.57	7.654e+38	0.00099
9054	diHPCARP_Ic.ptmmpptpu	4.902e+44	7.98	7.98	7.583e+38	0.000981
9055	diHPCARP_Ic.ptmmpptpu	4.674e+43	6.58	6.58	7.543e+38	0.000976
9056	diHPCARP_Ic.tmpmpptpmu	1.822e+43	6.02	6.02	7.475e+38	0.000967
9057	diHPCARP_Ic.tpttptpmu	4.478e+44	7.94	7.94	7.339e+38	0.000949
9058	diHPCARP_Ic.ttttmtmpu	1.597e+44	7.34	7.34	7.192e+38	0.00093
9059	diHPCARP_Ic.pptmmtpmu	9.329e+43	7.02	7.02	7.123e+38	0.000921
9060	diHPCARP_Ic.tpttmttmu	2.701e+44	7.66	7.66	7.044e+38	0.000911
9061	diHPCARP_Ic.mptmpttpu	8.413e+43	6.99	6.99	6.859e+38	0.000887
9062	diHPCARP_Ic.tpptmttmu	4.390e+44	7.98	7.98	6.719e+38	0.000869
9063	diHPCARP_Ic.mmtmmtppu	6.088e+43	6.81	6.81	6.682e+38	0.000864
9064	diHPCARP_Ic.tmpppptpmu	5.786e+43	6.78	6.78	6.670e+38	0.000863
9065	diHPCARP_Ic.tpmpttpu	8.092e+44	8.35	8.35	6.631e+38	0.000858
9066	diHPCARP_Ic.tmmmpmtpmu	9.790e+43	7.10	7.10	6.597e+38	0.000853
9067	diHPCARP_Ic.mmpmpmtpmu	8.991e+43	7.05	7.05	6.546e+38	0.000847
9068	diHPCARP_Ic.pmttptmmu	9.228e+44	8.45	8.45	6.482e+38	0.000839
9069	diHPCARP_Ic.mmpmmtpmu	1.969e+43	6.15	6.15	6.480e+38	0.000838
9070	diHPCARP_Ic.tppmpttmu	4.306e+44	8.00	8.00	6.438e+38	0.000833
9071	diHPCARP_Ic.pmppppppu	9.369e+43	7.09	7.09	6.373e+38	0.000824
9072	diHPCARP_Ic.mppppmtmpu	4.412e+43	6.65	6.65	6.360e+38	0.000823
9073	diHPCARP_Ic.tpppptmpu	4.661e+43	6.68	6.68	6.346e+38	0.000821
9074	diHPCARP_Ic.mmppttmu	3.845e+44	7.95	7.95	6.236e+38	0.000807
9075	diHPCARP_Ic.tmmppptpmu	1.443e+43	6.00	6.00	6.159e+38	0.000797
9076	diHPCARP_Ic.tptmpttpu	2.153e+44	7.61	7.61	6.129e+38	0.000793
9077	diHPCARP_Ic.ptptpttpu	1.049e+44	7.19	7.19	6.048e+38	0.000782
9078	diHPCARP_Ic.tmmmpmpu	2.762e+43	6.40	6.40	6.020e+38	0.000779
9079	diHPCARP_Ic.pppppptmpu	3.795e+43	6.60	6.60	5.886e+38	0.000761
9080	diHPCARP_Ic.mptpptpmu	4.143e+43	6.66	6.66	5.868e+38	0.000759
9081	diHPCARP_Ic.ptppmpmpu	2.061e+43	6.24	6.24	5.866e+38	0.000759
9082	diHPCARP_Ic.tmmmpptmu	4.215e+43	6.67	6.67	5.796e+38	0.00075
9083	diHPCARP_Ic.pmmppmmmu	6.782e+43	6.96	6.96	5.788e+38	0.000749
9084	diHPCARP_Ic.mpppttpu	6.712e+43	6.96	6.96	5.744e+38	0.000743
9085	diHPCARP_Ic.pppppmmmu	1.907e+43	6.21	6.21	5.733e+38	0.000742
9086	diHPCARP_Ic.pptmtmmu	1.361e+44	7.38	7.38	5.721e+38	0.00074
9087	diHPCARP_Ic.mmmmmpppu	3.358e+43	6.55	6.55	5.687e+38	0.000736
9088	diHPCARP_Ic.tmttppmpu	3.060e+44	7.88	7.88	5.596e+38	0.000724
9089	diHPCARP_Ic.pppmptmmu	3.111e+43	6.52	6.52	5.549e+38	0.000718
9090	diHPCARP_Ic.mmpptpppu	9.374e+43	7.18	7.18	5.491e+38	0.00071
9091	diHPCARP_Ic.mmpmpmtpmu	1.503e+44	7.47	7.47	5.475e+38	0.000708
9092	diHPCARP_Ic.ttpmmmpmu	2.508e+43	6.40	6.40	5.417e+38	0.000701
9093	diHPCARP_Ic.mptpptmpu	3.242e+43	6.56	6.56	5.370e+38	0.000695
9094	diHPCARP_Ic.pttmppmpu	2.718e+43	6.47	6.47	5.273e+38	0.000682
9095	diHPCARP_Ic.tmtmmtppu	1.704e+44	7.57	7.57	5.224e+38	0.000676
9096	diHPCARP_Ic.mmttptpmu	3.651e+44	8.02	8.02	5.215e+38	0.000675
9097	diHPCARP_Ic.tmmmtppu	8.454e+43	7.16	7.16	5.103e+38	0.00066
9098	diHPCARP_Ic.mmttmtmpu	1.363e+44	7.47	7.47	4.969e+38	0.000643
9099	diHPCARP_Ic.mmtmmtpmu	1.709e+44	7.60	7.60	4.968e+38	0.000643
9100	diHPCARP_Ic.mmmmtmtmu	1.621e+45	8.95	8.95	4.935e+38	0.000638
9101	diHPCARP_Ic.mmmmtmtppu	1.665e+44	7.59	7.59	4.915e+38	0.000636
9102	diHPCARP_Ic.mmmmpmttmu	2.485e+44	7.83	7.83	4.900e+38	0.000634
9103	diHPCARP_Ic.pptmptmmu	1.905e+44	7.68	7.68	4.828e+38	0.000625
9104	diHPCARP_Ic.tppmptmpu	3.201e+43	6.63	6.63	4.770e+38	0.000617
9105	diHPCARP_Ic.tmtmmttmu	6.726e+44	8.44	8.44	4.745e+38	0.000614
9106	diHPCARP_Ic.tmmpttmu	3.618e+44	8.08	8.08	4.686e+38	0.000606
9107	diHPCARP_Ic.tpttpppmu	1.491e+44	7.57	7.57	4.549e+38	0.000589
9108	diHPCARP_Ic.mppptmmu	4.251e+43	6.82	6.82	4.546e+38	0.000588
9109	diHPCARP_Ic.tmtptmpu	6.761e+43	7.10	7.10	4.541e+38	0.000587
9110	diHPCARP_Ic.pptppttpu	1.234e+44	7.46	7.46	4.516e+38	0.000584
9111	diHPCARP_Ic.mttmmtmpu	8.111e+43	7.22	7.22	4.475e+38	0.000579
9112	diHPCARP_Ic.pttmmpmu	3.190e+43	6.67	6.67	4.424e+38	0.000572
9113	diHPCARP_Ic.tttmptppu	1.290e+44	7.51	7.51	4.332e+38	0.00056
9114	diHPCARP_Ic.ppttmttmu	1.684e+44	7.67	7.67	4.321e+38	0.000559
9115	diHPCARP_Ic.tmttmtmpu	1.423e+44	7.58	7.58	4.306e+38	0.000557
9116	diHPCARP_Ic.pmtmpmtpmu	1.025e+44	7.38	7.38	4.300e+38	0.000556
9117	diHPCARP_Ic.tmpmtmpmu	4.317e+44	8.25	8.25	4.228e+38	0.000547
9118	diHPCARP_Ic.mmppttpu	2.665e+44	7.97	7.97	4.163e+38	0.000539
9119	diHPCARP_Ic.tmpppmmmpu	1.833e+44	7.75	7.75	4.145e+38	0.000536
9120	diHPCARP_Ic.ttpmptmpu	7.972e+43	7.26	7.26	4.102e+38	0.000531

9121	diHPCARP_Ic.tttptmpu	1.052e+44	7.43	7.43	4.101e+38	0.00053
9122	diHPCARP_Ic.pptpmtmpu	4.712e+43	6.95	6.95	4.077e+38	0.000527
9123	diHPCARP_Ic.pppmpmpu	6.149e+43	7.11	7.11	4.073e+38	0.000527
9124	diHPCARP_Ic.pmpmttptu	1.448e+44	7.62	7.62	4.061e+38	0.000525
9125	diHPCARP_Ic.tttmntmpu	5.574e+43	7.06	7.06	4.014e+38	0.000519
9126	diHPCARP_Ic.mptmntppu	1.851e+44	7.79	7.79	3.907e+38	0.000505
9127	diHPCARP_Ic.pppmptppu	1.815e+43	6.41	6.41	3.899e+38	0.000504
9128	diHPCARP_Ic.mptmntmpu	1.254e+44	7.56	7.56	3.893e+38	0.000504
9129	diHPCARP_Ic.pppmtmpu	5.830e+43	7.11	7.11	3.856e+38	0.000499
9130	diHPCARP_Ic.pmttptmpu	1.791e+44	7.78	7.78	3.846e+38	0.000497
9131	diHPCARP_Ic.mmtmpmpu	8.919e+43	7.37	7.37	3.833e+38	0.000496
9132	diHPCARP_Ic.tpttptmpu	2.476e+44	7.98	7.98	3.813e+38	0.000493
9133	diHPCARP_Ic.pmtmptmpu	4.404e+43	6.96	6.96	3.740e+38	0.000484
9134	diHPCARP_Ic.ptpmmmpu	2.320e+43	6.58	6.58	3.740e+38	0.000484
9135	diHPCARP_Ic.pppmtmpu	2.660e+43	6.67	6.67	3.698e+38	0.000478
9136	diHPCARP_Ic.pppmpmpu	1.055e+43	6.12	6.12	3.670e+38	0.000475
9137	diHPCARP_Ic.mmtmmpmpu	8.498e+44	8.74	8.74	3.657e+38	0.000473
9138	diHPCARP_Ic.tmpmtmpu	3.032e+44	8.13	8.13	3.646e+38	0.000472
9139	diHPCARP_Ic.tptpmtmpu	2.277e+44	7.96	7.96	3.642e+38	0.000471
9140	diHPCARP_Ic.pppmtmpmpu	2.631e+43	6.67	6.67	3.619e+38	0.000468
9141	diHPCARP_Ic.pppmpmpu	9.263e+42	6.05	6.05	3.613e+38	0.000467
9142	diHPCARP_Ic.mtmmpmpmpu	8.751e+43	7.39	7.39	3.611e+38	0.000467
9143	diHPCARP_Ic.ptmtpmpmpu	1.129e+44	7.55	7.55	3.599e+38	0.000466
9144	diHPCARP_Ic.tpptmtmpu	4.471e+44	8.37	8.37	3.588e+38	0.000464
9145	diHPCARP_Ic.mtttppmpu	8.804e+43	7.40	7.40	3.575e+38	0.000462
9146	diHPCARP_Ic.ptmtptmpu	3.827e+44	8.28	8.28	3.557e+38	0.00046
9147	diHPCARP_Ic.mpppmtmpu	5.886e+43	7.16	7.16	3.553e+38	0.00046
9148	diHPCARP_Ic.mmtmntmpu	7.163e+44	8.65	8.65	3.551e+38	0.000459
9149	diHPCARP_Ic.tptmtmpu	2.261e+44	7.98	7.98	3.505e+38	0.000453
9150	diHPCARP_Ic.tppmmtppu	9.306e+44	8.82	8.82	3.476e+38	0.00045
9151	diHPCARP_Ic.mptmntppu	8.700e+44	8.79	8.79	3.458e+38	0.000447
9152	diHPCARP_Ic.mmtmmpmpu	7.625e+44	8.71	8.71	3.438e+38	0.000445
9153	diHPCARP_Ic.ttpptmpu	2.128e+44	7.96	7.96	3.410e+38	0.000441
9154	diHPCARP_Ic.pttptmpu	8.965e+43	7.44	7.44	3.392e+38	0.000439
9155	diHPCARP_Ic.mtttptmpu	8.048e+43	7.38	7.38	3.391e+38	0.000439
9156	diHPCARP_Ic.mmtmntmpu	1.595e+44	7.79	7.79	3.389e+38	0.000438
9157	diHPCARP_Ic.ppppmtmpu	2.470e+43	6.68	6.68	3.355e+38	0.000434
9158	diHPCARP_Ic.mptmntmpu	6.223e+43	7.24	7.24	3.295e+38	0.000426
9159	diHPCARP_Ic.tppmmpmpu	2.678e+43	6.74	6.74	3.282e+38	0.000425
9160	diHPCARP_Ic.ttpmtmpu	1.098e+44	7.59	7.59	3.256e+38	0.000421
9161	diHPCARP_Ic.mmtpmtmpu	1.115e+44	7.60	7.60	3.255e+38	0.000421
9162	diHPCARP_Ic.tpptptmpu	5.062e+43	7.13	7.13	3.237e+38	0.000419
9163	diHPCARP_Ic.mptmntmpu	1.783e+44	7.89	7.89	3.210e+38	0.000415
9164	diHPCARP_Ic.tpppmtmpu	9.263e+43	7.50	7.50	3.168e+38	0.00041
9165	diHPCARP_Ic.pttppmpu	5.064e+43	7.15	7.15	3.132e+38	0.000405
9166	diHPCARP_Ic.mptmptmpu	1.534e+44	7.81	7.81	3.122e+38	0.000404
9167	diHPCARP_Ic.tmtptmpu	4.031e+44	8.39	8.39	3.095e+38	0.0004
9168	diHPCARP_Ic.mmtmptmpu	1.080e+44	7.61	7.61	3.081e+38	0.000399
9169	diHPCARP_Ic.pmttptmpu	1.188e+44	7.67	7.67	3.052e+38	0.000395
9170	diHPCARP_Ic.ppttptmpu	2.028e+44	8.00	8.00	3.023e+38	0.000391
9171	diHPCARP_Ic.tmtmptmpu	2.125e+44	8.03	8.03	2.985e+38	0.000386
9172	diHPCARP_Ic.pptmptmpu	8.014e+43	7.46	7.46	2.952e+38	0.000382
9173	diHPCARP_Ic.tttmptmpu	1.838e+44	7.96	7.96	2.943e+38	0.000381
9174	diHPCARP_Ic.tmpptmpu	1.219e+44	7.71	7.71	2.941e+38	0.00038
9175	diHPCARP_Ic.tttmntppu	3.299e+44	8.32	8.32	2.843e+38	0.000368
9176	diHPCARP_Ic.pptptmpu	7.864e+44	8.85	8.85	2.813e+38	0.000364
9177	diHPCARP_Ic.pttptmpu	6.377e+43	7.35	7.35	2.805e+38	0.000363
9178	diHPCARP_Ic.mpppmtmpu	5.344e+44	8.63	8.63	2.764e+38	0.000358
9179	diHPCARP_Ic.ptmppppu	1.351e+44	7.81	7.81	2.753e+38	0.000356
9180	diHPCARP_Ic.tmtmmtmpu	2.661e+44	8.23	8.23	2.685e+38	0.000347
9181	diHPCARP_Ic.ptppmpu	2.704e+43	6.87	6.87	2.678e+38	0.000346
9182	diHPCARP_Ic.mptmptmpu	1.091e+44	7.70	7.70	2.674e+38	0.000346
9183	diHPCARP_Ic.ptpmpptmpu	4.081e+43	7.12	7.12	2.663e+38	0.000344
9184	diHPCARP_Ic.tmmpmtmpu	1.916e+44	8.04	8.04	2.650e+38	0.000343
9185	diHPCARP_Ic.ttpptmpu	5.690e+43	7.32	7.32	2.643e+38	0.000342
9186	diHPCARP_Ic.pptptmpu	3.894e+43	7.10	7.10	2.613e+38	0.000338
9187	diHPCARP_Ic.mmtmptmpu	2.572e+44	8.23	8.23	2.611e+38	0.000338
9188	diHPCARP_Ic.tmtptmpu	6.772e+43	7.43	7.43	2.610e+38	0.000338
9189	diHPCARP_Ic.tmtmptmpu	9.723e+43	7.65	7.65	2.602e+38	0.000337
9190	diHPCARP_Ic.mmtmptmpu	3.015e+44	8.33	8.33	2.563e+38	0.000332
9191	diHPCARP_Ic.tppmmpmpu	1.075e+44	7.72	7.72	2.555e+38	0.00033
9192	diHPCARP_Ic.mppptmpu	3.815e+43	7.11	7.11	2.533e+38	0.000328

9193	diHPCARP_Ic.tmpmmtmu	3.793e+44	8.48	8.48	2.519e+38	0.000326
9194	diHPCARP_Ic.ptppmmmmu	1.042e+44	7.72	7.72	2.476e+38	0.00032
9195	diHPCARP_Ic.mtmtptmmu	1.028e+44	7.72	7.72	2.438e+38	0.000315
9196	diHPCARP_Ic.tpptmtppu	5.820e+44	8.76	8.76	2.423e+38	0.000313
9197	diHPCARP_Ic.tpttptmmu	2.448e+44	8.25	8.25	2.404e+38	0.000311
9198	diHPCARP_Ic.mppppppmu	2.477e+43	6.88	6.88	2.401e+38	0.000311
9199	diHPCARP_Ic.mppppppmu	3.745e+43	7.13	7.13	2.381e+38	0.000308
9200	diHPCARP_Ic.mpppttptu	7.822e+43	7.58	7.58	2.371e+38	0.000307
9201	diHPCARP_Ic.mmpptptmu	1.643e+44	8.02	8.02	2.366e+38	0.000306
9202	diHPCARP_Ic.mpttmtpmu	2.432e+44	8.26	8.26	2.356e+38	0.000305
9203	diHPCARP_Ic.ttptptpmu	4.484e+44	8.62	8.62	2.349e+38	0.000304
9204	diHPCARP_Ic.tptpptpmu	2.476e+44	8.28	8.28	2.314e+38	0.000299
9205	diHPCARP_Ic.ptmtppppu	7.511e+43	7.59	7.59	2.231e+38	0.000289
9206	diHPCARP_Ic.tttmpttptu	2.367e+44	8.27	8.27	2.225e+38	0.000288
9207	diHPCARP_Ic.pmttptmtpu	2.322e+44	8.28	8.28	2.165e+38	0.00028
9208	diHPCARP_Ic.ttptmtpmu	2.638e+44	8.36	8.36	2.144e+38	0.000277
9209	diHPCARP_Ic.mttppppmu	4.558e+43	7.32	7.32	2.132e+38	0.000276
9210	diHPCARP_Ic.tttmptpmu	6.592e+43	7.54	7.54	2.103e+38	0.000272
9211	diHPCARP_Ic.ttmtptpmu	1.386e+44	7.99	7.99	2.094e+38	0.000271
9212	diHPCARP_Ic.tpttmtpmu	1.938e+44	8.19	8.19	2.087e+38	0.00027
9213	diHPCARP_Ic.mmtptmmtmu	1.168e+45	9.26	9.26	2.083e+38	0.000269
9214	diHPCARP_Ic.tmttptppu	2.186e+44	8.27	8.27	2.061e+38	0.000267
9215	diHPCARP_Ic.mptmmpmmu	7.705e+43	7.65	7.65	2.059e+38	0.000266
9216	diHPCARP_Ic.ttttmmmpmu	6.221e+43	7.54	7.54	2.005e+38	0.000259
9217	diHPCARP_Ic.tpppmtmmu	9.769e+43	7.81	7.81	1.983e+38	0.000256
9218	diHPCARP_Ic.ppptpmppu	1.185e+44	7.94	7.94	1.952e+38	0.000253
9219	diHPCARP_Ic.mmpptptpu	1.360e+44	8.03	8.03	1.926e+38	0.000249
9220	diHPCARP_Ic.pmpmttppu	7.410e+43	7.67	7.67	1.917e+38	0.000248
9221	diHPCARP_Ic.ptppptpmu	1.454e+44	8.08	8.08	1.905e+38	0.000246
9222	diHPCARP_Ic.tpmpttptu	8.125e+43	7.73	7.73	1.903e+38	0.000246
9223	diHPCARP_Ic.tpmpttptu	1.690e+44	8.17	8.17	1.891e+38	0.000245
9224	diHPCARP_Ic.mtmmtptmu	5.424e+43	7.49	7.49	1.888e+38	0.000244
9225	diHPCARP_Ic.tptpmtmmu	2.347e+44	8.37	8.37	1.879e+38	0.000243
9226	diHPCARP_Ic.mmtptmtpmu	5.859e+43	7.54	7.54	1.873e+38	0.000242
9227	diHPCARP_Ic.mmttmttmu	2.253e+44	8.35	8.35	1.849e+38	0.000239
9228	diHPCARP_Ic.tpptmmmmu	1.128e+44	7.94	7.94	1.842e+38	0.000238
9229	diHPCARP_Ic.ppptmmmpu	2.258e+43	6.99	6.99	1.826e+38	0.000236
9230	diHPCARP_Ic.ptpmmmtmu	3.085e+43	7.18	7.18	1.819e+38	0.000235
9231	diHPCARP_Ic.ttmtmtmmu	3.756e+44	8.69	8.69	1.757e+38	0.000227
9232	diHPCARP_Ic.tmtmppmmu	4.278e+44	8.77	8.77	1.754e+38	0.000227
9233	diHPCARP_Ic.mttmmtpmu	3.741e+43	7.32	7.32	1.747e+38	0.000226
9234	diHPCARP_Ic.pmttmtmmu	3.906e+44	8.72	8.72	1.742e+38	0.000225
9235	diHPCARP_Ic.tmttmmmpu	1.533e+45	9.54	9.54	1.724e+38	0.000223
9236	diHPCARP_Ic.mptmppmpu	3.787e+43	7.34	7.34	1.711e+38	0.000221
9237	diHPCARP_Ic.pmpppmpu	5.241e+43	7.53	7.53	1.711e+38	0.000221
9238	diHPCARP_Ic.ptpmmtpmu	3.285e+43	7.25	7.25	1.710e+38	0.000221
9239	diHPCARP_Ic.mpppmtppu	2.425e+43	7.07	7.07	1.706e+38	0.000221
9240	diHPCARP_Ic.mttptptpmu	3.714e+43	7.34	7.34	1.674e+38	0.000217
9241	diHPCARP_Ic.tpmmtptmu	3.550e+43	7.32	7.32	1.649e+38	0.000213
9242	diHPCARP_Ic.tppmptpmu	9.293e+43	7.90	7.90	1.641e+38	0.000212
9243	diHPCARP_Ic.tppmptppu	2.152e+44	8.40	8.40	1.637e+38	0.000212
9244	diHPCARP_Ic.mmttmtppu	1.153e+44	8.03	8.03	1.631e+38	0.000211
9245	diHPCARP_Ic.pmmtpptmu	3.367e+43	7.30	7.30	1.624e+38	0.00021
9246	diHPCARP_Ic.tppmptpmu	3.715e+43	7.36	7.36	1.607e+38	0.000208
9247	diHPCARP_Ic.tmttmtppu	4.211e+44	8.81	8.81	1.607e+38	0.000208
9248	diHPCARP_Ic.mttmpttptu	9.313e+43	7.92	7.92	1.595e+38	0.000206
9249	diHPCARP_Ic.ptptptpmu	2.871e+44	8.59	8.59	1.584e+38	0.000205
9250	diHPCARP_Ic.tpptptppu	3.645e+44	8.74	8.74	1.560e+38	0.000202
9251	diHPCARP_Ic.tmmppmtmu	1.720e+44	8.30	8.30	1.551e+38	0.000201
9252	diHPCARP_Ic.pptmptppu	2.884e+44	8.62	8.62	1.517e+38	0.000196
9253	diHPCARP_Ic.tmmtmtppu	1.358e+44	8.18	8.18	1.496e+38	0.000194
9254	diHPCARP_Ic.ptmtptpmu	1.030e+44	8.02	8.02	1.473e+38	0.00019
9255	diHPCARP_Ic.ptppmpmmu	3.065e+43	7.30	7.30	1.468e+38	0.00019
9256	diHPCARP_Ic.tmtmptpmu	1.395e+44	8.21	8.21	1.465e+38	0.000189
9257	diHPCARP_Ic.mptppmpu	1.460e+43	6.86	6.86	1.461e+38	0.000189
9258	diHPCARP_Ic.ptptmtpmu	6.055e+43	7.71	7.71	1.460e+38	0.000189
9259	diHPCARP_Ic.mmtptptpmu	2.162e+44	8.47	8.47	1.459e+38	0.000189
9260	diHPCARP_Ic.mpttppppu	3.261e+43	7.35	7.35	1.434e+38	0.000186
9261	diHPCARP_Ic.ptpmpppmu	3.180e+43	7.34	7.34	1.424e+38	0.000184
9262	diHPCARP_Ic.mtpptptmu	2.361e+43	7.17	7.17	1.406e+38	0.000182
9263	diHPCARP_Ic.ttpmpttptu	2.464e+44	8.57	8.57	1.396e+38	0.000181
9264	diHPCARP_Ic.mppmmtmmu	1.922e+43	7.05	7.05	1.396e+38	0.000181

9265	diHPCARP_Ic.tmtptmtmu	3.099e+44	8.71	8.71	1.394e+38	0.00018
9266	diHPCARP_Ic.mtttmtmpu	1.435e+44	8.25	8.25	1.392e+38	0.00018
9267	diHPCARP_Ic.mttmtmtmu	6.152e+44	9.12	9.12	1.392e+38	0.00018
9268	diHPCARP_Ic.tmttpttptu	2.186e+44	8.51	8.51	1.384e+38	0.000179
9269	diHPCARP_Ic.tttmptmtmu	2.007e+44	8.46	8.46	1.367e+38	0.000177
9270	diHPCARP_Ic.mmtptmmmmu	8.580e+44	9.33	9.33	1.362e+38	0.000176
9271	diHPCARP_Ic.mpppmtmtmu	8.964e+43	7.99	7.99	1.353e+38	0.000175
9272	diHPCARP_Ic.tpttmttptu	4.626e+44	8.97	8.97	1.350e+38	0.000175
9273	diHPCARP_Ic.ptptmttptu	2.123e+45	9.88	9.88	1.337e+38	0.000173
9274	diHPCARP_Ic.ttmmpmtmu	4.447e+44	8.95	8.95	1.333e+38	0.000172
9275	diHPCARP_Ic.ptmmppmtmu	5.020e+43	7.66	7.66	1.325e+38	0.000171
9276	diHPCARP_Ic.tptmmmtmpu	2.302e+43	7.20	7.20	1.305e+38	0.000169
9277	diHPCARP_Ic.pptmmmtmpu	3.480e+43	7.45	7.45	1.297e+38	0.000168
9278	diHPCARP_Ic.tttmmmtmu	2.353e+44	8.60	8.60	1.288e+38	0.000167
9279	diHPCARP_Ic.mpttmttptu	5.219e+44	9.07	9.07	1.285e+38	0.000166
9280	diHPCARP_Ic.mptmtptmu	6.746e+43	7.85	7.85	1.283e+38	0.000166
9281	diHPCARP_Ic.tmmmpptmu	2.094e+43	7.16	7.16	1.283e+38	0.000166
9282	diHPCARP_Ic.ttpttptu	4.601e+44	9.00	9.00	1.268e+38	0.000164
9283	diHPCARP_Ic.ttppttmtmu	3.832e+44	8.90	8.90	1.264e+38	0.000164
9284	diHPCARP_Ic.tptmtptmu	7.935e+43	7.96	7.96	1.256e+38	0.000162
9285	diHPCARP_Ic.mmpptmtmu	1.344e+44	8.28	8.28	1.246e+38	0.000161
9286	diHPCARP_Ic.mtmtmtmpu	1.353e+44	8.29	8.29	1.244e+38	0.000161
9287	diHPCARP_Ic.mmmptmtmu	1.191e+44	8.21	8.21	1.235e+38	0.00016
9288	diHPCARP_Ic.mmttpttmu	4.475e+44	9.01	9.01	1.217e+38	0.000157
9289	diHPCARP_Ic.mpttmtmtmu	2.295e+44	8.62	8.62	1.209e+38	0.000156
9290	diHPCARP_Ic.pmpptmtmu	1.904e+43	7.14	7.14	1.202e+38	0.000155
9291	diHPCARP_Ic.mtptmptmu	1.990e+43	7.16	7.16	1.202e+38	0.000155
9292	diHPCARP_Ic.tmtmtmpu	1.649e+44	8.44	8.44	1.180e+38	0.000153
9293	diHPCARP_Ic.ttmmpmtmu	8.589e+43	8.05	8.05	1.172e+38	0.000152
9294	diHPCARP_Ic.ttttpttmu	2.810e+44	8.76	8.76	1.169e+38	0.000151
9295	diHPCARP_Ic.tttmmmpmu	2.936e+43	7.41	7.41	1.167e+38	0.000151
9296	diHPCARP_Ic.pttmtptmu	3.685e+43	7.55	7.55	1.166e+38	0.000151
9297	diHPCARP_Ic.mpttpttptu	2.125e+44	8.61	8.61	1.142e+38	0.000148
9298	diHPCARP_Ic.mtmmtmtmu	7.401e+43	7.99	7.99	1.111e+38	0.000144
9299	diHPCARP_Ic.ptmtptmtmu	4.841e+44	9.12	9.12	1.092e+38	0.000141
9300	diHPCARP_Ic.mmpptmtmu	1.729e+44	8.51	8.51	1.089e+38	0.000141
9301	diHPCARP_Ic.mpttmtmpu	9.959e+43	8.19	8.19	1.080e+38	0.00014
9302	diHPCARP_Ic.tmmtpptmu	6.521e+43	7.94	7.94	1.080e+38	0.00014
9303	diHPCARP_Ic.pptptmtmu	6.888e+43	7.97	7.97	1.072e+38	0.000139
9304	diHPCARP_Ic.mtptmtmpu	7.566e+43	8.04	8.04	1.060e+38	0.000137
9305	diHPCARP_Ic.tttmptmtmu	2.839e+44	8.83	8.83	1.057e+38	0.000137
9306	diHPCARP_Ic.ptmmpmtmu	2.693e+43	7.42	7.42	1.053e+38	0.000136
9307	diHPCARP_Ic.pmpptmtmu	7.890e+43	8.07	8.07	1.045e+38	0.000135
9308	diHPCARP_Ic.pmpptmtmu	4.481e+43	7.73	7.73	1.042e+38	0.000135
9309	diHPCARP_Ic.tppmpptmu	1.557e+43	7.11	7.11	1.038e+38	0.000134
9310	diHPCARP_Ic.mtmmpptmu	6.427e+43	7.95	7.95	1.037e+38	0.000134
9311	diHPCARP_Ic.tttptmtmu	5.565e+43	7.88	7.88	1.019e+38	0.000132
9312	diHPCARP_Ic.tmttptmtmu	3.814e+44	9.02	9.02	1.018e+38	0.000132
9313	diHPCARP_Ic.mtmmpmtmu	4.814e+43	7.81	7.81	9.896e+37	0.000128
9314	diHPCARP_Ic.tmpptmtmu	1.715e+45	9.94	9.94	9.776e+37	0.000126
9315	diHPCARP_Ic.tttmtmtmu	3.144e+44	8.93	8.93	9.757e+37	0.000126
9316	diHPCARP_Ic.ptptmtmtmu	5.445e+43	7.90	7.90	9.588e+37	0.000124
9317	diHPCARP_Ic.ttpmmpmtmu	5.715e+43	7.94	7.94	9.457e+37	0.000122
9318	diHPCARP_Ic.mmpptmtmu	2.325e+44	8.77	8.77	9.431e+37	0.000122
9319	diHPCARP_Ic.ptptmtmtmu	7.175e+44	9.45	9.45	9.429e+37	0.000122
9320	diHPCARP_Ic.mptmtmtmu	9.015e+43	8.21	8.21	9.414e+37	0.000122
9321	diHPCARP_Ic.ptppmtmtmu	1.413e+44	8.48	8.48	9.370e+37	0.000121
9322	diHPCARP_Ic.mppppptmu	2.174e+43	7.37	7.37	9.322e+37	0.000121
9323	diHPCARP_Ic.ttttmtmtmu	1.020e+44	8.29	8.29	9.313e+37	0.00012
9324	diHPCARP_Ic.pmtmtmtmu	1.488e+44	8.52	8.52	9.171e+37	0.000119
9325	diHPCARP_Ic.tptppptmu	7.127e+43	8.09	8.09	9.148e+37	0.000118
9326	diHPCARP_Ic.tmtmpttptu	2.810e+44	8.91	8.91	9.135e+37	0.000118
9327	diHPCARP_Ic.pmpmttptu	1.639e+44	8.59	8.59	9.096e+37	0.000118
9328	diHPCARP_Ic.tmtptmtmu	8.531e+44	9.57	9.57	9.041e+37	0.000117
9329	diHPCARP_Ic.ttttpttptu	2.835e+44	8.92	8.92	9.033e+37	0.000117
9330	diHPCARP_Ic.ptmmpmtmu	4.641e+43	7.84	7.84	8.955e+37	0.000116
9331	diHPCARP_Ic.tpptmtmtmu	1.234e+44	8.43	8.43	8.873e+37	0.000115
9332	diHPCARP_Ic.ptppmttptu	2.568e+44	8.87	8.87	8.856e+37	0.000115
9333	diHPCARP_Ic.mmtmtmtmu	6.689e+44	9.45	9.45	8.770e+37	0.000113
9334	diHPCARP_Ic.ttpttptmu	1.040e+45	9.72	9.72	8.637e+37	0.000112
9335	diHPCARP_Ic.pmpptmtmu	2.109e+44	8.78	8.78	8.454e+37	0.000109
9336	diHPCARP_Ic.mptmmmtmpu	1.164e+44	8.43	8.43	8.365e+37	0.000108

9337	diHPCARP_Ic.ptpppttpu	2.251e+44	8.84	8.84	8.214e+37	0.000106
9338	diHPCARP_Ic.pptmmmtmu	9.758e+43	8.34	8.34	8.190e+37	0.000106
9339	diHPCARP_Ic.mtppptmmu	2.320e+44	8.86	8.86	8.089e+37	0.000105
9340	diHPCARP_Ic.ppnmmtpmu	2.125e+43	7.44	7.44	8.065e+37	0.000104
9341	diHPCARP_Ic.tpmptmtmu	2.527e+44	8.92	8.92	8.017e+37	0.000104
9342	diHPCARP_Ic.pttptmpmu	4.001e+43	7.82	7.82	7.997e+37	0.000103
9343	diHPCARP_Ic.tmtmmtmu	2.771e+44	8.98	8.98	7.957e+37	0.000103
9344	diHPCARP_Ic.pmttptmpu	6.532e+43	8.14	8.14	7.620e+37	9.86e-05
9345	diHPCARP_Ic.mpppmmmpu	5.369e+43	8.03	8.03	7.536e+37	9.75e-05
9346	diHPCARP_Ic.tptmtmpu	1.257e+44	8.55	8.55	7.439e+37	9.62e-05
9347	diHPCARP_Ic.pptmptmpu	5.938e+43	8.10	8.10	7.412e+37	9.59e-05
9348	diHPCARP_Ic.pmpmtpppu	5.775e+43	8.10	8.10	7.215e+37	9.33e-05
9349	diHPCARP_Ic.tpttpttpu	3.768e+44	9.22	9.22	7.192e+37	9.3e-05
9350	diHPCARP_Ic.tmmmmmtmu	5.923e+43	8.12	8.12	7.190e+37	9.3e-05
9351	diHPCARP_Ic.mmttmmmtmu	8.413e+44	9.70	9.70	7.176e+37	9.28e-05
9352	diHPCARP_Ic.ppttptmmu	2.780e+44	9.04	9.04	7.162e+37	9.26e-05
9353	diHPCARP_Ic.mtppmtpmu	2.571e+43	7.63	7.63	7.119e+37	9.21e-05
9354	diHPCARP_Ic.pptmtmpu	6.183e+43	8.16	8.16	7.080e+37	9.16e-05
9355	diHPCARP_Ic.pmtppmtmu	1.559e+44	8.71	8.71	7.070e+37	9.15e-05
9356	diHPCARP_Ic.mppmmmtmu	3.034e+43	7.73	7.73	7.063e+37	9.14e-05
9357	diHPCARP_Ic.mttptmpu	3.066e+43	7.74	7.74	7.030e+37	9.09e-05
9358	diHPCARP_Ic.ttttmtppu	8.733e+44	9.74	9.74	7.004e+37	9.06e-05
9359	diHPCARP_Ic.ppmmtmtmu	3.329e+44	9.17	9.17	6.925e+37	8.96e-05
9360	diHPCARP_Ic.mtmmmmmtmu	1.060e+44	8.50	8.50	6.868e+37	8.88e-05
9361	diHPCARP_Ic.tttmmtmmu	2.302e+44	8.96	8.96	6.848e+37	8.86e-05
9362	diHPCARP_Ic.mpttmttmu	2.151e+44	8.92	8.92	6.812e+37	8.81e-05
9363	diHPCARP_Ic.ppmtpmpu	3.093e+43	7.78	7.78	6.598e+37	8.54e-05
9364	diHPCARP_Ic.tpmtmmpu	4.644e+43	8.03	8.03	6.586e+37	8.52e-05
9365	diHPCARP_Ic.mpptmttpu	1.442e+44	8.71	8.71	6.568e+37	8.5e-05
9366	diHPCARP_Ic.tmmmtmpu	1.332e+44	8.66	8.66	6.555e+37	8.48e-05
9367	diHPCARP_Ic.ptppppmmu	5.574e+43	8.14	8.14	6.550e+37	8.47e-05
9368	diHPCARP_Ic.mtpppppmu	2.606e+43	7.69	7.69	6.541e+37	8.46e-05
9369	diHPCARP_Ic.mttptmpu	9.150e+43	8.45	8.45	6.422e+37	8.31e-05
9370	diHPCARP_Ic.tpptptmmu	1.089e+44	8.58	8.58	6.140e+37	7.94e-05
9371	diHPCARP_Ic.mtmmmtmpu	8.352e+43	8.43	8.43	6.081e+37	7.87e-05
9372	diHPCARP_Ic.pppppmmpu	6.469e+43	8.28	8.28	6.025e+37	7.79e-05
9373	diHPCARP_Ic.mtmptpmu	3.223e+43	7.87	7.87	5.954e+37	7.7e-05
9374	diHPCARP_Ic.mpptppmpu	2.620e+43	7.75	7.75	5.897e+37	7.63e-05
9375	diHPCARP_Ic.tpmtpttmu	7.915e+44	9.79	9.79	5.884e+37	7.61e-05
9376	diHPCARP_Ic.mmmmtmpu	2.833e+44	9.18	9.18	5.811e+37	7.52e-05
9377	diHPCARP_Ic.pmppptmu	7.583e+43	8.40	8.40	5.781e+37	7.48e-05
9378	diHPCARP_Ic.mppmpttpu	6.412e+43	8.30	8.30	5.763e+37	7.45e-05
9379	diHPCARP_Ic.mptppppmu	3.221e+43	7.90	7.90	5.710e+37	7.39e-05
9380	diHPCARP_Ic.mtptmtmpu	2.645e+44	9.16	9.16	5.624e+37	7.28e-05
9381	diHPCARP_Ic.ttpmptmpu	4.473e+43	8.11	8.11	5.567e+37	7.2e-05
9382	diHPCARP_Ic.pmtmpmpu	1.452e+44	8.81	8.81	5.510e+37	7.13e-05
9383	diHPCARP_Ic.mmmmpmtmu	1.315e+44	8.76	8.76	5.477e+37	7.09e-05
9384	diHPCARP_Ic.ptppmtppu	5.689e+43	8.26	8.26	5.468e+37	7.07e-05
9385	diHPCARP_Ic.ptppptpmu	4.766e+43	8.16	8.16	5.411e+37	7e-05
9386	diHPCARP_Ic.mpppmtppu	9.186e+43	8.57	8.57	5.287e+37	6.84e-05
9387	diHPCARP_Ic.pmmmpmtmu	3.302e+43	7.96	7.96	5.280e+37	6.83e-05
9388	diHPCARP_Ic.mptpmtpmu	1.166e+44	8.71	8.71	5.271e+37	6.82e-05
9389	diHPCARP_Ic.ttpptpmu	3.308e+43	7.96	7.96	5.270e+37	6.82e-05
9390	diHPCARP_Ic.tmtmtmmu	6.478e+44	9.74	9.74	5.238e+37	6.78e-05
9391	diHPCARP_Ic.ptppmptmu	6.014e+43	8.32	8.32	5.235e+37	6.77e-05
9392	diHPCARP_Ic.mmtmmttpu	4.611e+44	9.54	9.54	5.197e+37	6.72e-05
9393	diHPCARP_Ic.tpmmttpu	7.389e+43	8.45	8.45	5.172e+37	6.69e-05
9394	diHPCARP_Ic.tpttptmpu	1.544e+44	8.89	8.89	5.148e+37	6.66e-05
9395	diHPCARP_Ic.tmtmmttpu	4.514e+44	9.53	9.53	5.113e+37	6.61e-05
9396	diHPCARP_Ic.tmmppptmu	6.310e+43	8.36	8.36	5.093e+37	6.59e-05
9397	diHPCARP_Ic.ppttptpmu	1.248e+44	8.77	8.77	5.092e+37	6.59e-05
9398	diHPCARP_Ic.tmppppppu	2.477e+44	9.18	9.18	5.050e+37	6.53e-05
9399	diHPCARP_Ic.tmttpttpu	5.027e+44	9.62	9.62	4.937e+37	6.39e-05
9400	diHPCARP_Ic.mpttpmpu	8.807e+43	8.59	8.59	4.900e+37	6.34e-05
9401	diHPCARP_Ic.tmttpttpu	2.106e+44	9.11	9.11	4.893e+37	6.33e-05
9402	diHPCARP_Ic.mmttpttpu	2.873e+45	10.67	10.67	4.876e+37	6.31e-05
9403	diHPCARP_Ic.mtpppttmu	2.434e+44	9.19	9.19	4.875e+37	6.31e-05
9404	diHPCARP_Ic.ttpmtmpu	5.835e+43	8.35	8.35	4.792e+37	6.2e-05
9405	diHPCARP_Ic.ptmmpmpu	3.918e+43	8.12	8.12	4.770e+37	6.17e-05
9406	diHPCARP_Ic.tptmttpu	5.457e+44	9.69	9.69	4.767e+37	6.17e-05
9407	diHPCARP_Ic.mppmptpmu	3.205e+43	8.00	8.00	4.761e+37	6.16e-05
9408	diHPCARP_Ic.ttppttmu	9.496e+43	8.66	8.66	4.671e+37	6.04e-05

9409	diHPCARP_Ic.mmtmmpmpu	7.368e+44	9.88	9.88	4.659e+37	6.03e-05
9410	diHPCARP_Ic.mpttpmtmu	1.637e+44	9.00	9.00	4.573e+37	5.92e-05
9411	diHPCARP_Ic.mttmtmpmu	7.402e+43	8.53	8.53	4.526e+37	5.85e-05
9412	diHPCARP_Ic.mpmmpmpmu	1.788e+43	7.69	7.69	4.460e+37	5.77e-05
9413	diHPCARP_Ic.mttppptpu	1.433e+44	8.94	8.94	4.430e+37	5.73e-05
9414	diHPCARP_Ic.mpttppmpu	8.065e+43	8.60	8.60	4.418e+37	5.71e-05
9415	diHPCARP_Ic.pptpmtmu	2.071e+44	9.16	9.16	4.398e+37	5.69e-05
9416	diHPCARP_Ic.mmmppmtmu	1.387e+45	10.30	10.30	4.325e+37	5.59e-05
9417	diHPCARP_Ic.mtttpttmu	1.891e+44	9.12	9.12	4.268e+37	5.52e-05
9418	diHPCARP_Ic.mmpmtmpu	5.182e+43	8.35	8.35	4.266e+37	5.52e-05
9419	diHPCARP_Ic.mpttpttmu	6.836e+43	8.52	8.52	4.214e+37	5.45e-05
9420	diHPCARP_Ic.ttttpttmu	3.287e+44	9.47	9.47	4.175e+37	5.4e-05
9421	diHPCARP_Ic.tttppttmu	2.546e+44	9.33	9.33	4.085e+37	5.28e-05
9422	diHPCARP_Ic.pmmppmtmu	8.008e+42	7.27	7.27	4.077e+37	5.27e-05
9423	diHPCARP_Ic.mptpmtmu	1.719e+44	9.10	9.10	4.016e+37	5.2e-05
9424	diHPCARP_Ic.pmpppmmpu	9.857e+43	8.77	8.77	4.007e+37	5.18e-05
9425	diHPCARP_Ic.pptpmtmu	3.479e+43	8.16	8.16	3.922e+37	5.07e-05
9426	diHPCARP_Ic.ptpppttmu	5.538e+44	9.83	9.83	3.854e+37	4.99e-05
9427	diHPCARP_Ic.mmmmmmtmu	2.245e+44	9.29	9.29	3.846e+37	4.98e-05
9428	diHPCARP_Ic.ttttpttmu	9.527e+43	8.79	8.79	3.785e+37	4.9e-05
9429	diHPCARP_Ic.pmpptmtmu	1.672e+44	9.12	9.12	3.774e+37	4.88e-05
9430	diHPCARP_Ic.pmpptmtmu	1.355e+44	9.00	9.00	3.741e+37	4.84e-05
9431	diHPCARP_Ic.ptpppttmu	3.008e+44	9.49	9.49	3.685e+37	4.77e-05
9432	diHPCARP_Ic.mtttmtppu	9.511e+43	8.82	8.82	3.581e+37	4.63e-05
9433	diHPCARP_Ic.ttmtpmtmu	1.605e+44	9.13	9.13	3.569e+37	4.62e-05
9434	diHPCARP_Ic.ptmmpmmpu	2.484e+44	9.40	9.40	3.513e+37	4.54e-05
9435	diHPCARP_Ic.tpmmttppu	1.003e+44	8.88	8.88	3.406e+37	4.41e-05
9436	diHPCARP_Ic.pmtppmtmu	4.098e+43	8.35	8.35	3.400e+37	4.4e-05
9437	diHPCARP_Ic.ppptmtmu	4.880e+43	8.46	8.46	3.372e+37	4.36e-05
9438	diHPCARP_Ic.mppmtmmpu	8.407e+43	8.79	8.79	3.348e+37	4.33e-05
9439	diHPCARP_Ic.tmttppmmpu	6.924e+44	10.04	10.04	3.344e+37	4.33e-05
9440	diHPCARP_Ic.mppmttmtmu	6.713e+44	10.03	10.03	3.302e+37	4.27e-05
9441	diHPCARP_Ic.mmmmtmmpu	4.048e+44	9.74	9.74	3.257e+37	4.21e-05
9442	diHPCARP_Ic.ttpmmpmpu	7.363e+43	8.73	8.73	3.228e+37	4.18e-05
9443	diHPCARP_Ic.ttmmpmtmu	1.598e+44	9.20	9.20	3.191e+37	4.13e-05
9444	diHPCARP_Ic.mmtmttmtmu	8.941e+44	10.23	10.23	3.166e+37	4.09e-05
9445	diHPCARP_Ic.pmttpttmu	7.303e+44	10.11	10.11	3.157e+37	4.08e-05
9446	diHPCARP_Ic.ptttppppu	6.352e+43	8.66	8.66	3.143e+37	4.07e-05
9447	diHPCARP_Ic.tttppmpmu	2.502e+43	8.11	8.11	3.086e+37	3.99e-05
9448	diHPCARP_Ic.ttttpttmu	3.294e+44	9.65	9.65	3.078e+37	3.98e-05
9449	diHPCARP_Ic.mttmmpmpu	1.229e+45	10.44	10.44	3.069e+37	3.97e-05
9450	diHPCARP_Ic.ppppmtmtmu	2.063e+44	9.37	9.37	3.065e+37	3.97e-05
9451	diHPCARP_Ic.tmppttmtmu	2.783e+44	9.56	9.56	3.022e+37	3.91e-05
9452	diHPCARP_Ic.ppppmtmtmu	7.423e+43	8.77	8.77	3.015e+37	3.9e-05
9453	diHPCARP_Ic.pptmmpmpu	5.697e+43	8.62	8.62	2.988e+37	3.87e-05
9454	diHPCARP_Ic.mtpmmtmpu	7.672e+43	8.80	8.80	2.980e+37	3.85e-05
9455	diHPCARP_Ic.ttmmtmtmu	3.963e+44	9.78	9.78	2.980e+37	3.85e-05
9456	diHPCARP_Ic.mtpmmpmpu	2.560e+43	8.16	8.16	2.914e+37	3.77e-05
9457	diHPCARP_Ic.mtpmtpmtmu	2.890e+43	8.24	8.24	2.896e+37	3.75e-05
9458	diHPCARP_Ic.pmmtpmtmu	2.540e+44	9.53	9.53	2.889e+37	3.74e-05
9459	diHPCARP_Ic.pttmmpmpu	8.114e+43	8.86	8.86	2.857e+37	3.7e-05
9460	diHPCARP_Ic.ppttptmtmu	9.356e+43	8.95	8.95	2.807e+37	3.63e-05
9461	diHPCARP_Ic.ptptpttmu	4.454e+44	9.89	9.89	2.792e+37	3.61e-05
9462	diHPCARP_Ic.tmppttmtmu	3.642e+44	9.77	9.77	2.792e+37	3.61e-05
9463	diHPCARP_Ic.mpmtpmpmu	5.355e+43	8.63	8.63	2.780e+37	3.6e-05
9464	diHPCARP_Ic.mppmtmtmu	7.650e+43	8.84	8.84	2.772e+37	3.59e-05
9465	diHPCARP_Ic.ttppttmtmu	1.171e+44	9.10	9.10	2.758e+37	3.57e-05
9466	diHPCARP_Ic.pmmtpmpmu	9.952e+43	9.01	9.01	2.721e+37	3.52e-05
9467	diHPCARP_Ic.tttpttmtmu	6.172e+43	8.74	8.74	2.635e+37	3.41e-05
9468	diHPCARP_Ic.mptpmtmpu	5.810e+43	8.71	8.71	2.625e+37	3.4e-05
9469	diHPCARP_Ic.tpmmpmtmu	6.177e+43	8.75	8.75	2.619e+37	3.39e-05
9470	diHPCARP_Ic.tpmppmtmu	6.436e+43	8.78	8.78	2.592e+37	3.35e-05
9471	diHPCARP_Ic.mmmmpmtmu	1.117e+44	9.11	9.11	2.570e+37	3.32e-05
9472	diHPCARP_Ic.ppmmpmpmu	5.716e+42	7.36	7.36	2.503e+37	3.24e-05
9473	diHPCARP_Ic.tpmmtmtmu	1.005e+45	10.44	10.44	2.487e+37	3.22e-05
9474	diHPCARP_Ic.ptmmpmtmu	7.445e+43	8.90	8.90	2.452e+37	3.17e-05
9475	diHPCARP_Ic.pttppmpmu	6.830e+43	8.85	8.85	2.446e+37	3.16e-05
9476	diHPCARP_Ic.pptmmtmu	1.080e+44	9.13	9.13	2.415e+37	3.12e-05
9477	diHPCARP_Ic.mppmtmpmu	7.697e+43	8.93	8.93	2.407e+37	3.11e-05
9478	diHPCARP_Ic.mtppttmtmu	1.919e+44	9.47	9.47	2.405e+37	3.11e-05
9479	diHPCARP_Ic.ttmtpmpmu	1.047e+44	9.12	9.12	2.383e+37	3.08e-05
9480	diHPCARP_Ic.mttmmpmpu	6.010e+43	8.80	8.80	2.324e+37	3.01e-05

9481	diHPCARP_Ic.ptppmptpu	6.803e+43	8.88	8.88	2.320e+37	3e-05
9482	diHPCARP_Ic.mpptmmmpu	5.093e+43	8.71	8.71	2.298e+37	2.97e-05
9483	diHPCARP_Ic.mpttmppmu	1.358e+44	9.30	9.30	2.286e+37	2.96e-05
9484	diHPCARP_Ic.tpmmtmtmu	6.648e+43	8.87	8.87	2.282e+37	2.95e-05
9485	diHPCARP_Ic.mtmmpmtpmu	3.526e+43	8.50	8.50	2.270e+37	2.94e-05
9486	diHPCARP_Ic.mtpptmtpu	1.832e+44	9.48	9.48	2.261e+37	2.92e-05
9487	diHPCARP_Ic.tmpmmmtmu	6.559e+43	8.88	8.88	2.238e+37	2.89e-05
9488	diHPCARP_Ic.tttmmmtmu	4.758e+43	8.69	8.69	2.227e+37	2.88e-05
9489	diHPCARP_Ic.mmmmmmmmu	4.043e+44	9.98	9.98	2.167e+37	2.8e-05
9490	diHPCARP_Ic.pmpppmpu	6.563e+43	8.90	8.90	2.142e+37	2.77e-05
9491	diHPCARP_Ic.tmpptmtmu	1.290e+45	10.69	10.69	2.102e+37	2.72e-05
9492	diHPCARP_Ic.ttpptmtmu	1.934e+44	9.56	9.56	2.086e+37	2.7e-05
9493	diHPCARP_Ic.tpmmtmtmu	2.055e+44	9.60	9.60	2.079e+37	2.69e-05
9494	diHPCARP_Ic.tttptmtmu	3.133e+44	9.86	9.86	2.063e+37	2.67e-05
9495	diHPCARP_Ic.ttpmmtpmu	5.984e+43	8.87	8.87	2.057e+37	2.66e-05
9496	diHPCARP_Ic.mptmtmtmu	6.004e+44	10.25	10.25	2.041e+37	2.64e-05
9497	diHPCARP_Ic.ptpmmtpu	4.969e+43	8.77	8.77	2.036e+37	2.63e-05
9498	diHPCARP_Ic.mpmppmpu	1.166e+43	7.91	7.91	2.008e+37	2.6e-05
9499	diHPCARP_Ic.tttmmmpu	4.632e+43	8.73	8.73	2.008e+37	2.6e-05
9500	diHPCARP_Ic.mtppmmpu	2.694e+43	8.41	8.41	2.006e+37	2.59e-05
9501	diHPCARP_Ic.tmpmmmtmu	1.043e+44	9.22	9.22	1.997e+37	2.58e-05
9502	diHPCARP_Ic.mtppmttmu	2.376e+44	9.71	9.71	1.991e+37	2.58e-05
9503	diHPCARP_Ic.pppmmtmu	5.730e+43	8.87	8.87	1.987e+37	2.57e-05
9504	diHPCARP_Ic.mptppmpu	3.578e+43	8.59	8.59	1.969e+37	2.55e-05
9505	diHPCARP_Ic.tmpmmmtmu	1.258e+44	9.34	9.34	1.966e+37	2.54e-05
9506	diHPCARP_Ic.tpmmtppu	6.099e+43	8.91	8.91	1.961e+37	2.54e-05
9507	diHPCARP_Ic.mttptmtmu	3.534e+43	8.59	8.59	1.939e+37	2.51e-05
9508	diHPCARP_Ic.pptptppu	4.211e+44	10.07	10.07	1.938e+37	2.51e-05
9509	diHPCARP_Ic.mmpptppmu	1.751e+44	9.56	9.56	1.888e+37	2.44e-05
9510	diHPCARP_Ic.pmmtpmtpu	3.323e+44	9.95	9.95	1.883e+37	2.44e-05
9511	diHPCARP_Ic.ptppmmtmu	1.259e+44	9.38	9.38	1.850e+37	2.39e-05
9512	diHPCARP_Ic.ttmppmpu	1.460e+44	9.47	9.47	1.842e+37	2.38e-05
9513	diHPCARP_Ic.tmtpttptu	3.800e+44	10.04	10.04	1.841e+37	2.38e-05
9514	diHPCARP_Ic.tpmmmmpu	2.157e+43	8.33	8.33	1.835e+37	2.37e-05
9515	diHPCARP_Ic.mtpppttmu	1.391e+44	9.45	9.45	1.818e+37	2.35e-05
9516	diHPCARP_Ic.ttmmtppu	5.399e+43	8.89	8.89	1.816e+37	2.35e-05
9517	diHPCARP_Ic.ptptptppu	6.150e+44	10.35	10.35	1.780e+37	2.3e-05
9518	diHPCARP_Ic.ptptpttmu	9.719e+44	10.64	10.64	1.728e+37	2.24e-05
9519	diHPCARP_Ic.tttmmppu	4.085e+43	8.75	8.75	1.715e+37	2.22e-05
9520	diHPCARP_Ic.tmpmmttmu	9.372e+43	9.26	9.26	1.676e+37	2.17e-05
9521	diHPCARP_Ic.mpmmtpmu	4.388e+43	8.81	8.81	1.669e+37	2.16e-05
9522	diHPCARP_Ic.tpmtpmtpu	1.129e+44	9.38	9.38	1.661e+37	2.15e-05
9523	diHPCARP_Ic.mmmtmpmpu	4.783e+44	10.26	10.26	1.613e+37	2.09e-05
9524	diHPCARP_Ic.mmmtmmmmu	4.772e+44	10.26	10.26	1.611e+37	2.08e-05
9525	diHPCARP_Ic.mmpmmtmu	4.265e+44	10.20	10.20	1.591e+37	2.06e-05
9526	diHPCARP_Ic.mtppmpmpu	3.283e+43	8.67	8.67	1.590e+37	2.06e-05
9527	diHPCARP_Ic.tptptmtpu	7.824e+43	9.20	9.20	1.562e+37	2.02e-05
9528	diHPCARP_Ic.mppptppmu	3.015e+43	8.63	8.63	1.552e+37	2.01e-05
9529	diHPCARP_Ic.mtpmmpmu	2.896e+43	8.62	8.62	1.528e+37	1.98e-05
9530	diHPCARP_Ic.pttptptmu	9.544e+43	9.33	9.33	1.522e+37	1.97e-05
9531	diHPCARP_Ic.mtppmmtmu	1.564e+44	9.64	9.64	1.496e+37	1.93e-05
9532	diHPCARP_Ic.mtppmptmu	3.341e+43	8.72	8.72	1.474e+37	1.91e-05
9533	diHPCARP_Ic.mmtmtpmu	9.876e+44	10.74	10.74	1.472e+37	1.9e-05
9534	diHPCARP_Ic.mptmmtmu	2.187e+44	9.85	9.85	1.468e+37	1.9e-05
9535	diHPCARP_Ic.pptpmmpu	3.025e+43	8.67	8.67	1.468e+37	1.9e-05
9536	diHPCARP_Ic.ptpmmtmu	4.321e+43	8.88	8.88	1.459e+37	1.89e-05
9537	diHPCARP_Ic.ptpmmtmu	7.454e+43	9.22	9.22	1.443e+37	1.87e-05
9538	diHPCARP_Ic.mpmmtmtpu	1.709e+43	8.35	8.35	1.421e+37	1.84e-05
9539	diHPCARP_Ic.ttpptppu	2.356e+44	9.93	9.93	1.374e+37	1.78e-05
9540	diHPCARP_Ic.pppmmmpu	1.256e+44	9.56	9.56	1.355e+37	1.75e-05
9541	diHPCARP_Ic.tmtmptmu	2.200e+44	9.91	9.91	1.323e+37	1.71e-05
9542	diHPCARP_Ic.ttpmtpmu	1.589e+44	9.72	9.72	1.320e+37	1.71e-05
9543	diHPCARP_Ic.pmptpmmpu	1.534e+44	9.71	9.71	1.292e+37	1.67e-05
9544	diHPCARP_Ic.mmpptmtmu	2.821e+44	10.08	10.08	1.290e+37	1.67e-05
9545	diHPCARP_Ic.ttmmtmtmu	7.945e+44	10.69	10.69	1.288e+37	1.67e-05
9546	diHPCARP_Ic.ptppmtmu	1.641e+44	9.76	9.76	1.279e+37	1.65e-05
9547	diHPCARP_Ic.mmpmtmtpu	7.969e+43	9.33	9.33	1.262e+37	1.63e-05
9548	diHPCARP_Ic.tpmmttptu	3.183e+44	10.16	10.16	1.253e+37	1.62e-05
9549	diHPCARP_Ic.pptptmtpu	6.657e+43	9.24	9.24	1.236e+37	1.6e-05
9550	diHPCARP_Ic.tmppttptu	8.364e+44	10.75	10.75	1.235e+37	1.6e-05
9551	diHPCARP_Ic.mmpmmttmu	2.918e+44	10.13	10.13	1.225e+37	1.58e-05
9552	diHPCARP_Ic.tpmmmmtmu	4.537e+44	10.40	10.40	1.206e+37	1.56e-05

9553	diHPCARP_Ic.tmpmttptpu	1.671e+44	9.81	9.81	1.195e+37	1.55e-05
9554	diHPCARP_Ic.tttmttptpu	4.459e+44	10.40	10.40	1.190e+37	1.54e-05
9555	diHPCARP_Ic.ttpmtmmu	1.159e+44	9.60	9.60	1.179e+37	1.52e-05
9556	diHPCARP_Ic.ptptmmpu	6.387e+43	9.25	9.25	1.157e+37	1.5e-05
9557	diHPCARP_Ic.mmpmtmtmu	2.455e+45	11.44	11.44	1.137e+37	1.47e-05
9558	diHPCARP_Ic.ttpmptpmu	6.055e+43	9.23	9.23	1.136e+37	1.47e-05
9559	diHPCARP_Ic.ttmmtmmpu	7.842e+43	9.40	9.40	1.121e+37	1.45e-05
9560	diHPCARP_Ic.tmtpttptpu	5.689e+44	10.58	10.58	1.115e+37	1.44e-05
9561	diHPCARP_Ic.mtptpttmu	2.217e+44	10.03	10.03	1.094e+37	1.41e-05
9562	diHPCARP_Ic.mtppmpmu	4.376e+43	9.08	9.08	1.068e+37	1.38e-05
9563	diHPCARP_Ic.mppmptmu	3.635e+44	10.34	10.34	1.067e+37	1.38e-05
9564	diHPCARP_Ic.mttmttptpu	1.176e+44	9.67	9.67	1.067e+37	1.38e-05
9565	diHPCARP_Ic.ptmtppmu	2.543e+43	8.78	8.78	1.019e+37	1.32e-05
9566	diHPCARP_Ic.tmtmttptpu	5.307e+44	10.61	10.61	9.935e+36	1.29e-05
9567	diHPCARP_Ic.mtpmmtpmu	2.384e+43	8.78	8.78	9.641e+36	1.25e-05
9568	diHPCARP_Ic.ttpppmpu	9.990e+43	9.63	9.63	9.593e+36	1.24e-05
9569	diHPCARP_Ic.tptmtmmu	3.868e+44	10.45	10.45	9.392e+36	1.22e-05
9570	diHPCARP_Ic.tppmtmtmu	7.317e+43	9.46	9.46	9.355e+36	1.21e-05
9571	diHPCARP_Ic.pppmmpmu	2.876e+43	8.91	8.91	9.340e+36	1.21e-05
9572	diHPCARP_Ic.ttmmttptpu	2.681e+44	10.24	10.24	9.250e+36	1.2e-05
9573	diHPCARP_Ic.mmpmmpu	5.031e+43	9.25	9.25	9.229e+36	1.19e-05
9574	diHPCARP_Ic.ttpmmpmu	1.503e+44	9.91	9.91	9.118e+36	1.18e-05
9575	diHPCARP_Ic.pttppmmu	1.164e+44	9.76	9.76	8.984e+36	1.16e-05
9576	diHPCARP_Ic.mptmmmtmu	1.499e+44	9.92	9.92	8.965e+36	1.16e-05
9577	diHPCARP_Ic.pttppmmu	1.178e+44	9.80	9.80	8.607e+36	1.11e-05
9578	diHPCARP_Ic.pppmmpu	2.772e+43	8.94	8.94	8.525e+36	1.1e-05
9579	diHPCARP_Ic.pttptptpu	2.614e+44	10.28	10.28	8.453e+36	1.09e-05
9580	diHPCARP_Ic.mtppmpu	5.997e+43	9.41	9.41	8.384e+36	1.08e-05
9581	diHPCARP_Ic.tmtptptpu	1.572e+44	9.98	9.98	8.375e+36	1.08e-05
9582	diHPCARP_Ic.mppmmtmu	3.432e+44	10.46	10.46	8.298e+36	1.07e-05
9583	diHPCARP_Ic.mpptmtptpu	1.960e+44	10.13	10.13	8.149e+36	1.05e-05
9584	diHPCARP_Ic.ttpmmpmu	2.889e+43	8.99	8.99	8.092e+36	1.05e-05
9585	diHPCARP_Ic.ttpmmpmu	5.898e+43	9.42	9.42	8.073e+36	1.04e-05
9586	diHPCARP_Ic.mtpppppu	3.436e+43	9.11	9.11	7.901e+36	1.02e-05
9587	diHPCARP_Ic.tppppppmu	4.033e+43	9.21	9.21	7.877e+36	1.02e-05
9588	diHPCARP_Ic.mtptmtptpu	1.625e+44	10.04	10.04	7.864e+36	1.02e-05
9589	diHPCARP_Ic.tppppmpu	4.624e+43	9.30	9.30	7.764e+36	1e-05
9590	diHPCARP_Ic.mptmmpu	1.089e+44	9.81	9.81	7.757e+36	1e-05
9591	diHPCARP_Ic.pttppmmu	2.463e+44	10.32	10.32	7.420e+36	9.6e-06
9592	diHPCARP_Ic.mtppppmu	6.234e+43	9.51	9.51	7.415e+36	9.59e-06
9593	diHPCARP_Ic.ttpmmpmu	3.811e+43	9.22	9.22	7.370e+36	9.53e-06
9594	diHPCARP_Ic.mtmtppmu	3.265e+43	9.12	9.12	7.362e+36	9.52e-06
9595	diHPCARP_Ic.mtppmpmu	5.173e+43	9.40	9.40	7.360e+36	9.52e-06
9596	diHPCARP_Ic.mtppppptpu	5.889e+43	9.48	9.48	7.317e+36	9.46e-06
9597	diHPCARP_Ic.mptmmpmu	7.947e+43	9.67	9.67	7.202e+36	9.32e-06
9598	diHPCARP_Ic.pptptmtmu	8.201e+43	9.69	9.69	7.167e+36	9.27e-06
9599	diHPCARP_Ic.mtppmptmu	3.404e+43	9.17	9.17	7.141e+36	9.24e-06
9600	diHPCARP_Ic.ttttppmu	1.010e+44	9.82	9.82	7.064e+36	9.14e-06
9601	diHPCARP_Ic.mtmtmtpmu	1.203e+44	9.94	9.94	6.963e+36	9.01e-06
9602	diHPCARP_Ic.mtptptptpu	2.399e+44	10.35	10.35	6.960e+36	9e-06
9603	diHPCARP_Ic.ppmmtmmpu	4.025e+43	9.29	9.29	6.927e+36	8.96e-06
9604	diHPCARP_Ic.mptmmpmu	4.244e+43	9.33	9.33	6.782e+36	8.77e-06
9605	diHPCARP_Ic.pptptptmu	6.600e+43	9.66	9.66	6.050e+36	7.83e-06
9606	diHPCARP_Ic.mtptppmu	9.213e+43	9.86	9.86	6.025e+36	7.79e-06
9607	diHPCARP_Ic.mtppppmu	3.607e+43	9.32	9.32	5.891e+36	7.62e-06
9608	diHPCARP_Ic.tppmmtmu	1.026e+44	9.94	9.94	5.854e+36	7.57e-06
9609	diHPCARP_Ic.mptmmpu	4.676e+44	10.85	10.85	5.811e+36	7.52e-06
9610	diHPCARP_Ic.tppmptptpu	1.547e+44	10.20	10.20	5.725e+36	7.41e-06
9611	diHPCARP_Ic.ptptmtmu	3.268e+44	10.66	10.66	5.639e+36	7.29e-06
9612	diHPCARP_Ic.mppmmtmu	2.377e+43	9.10	9.10	5.598e+36	7.24e-06
9613	diHPCARP_Ic.tppmptmu	1.529e+44	10.22	10.22	5.506e+36	7.12e-06
9614	diHPCARP_Ic.tmtptmtmu	2.504e+44	10.54	10.54	5.282e+36	6.83e-06
9615	diHPCARP_Ic.tptmtptpu	3.084e+44	10.67	10.67	5.215e+36	6.75e-06
9616	diHPCARP_Ic.tmpmptptpu	1.461e+44	10.23	10.23	5.123e+36	6.63e-06
9617	diHPCARP_Ic.pppmptptpu	1.753e+43	8.97	8.97	5.093e+36	6.59e-06
9618	diHPCARP_Ic.tppmptmu	7.042e+43	9.82	9.82	4.961e+36	6.42e-06
9619	diHPCARP_Ic.mtppmmpmu	3.147e+43	9.35	9.35	4.831e+36	6.25e-06
9620	diHPCARP_Ic.mtptptptpu	2.361e+44	10.56	10.56	4.822e+36	6.24e-06
9621	diHPCARP_Ic.mtptmtptpu	4.039e+44	10.88	10.88	4.784e+36	6.19e-06
9622	diHPCARP_Ic.tptmmpmu	1.122e+44	10.12	10.12	4.766e+36	6.17e-06
9623	diHPCARP_Ic.tttmmpmu	8.845e+43	9.98	9.98	4.731e+36	6.12e-06
9624	diHPCARP_Ic.tppmmpmu	4.305e+43	9.55	9.55	4.729e+36	6.12e-06

9625	diHPCARP_Ic.tmpmtttmu	8.628e+44	11.34	11.34	4.714e+36	6.1e-06
9626	diHPCARP_Ic.mmpmmttmu	6.558e+43	9.81	9.81	4.713e+36	6.1e-06
9627	diHPCARP_Ic.tpmmmppmu	4.741e+43	9.62	9.62	4.677e+36	6.05e-06
9628	diHPCARP_Ic.mpmmtppmu	9.756e+43	10.05	10.05	4.638e+36	6e-06
9629	diHPCARP_Ic.mptmmmmu	4.322e+44	10.96	10.96	4.471e+36	5.78e-06
9630	diHPCARP_Ic.tttmttptmu	1.163e+44	10.19	10.19	4.421e+36	5.72e-06
9631	diHPCARP_Ic.tmpppmmu	3.004e+44	10.76	10.76	4.365e+36	5.65e-06
9632	diHPCARP_Ic.tmpppptmu	1.886e+44	10.48	10.48	4.343e+36	5.62e-06
9633	diHPCARP_Ic.mpppmppmu	4.214e+44	10.98	10.98	4.247e+36	5.49e-06
9634	diHPCARP_Ic.mtpmppmmu	2.518e+43	9.30	9.30	4.221e+36	5.46e-06
9635	diHPCARP_Ic.mpttmmppu	3.816e+45	12.30	12.30	4.216e+36	5.45e-06
9636	diHPCARP_Ic.tttmmppmu	7.958e+43	9.99	9.99	4.177e+36	5.4e-06
9637	diHPCARP_Ic.tmpppptpu	1.703e+44	10.45	10.45	4.172e+36	5.4e-06
9638	diHPCARP_Ic.tttmmmmu	2.090e+44	10.58	10.58	4.119e+36	5.33e-06
9639	diHPCARP_Ic.mtmmtttmu	6.855e+44	11.29	11.29	4.096e+36	5.3e-06
9640	diHPCARP_Ic.mtptmmttptmu	7.378e+43	9.96	9.96	4.094e+36	5.3e-06
9641	diHPCARP_Ic.mmmppmmmu	6.194e+44	11.23	11.23	4.090e+36	5.29e-06
9642	diHPCARP_Ic.ptmmpmmpmu	2.132e+43	9.25	9.25	3.910e+36	5.06e-06
9643	diHPCARP_Ic.ptpmmmppu	1.026e+44	10.19	10.19	3.904e+36	5.05e-06
9644	diHPCARP_Ic.mptmttppu	5.094e+43	9.77	9.77	3.894e+36	5.04e-06
9645	diHPCARP_Ic.tmttptptpu	4.823e+44	11.12	11.12	3.853e+36	4.98e-06
9646	diHPCARP_Ic.pmmppttmu	2.016e+44	10.60	10.60	3.849e+36	4.98e-06
9647	diHPCARP_Ic.mptmmmtptmu	1.026e+45	11.57	11.57	3.843e+36	4.97e-06
9648	diHPCARP_Ic.mptmmpmmu	9.930e+43	10.18	10.18	3.804e+36	4.92e-06
9649	diHPCARP_Ic.mmpmtmptmu	1.337e+45	11.74	11.74	3.773e+36	4.88e-06
9650	diHPCARP_Ic.tmpmmmmmu	7.247e+43	10.01	10.01	3.728e+36	4.82e-06
9651	diHPCARP_Ic.ttttmtptmu	1.427e+44	10.41	10.41	3.715e+36	4.81e-06
9652	diHPCARP_Ic.mtppppptmu	7.869e+43	10.07	10.07	3.627e+36	4.69e-06
9653	diHPCARP_Ic.ttmmpmtmu	2.093e+44	10.67	10.67	3.554e+36	4.6e-06
9654	diHPCARP_Ic.mpppmmtptmu	3.038e+44	10.89	10.89	3.539e+36	4.58e-06
9655	diHPCARP_Ic.tttmtptptmu	1.017e+44	10.24	10.24	3.534e+36	4.57e-06
9656	diHPCARP_Ic.mmpmmmtppu	5.176e+43	9.84	9.84	3.531e+36	4.57e-06
9657	diHPCARP_Ic.pmpptppmpu	1.098e+44	10.30	10.30	3.452e+36	4.47e-06
9658	diHPCARP_Ic.tmmtpptmu	1.309e+44	10.41	10.41	3.410e+36	4.41e-06
9659	diHPCARP_Ic.mtmmtttptmu	9.376e+44	11.60	11.60	3.326e+36	4.3e-06
9660	diHPCARP_Ic.mtpttptptmu	1.960e+44	10.69	10.69	3.223e+36	4.17e-06
9661	diHPCARP_Ic.tmpmptttmu	8.977e+43	10.22	10.22	3.214e+36	4.16e-06
9662	diHPCARP_Ic.tmpmmmtmu	1.312e+44	10.45	10.45	3.209e+36	4.15e-06
9663	diHPCARP_Ic.ttpppppmu	9.697e+43	10.28	10.28	3.131e+36	4.05e-06
9664	diHPCARP_Ic.mtpttptptmu	1.563e+44	10.57	10.57	3.120e+36	4.04e-06
9665	diHPCARP_Ic.tmpmtttptmu	5.389e+44	11.31	11.31	3.119e+36	4.03e-06
9666	diHPCARP_Ic.pptmmmmmu	7.900e+43	10.17	10.17	3.097e+36	4.01e-06
9667	diHPCARP_Ic.tpmppmmpu	3.661e+43	9.72	9.72	3.041e+36	3.93e-06
9668	diHPCARP_Ic.mtmmmppmu	3.724e+43	9.74	9.74	2.991e+36	3.87e-06
9669	diHPCARP_Ic.mptpmmpu	9.902e+43	10.33	10.33	2.957e+36	3.83e-06
9670	diHPCARP_Ic.tptppmppu	4.254e+43	9.84	9.84	2.907e+36	3.76e-06
9671	diHPCARP_Ic.mppmmmpu	1.593e+44	10.63	10.63	2.853e+36	3.69e-06
9672	diHPCARP_Ic.tmpmmttmu	1.760e+44	10.72	10.72	2.720e+36	3.52e-06
9673	diHPCARP_Ic.tmpppptmu	1.839e+44	10.75	10.75	2.696e+36	3.49e-06
9674	diHPCARP_Ic.mmpmmmtptmu	6.205e+43	10.11	10.11	2.685e+36	3.47e-06
9675	diHPCARP_Ic.mpppmmtmu	1.606e+44	10.72	10.72	2.510e+36	3.25e-06
9676	diHPCARP_Ic.tpptpmmpu	4.560e+43	9.99	9.99	2.397e+36	3.1e-06
9677	diHPCARP_Ic.mtmmttptmu	5.518e+43	10.13	10.13	2.293e+36	2.97e-06
9678	diHPCARP_Ic.mpttmttmu	2.270e+44	11.00	11.00	2.219e+36	2.87e-06
9679	diHPCARP_Ic.mttptmttmu	2.933e+44	11.15	11.15	2.211e+36	2.86e-06
9680	diHPCARP_Ic.tmppppmmu	2.582e+44	11.11	11.11	2.079e+36	2.69e-06
9681	diHPCARP_Ic.pmpmmmmu	2.407e+44	11.10	11.10	1.965e+36	2.54e-06
9682	diHPCARP_Ic.tppppptmu	3.365e+44	11.30	11.30	1.963e+36	2.54e-06
9683	diHPCARP_Ic.ppppmmmmu	3.672e+43	9.99	9.99	1.938e+36	2.51e-06
9684	diHPCARP_Ic.tttttmpmmu	1.424e+44	10.80	10.80	1.922e+36	2.49e-06
9685	diHPCARP_Ic.mttmmttmu	3.001e+44	11.27	11.27	1.847e+36	2.39e-06
9686	diHPCARP_Ic.ttmmtptmu	3.954e+43	10.07	10.07	1.839e+36	2.38e-06
9687	diHPCARP_Ic.ptpmppmmu	5.494e+43	10.27	10.27	1.821e+36	2.36e-06
9688	diHPCARP_Ic.mtttmttptmu	5.146e+44	11.61	11.61	1.794e+36	2.32e-06
9689	diHPCARP_Ic.ttmmttmtmu	2.276e+44	11.13	11.13	1.779e+36	2.3e-06
9690	diHPCARP_Ic.ttmmttptmu	3.908e+43	10.09	10.09	1.733e+36	2.24e-06
9691	diHPCARP_Ic.mptmpttptmu	1.091e+44	10.71	10.71	1.730e+36	2.24e-06
9692	diHPCARP_Ic.ttttmmppmu	6.045e+43	10.36	10.36	1.713e+36	2.22e-06
9693	diHPCARP_Ic.mtpmpttmu	7.426e+43	10.50	10.50	1.672e+36	2.16e-06
9694	diHPCARP_Ic.tmpmpttptmu	9.289e+43	10.64	10.64	1.639e+36	2.12e-06
9695	diHPCARP_Ic.tptmmpmu	1.123e+44	10.76	10.76	1.629e+36	2.11e-06
9696	diHPCARP_Ic.tmpmptptmu	1.400e+44	10.89	10.89	1.623e+36	2.1e-06

9697	diHPCARP_Ic.tppppmtpu	3.299e+44	11.42	11.42	1.593e+36	2.06e-06
9698	diHPCARP_Ic.tttppmmpmu	3.063e+44	11.38	11.38	1.583e+36	2.05e-06
9699	diHPCARP_Ic.mpttpmppu	1.138e+44	10.79	10.79	1.570e+36	2.03e-06
9700	diHPCARP_Ic.ttmtppppu	9.321e+43	10.67	10.67	1.567e+36	2.03e-06
9701	diHPCARP_Ic.ppppptppu	1.447e+44	10.94	10.94	1.545e+36	2e-06
9702	diHPCARP_Ic.tmpmmmtmpu	7.773e+43	10.57	10.57	1.542e+36	1.99e-06
9703	diHPCARP_Ic.tpttpmpu	2.245e+44	11.21	11.21	1.532e+36	1.98e-06
9704	diHPCARP_Ic.tmpmmmmmpu	5.260e+43	10.35	10.35	1.519e+36	1.96e-06
9705	diHPCARP_Ic.mtpmptppu	1.102e+44	10.82	10.82	1.455e+36	1.88e-06
9706	diHPCARP_Ic.mpmtpppmu	3.353e+43	10.12	10.12	1.422e+36	1.84e-06
9707	diHPCARP_Ic.mppppptpu	8.474e+43	10.68	10.68	1.412e+36	1.83e-06
9708	diHPCARP_Ic.ppttmppmu	1.855e+44	11.16	11.16	1.387e+36	1.79e-06
9709	diHPCARP_Ic.ttptpppmu	1.227e+44	10.92	10.92	1.365e+36	1.77e-06
9710	diHPCARP_Ic.mppmmmtmu	6.931e+44	11.95	11.95	1.361e+36	1.76e-06
9711	diHPCARP_Ic.ttttmmmmu	2.766e+44	11.43	11.43	1.306e+36	1.69e-06
9712	diHPCARP_Ic.tmpptptmu	4.534e+44	11.74	11.74	1.280e+36	1.66e-06
9713	diHPCARP_Ic.mtpmptppu	5.151e+43	10.44	10.44	1.274e+36	1.65e-06
9714	diHPCARP_Ic.pmmpttptu	3.958e+43	10.32	10.32	1.208e+36	1.56e-06
9715	diHPCARP_Ic.ttpmmmtmu	8.610e+43	10.79	10.79	1.184e+36	1.53e-06
9716	diHPCARP_Ic.mpmmmmtmu	8.184e+43	10.76	10.76	1.179e+36	1.53e-06
9717	diHPCARP_Ic.mmpmmmtmu	6.236e+43	10.61	10.61	1.167e+36	1.51e-06
9718	diHPCARP_Ic.ttpmpptpu	6.216e+43	10.64	10.64	1.111e+36	1.44e-06
9719	diHPCARP_Ic.ttttmtptu	2.481e+44	11.48	11.48	1.073e+36	1.39e-06
9720	diHPCARP_Ic.mtpmpttptu	6.356e+43	10.67	10.67	1.065e+36	1.38e-06
9721	diHPCARP_Ic.pptpmppmu	2.623e+44	11.52	11.52	1.064e+36	1.38e-06
9722	diHPCARP_Ic.mptpmmmmu	1.040e+45	12.35	12.35	1.056e+36	1.37e-06
9723	diHPCARP_Ic.tptppmtmu	1.667e+44	11.26	11.26	1.054e+36	1.36e-06
9724	diHPCARP_Ic.mtttmttmu	5.354e+44	11.95	11.95	1.049e+36	1.36e-06
9725	diHPCARP_Ic.ttpmpppmu	3.745e+43	10.38	10.38	1.023e+36	1.32e-06
9726	diHPCARP_Ic.mpmmpppmu	1.094e+43	9.66	9.66	1.001e+36	1.29e-06
9727	diHPCARP_Ic.tppmppmpu	1.443e+44	11.21	11.21	9.865e+35	1.28e-06
9728	diHPCARP_Ic.mtmmtmtmu	6.222e+44	12.09	12.09	9.772e+35	1.26e-06
9729	diHPCARP_Ic.mtptmttmu	6.905e+44	12.15	12.15	9.738e+35	1.26e-06
9730	diHPCARP_Ic.tmpptptpu	4.907e+44	11.96	11.96	9.547e+35	1.24e-06
9731	diHPCARP_Ic.tmpptppmu	1.119e+45	12.46	12.46	9.438e+35	1.22e-06
9732	diHPCARP_Ic.tmpmpmmpmu	2.173e+44	11.49	11.49	9.259e+35	1.2e-06
9733	diHPCARP_Ic.mpmmtmtmu	9.635e+43	11.01	11.01	9.169e+35	1.19e-06
9734	diHPCARP_Ic.ttmppmmpmu	1.275e+44	11.19	11.19	8.966e+35	1.16e-06
9735	diHPCARP_Ic.tpmmpmmmu	4.590e+43	10.59	10.59	8.862e+35	1.15e-06
9736	diHPCARP_Ic.tmttppmmu	1.988e+44	11.50	11.50	8.315e+35	1.08e-06
9737	diHPCARP_Ic.mppppmmmu	4.835e+43	10.68	10.68	7.991e+35	1.03e-06
9738	diHPCARP_Ic.mpttpmmpmu	1.782e+44	11.47	11.47	7.886e+35	1.02e-06
9739	diHPCARP_Ic.mpmmpptmu	2.033e+43	10.18	10.18	7.746e+35	1e-06
9740	diHPCARP_Ic.ttpppptpu	2.687e+44	11.72	11.72	7.729e+35	1e-06
9741	diHPCARP_Ic.mppmtmtmu	4.605e+44	12.07	12.07	7.378e+35	9.54e-07
9742	diHPCARP_Ic.tptmpppmu	2.448e+44	11.73	11.73	7.007e+35	9.06e-07
9743	diHPCARP_Ic.tptmpmtmu	3.311e+44	11.91	11.91	7.005e+35	9.06e-07
9744	diHPCARP_Ic.mtptmttmu	3.952e+43	10.66	10.66	6.803e+35	8.8e-07
9745	diHPCARP_Ic.tmpmtmtmu	5.411e+44	12.23	12.23	6.701e+35	8.67e-07
9746	diHPCARP_Ic.mtttmtptmu	4.158e+44	12.13	12.13	6.053e+35	7.83e-07
9747	diHPCARP_Ic.tmpmptmnu	8.843e+43	11.21	11.21	6.042e+35	7.82e-07
9748	diHPCARP_Ic.ppttmmmmu	1.295e+44	11.44	11.44	6.041e+35	7.81e-07
9749	diHPCARP_Ic.tmpptptmu	6.028e+44	12.37	12.37	5.915e+35	7.65e-07
9750	diHPCARP_Ic.tpmmpmmpu	5.055e+43	10.91	10.91	5.671e+35	7.34e-07
9751	diHPCARP_Ic.mpttmmmmu	4.968e+44	12.28	12.28	5.612e+35	7.26e-07
9752	diHPCARP_Ic.tppmpmtmu	4.124e+44	12.17	12.17	5.580e+35	7.22e-07
9753	diHPCARP_Ic.mttptmtmu	8.171e+44	12.60	12.60	5.375e+35	6.95e-07
9754	diHPCARP_Ic.tmmptmptu	6.687e+44	12.50	12.50	5.233e+35	6.77e-07
9755	diHPCARP_Ic.mpmppmtmu	4.377e+43	10.91	10.91	4.905e+35	6.35e-07
9756	diHPCARP_Ic.pmpmptmnu	6.607e+43	11.16	11.16	4.873e+35	6.3e-07
9757	diHPCARP_Ic.pppmmpmmpu	3.210e+43	10.74	10.74	4.787e+35	6.19e-07
9758	diHPCARP_Ic.ttmmmmpmu	2.201e+43	10.52	10.52	4.755e+35	6.15e-07
9759	diHPCARP_Ic.ttpmmmpmu	7.275e+43	11.24	11.24	4.725e+35	6.11e-07
9760	diHPCARP_Ic.tptppmpu	1.474e+44	11.67	11.67	4.639e+35	6e-07
9761	diHPCARP_Ic.mtptmptpu	1.691e+44	11.76	11.76	4.604e+35	5.96e-07
9762	diHPCARP_Ic.mptppmmpmu	9.902e+43	11.46	11.46	4.417e+35	5.71e-07
9763	diHPCARP_Ic.ppttmmmmu	4.875e+43	11.08	11.08	4.128e+35	5.34e-07
9764	diHPCARP_Ic.mtmptmtmu	9.015e+43	11.46	11.46	4.059e+35	5.25e-07
9765	diHPCARP_Ic.pptpmmmmu	8.556e+43	11.43	11.43	4.007e+35	5.18e-07
9766	diHPCARP_Ic.mttmmtmnu	2.241e+44	12.06	12.06	3.683e+35	4.76e-07
9767	diHPCARP_Ic.ppmppmmpmu	2.785e+43	10.84	10.84	3.529e+35	4.57e-07
9768	diHPCARP_Ic.tpmmpmtmu	5.157e+43	11.21	11.21	3.526e+35	4.56e-07

9769	diHPCARP_Ic.ttptpoptpu	3.153e+44	12.31	12.31	3.394e+35	4.39e-07
9770	diHPCARP_Ic.mpptpoptpu	1.185e+44	11.73	11.73	3.355e+35	4.34e-07
9771	diHPCARP_Ic.mpppmmmmu	1.741e+44	11.99	11.99	3.227e+35	4.17e-07
9772	diHPCARP_Ic.mttmtmtmu	8.318e+44	12.94	12.94	3.090e+35	4e-07
9773	diHPCARP_Ic.mptmptmtmu	8.364e+43	11.64	11.64	2.790e+35	3.61e-07
9774	diHPCARP_Ic.pppttpptpu	1.315e+44	11.92	11.92	2.712e+35	3.51e-07
9775	diHPCARP_Ic.mptmtmtmu	1.096e+45	13.20	13.20	2.659e+35	3.44e-07
9776	diHPCARP_Ic.mpttpmtpu	3.936e+44	12.62	12.62	2.525e+35	3.27e-07
9777	diHPCARP_Ic.tmmmpmtpu	1.463e+44	12.10	12.10	2.233e+35	2.89e-07
9778	diHPCARP_Ic.tpttpmmmu	1.283e+44	12.03	12.03	2.216e+35	2.87e-07
9779	diHPCARP_Ic.tptppmmmu	5.692e+44	12.93	12.93	2.156e+35	2.79e-07
9780	diHPCARP_Ic.pmpmtmmmu	2.597e+44	12.47	12.47	2.140e+35	2.77e-07
9781	diHPCARP_Ic.mpmtmttpu	3.865e+44	12.72	12.72	2.100e+35	2.72e-07
9782	diHPCARP_Ic.mttmtmtpu	4.169e+44	12.79	12.79	2.005e+35	2.59e-07
9783	diHPCARP_Ic.tmmmpmmmu	1.903e+44	12.33	12.33	1.990e+35	2.57e-07
9784	diHPCARP_Ic.mtptmtmtmu	2.145e+44	12.41	12.41	1.944e+35	2.51e-07
9785	diHPCARP_Ic.tmmtpmmmu	3.137e+44	12.72	12.72	1.690e+35	2.19e-07
9786	diHPCARP_Ic.mppmmmmmu	2.423e+43	11.21	11.21	1.660e+35	2.15e-07
9787	diHPCARP_Ic.pmmppmtmu	7.678e+43	11.90	11.90	1.648e+35	2.13e-07
9788	diHPCARP_Ic.tppmmppmu	1.178e+44	12.16	12.16	1.638e+35	2.12e-07
9789	diHPCARP_Ic.ttpmptmtmu	1.309e+44	12.25	12.25	1.562e+35	2.02e-07
9790	diHPCARP_Ic.tpttpmppu	4.773e+44	13.04	13.04	1.519e+35	1.96e-07
9791	diHPCARP_Ic.mppmptmtmu	2.823e+43	11.36	11.36	1.494e+35	1.93e-07
9792	diHPCARP_Ic.mtppmmptpu	5.942e+43	11.81	11.81	1.476e+35	1.91e-07
9793	diHPCARP_Ic.mppmpmtmu	7.897e+43	11.99	11.99	1.446e+35	1.87e-07
9794	diHPCARP_Ic.mtppmmmtmu	1.987e+44	12.60	12.60	1.314e+35	1.7e-07
9795	diHPCARP_Ic.mtttmmmu	4.691e+44	13.12	13.12	1.290e+35	1.67e-07
9796	diHPCARP_Ic.tpttpmtmu	1.991e+44	12.63	12.63	1.250e+35	1.62e-07
9797	diHPCARP_Ic.mtppmptpu	7.371e+43	12.05	12.05	1.225e+35	1.58e-07
9798	diHPCARP_Ic.mppmmmmppu	6.623e+43	11.99	11.99	1.215e+35	1.57e-07
9799	diHPCARP_Ic.mpttpptmu	1.675e+44	12.61	12.61	1.082e+35	1.4e-07
9800	diHPCARP_Ic.tptppmmmu	1.114e+44	12.39	12.39	1.052e+35	1.36e-07
9801	diHPCARP_Ic.tppmptmtmu	9.492e+43	12.32	12.32	1.006e+35	1.3e-07
9802	diHPCARP_Ic.pppmmmmmu	1.850e+43	11.35	11.35	9.971e+34	1.29e-07
9803	diHPCARP_Ic.mpptpmmmu	4.823e+43	11.95	11.95	9.433e+34	1.22e-07
9804	diHPCARP_Ic.pppmmmmmu	4.365e+43	12.08	12.08	6.933e+34	8.97e-08
9805	diHPCARP_Ic.pppmmmmmu	1.926e+44	12.97	12.97	6.870e+34	8.89e-08
9806	diHPCARP_Ic.mttmtmtpu	3.184e+44	13.31	13.31	6.461e+34	8.36e-08
9807	diHPCARP_Ic.mtmtmtmtmu	1.101e+45	14.06	14.06	6.333e+34	8.19e-08
9808	diHPCARP_Ic.mppmtmmppu	4.828e+43	12.22	12.22	6.030e+34	7.8e-08
9809	diHPCARP_Ic.pppmmmmmu	2.799e+43	11.90	11.90	5.970e+34	7.72e-08
9810	diHPCARP_Ic.mppmmmttpu	1.455e+44	12.91	12.91	5.779e+34	7.48e-08
9811	diHPCARP_Ic.mppmmmtmtmu	4.056e+44	13.55	13.55	5.487e+34	7.1e-08
9812	diHPCARP_Ic.mppmmmmmu	3.046e+43	12.01	12.01	5.438e+34	7.03e-08
9813	diHPCARP_Ic.mppmmmtmtmu	2.316e+44	13.22	13.22	5.399e+34	6.98e-08
9814	diHPCARP_Ic.mppmmmtmtmu	4.700e+43	12.27	12.27	5.395e+34	6.98e-08
9815	diHPCARP_Ic.mtptmtmtmu	5.180e+44	13.84	13.84	4.304e+34	5.57e-08
9816	diHPCARP_Ic.mppmtmmmu	1.506e+44	13.16	13.16	3.919e+34	5.07e-08
9817	diHPCARP_Ic.mppmmmmppu	8.013e+43	12.83	12.83	3.616e+34	4.68e-08
9818	diHPCARP_Ic.mppmptmppu	1.439e+44	13.28	13.28	3.051e+34	3.95e-08
9819	diHPCARP_Ic.mtppmptpu	1.500e+44	13.35	13.35	2.802e+34	3.62e-08
9820	diHPCARP_Ic.mppmmmttpu	4.450e+43	12.73	12.73	2.359e+34	3.05e-08
9821	diHPCARP_Ic.mppmptmtmu	5.362e+44	14.25	14.25	2.219e+34	2.87e-08
9822	diHPCARP_Ic.tppppmmmu	1.556e+44	13.66	13.66	1.729e+34	2.24e-08
9823	diHPCARP_Ic.ttpmppmmmu	8.987e+43	13.38	13.38	1.599e+34	2.07e-08
9824	diHPCARP_Ic.ttpmtmmmu	3.889e+44	14.34	14.34	1.400e+34	1.81e-08
9825	diHPCARP_Ic.tpptpmmmu	2.720e+44	14.15	14.15	1.340e+34	1.73e-08
9826	diHPCARP_Ic.mppmptmmtmu	1.444e+44	14.01	14.01	9.045e+33	1.17e-08
9827	diHPCARP_Ic.tppmptmtmu	5.361e+44	14.79	14.79	8.949e+33	1.16e-08
9828	diHPCARP_Ic.tppmmmmmu	9.883e+43	13.81	13.81	8.539e+33	1.1e-08
9829	diHPCARP_Ic.mppmmmmmu	2.679e+43	13.20	13.20	6.498e+33	8.41e-09
9830	diHPCARP_Ic.mptppoptpu	1.755e+44	14.37	14.37	5.979e+33	7.73e-09
9831	diHPCARP_Ic.pppmppmppu	4.561e+43	13.59	13.59	5.709e+33	7.39e-09
9832	diHPCARP_Ic.mppmmmmmu	1.031e+44	14.19	14.19	4.774e+33	6.18e-09
9833	diHPCARP_Ic.mppmmtmmmu	3.531e+44	14.95	14.95	4.542e+33	5.88e-09
9834	diHPCARP_Ic.mtppmmtmtmu	2.105e+44	14.67	14.67	4.344e+33	5.62e-09
9835	diHPCARP_Ic.tppmptmppu	2.052e+44	14.78	14.78	3.519e+33	4.55e-09
9836	diHPCARP_Ic.tppmppmmmu	7.591e+43	14.31	14.31	2.845e+33	3.68e-09
9837	diHPCARP_Ic.mppmmmmmu	1.037e+44	14.51	14.51	2.768e+33	3.58e-09
9838	diHPCARP_Ic.mtppmptmtmu	1.508e+44	15.41	15.41	8.932e+32	1.16e-09
9839	diHPCARP_Ic.mtppmptmtmu	7.621e+43	15.19	15.19	6.579e+32	8.51e-10
9840	Total				7.730e+43	100

9841
9842
9843
9844 1,4-aldehyde-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-
9845 Ia)
9846 =====
9847 =
9848
9849 Population analysis at 300K. Vibrational scaling: 0.971.
9850 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
9851 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
9852 %: contribution to the population (with current data set assumed 100%)
9853 Compound Qtot Erel Erel2 n*Q*MB %
9854 -----
9855 TS.diHPCARP_I.14aldHshift.ttmmmpu 4.227e+42 0.00 0.00 4.227e+42 56.8
9856 TS.diHPCARP_I.14aldHshift.tppppmu 1.057e+43 1.36 1.36 1.085e+42 14.6
9857 TS.diHPCARP_I.14aldHshift.tptmmpu 5.632e+42 1.50 1.50 4.576e+41 6.15
9858 TS.diHPCARP_I.14aldHshift.mmpmpmu 6.175e+42 1.99 1.99 2.199e+41 2.95
9859 TS.diHPCARP_I.14aldHshift.tpptpmu 1.078e+43 2.45 2.45 1.764e+41 2.37
9860 TS.diHPCARP_I.14aldHshift.mtmmpmu 8.907e+42 2.35 2.35 1.733e+41 2.33
9861 TS.diHPCARP_I.14aldHshift.tmmppmu 1.564e+43 2.80 2.80 1.416e+41 1.9
9862 TS.diHPCARP_I.14aldHshift.mppppmu 5.248e+43 3.59 3.59 1.265e+41 1.7
9863 TS.diHPCARP_I.14aldHshift.tpmmpmu 1.435e+43 3.01 3.01 9.141e+40 1.23
9864 TS.diHPCARP_I.14aldHshift.tmmmpmu 1.504e+43 3.29 3.29 6.016e+40 0.808
9865 TS.diHPCARP_I.14aldHshift.tppppmu 1.002e+43 3.08 3.08 5.730e+40 0.77
9866 TS.diHPCARP_I.14aldHshift.ttpmmpu 1.423e+43 3.42 3.42 4.585e+40 0.616
9867 TS.diHPCARP_I.14aldHshift.mmmmpmu 7.872e+42 3.20 3.20 3.677e+40 0.494
9868 TS.diHPCARP_I.14aldHshift.tpptpmu 1.800e+43 3.71 3.71 3.551e+40 0.477
9869 TS.diHPCARP_I.14aldHshift.mmpmpmu 7.807e+42 3.26 3.26 3.311e+40 0.445
9870 TS.diHPCARP_I.14aldHshift.ttmmmmu 1.333e+43 3.59 3.59 3.242e+40 0.435
9871 TS.diHPCARP_I.14aldHshift.tppppmu 2.630e+43 4.04 4.04 2.998e+40 0.403
9872 TS.diHPCARP_I.14aldHshift.ttmppmu 2.133e+43 3.98 3.98 2.698e+40 0.362
9873 TS.diHPCARP_I.14aldHshift.tpmmpmu 1.153e+43 3.80 3.80 1.956e+40 0.263
9874 TS.diHPCARP_I.14aldHshift.pppppmu 6.638e+42 3.49 3.49 1.903e+40 0.256
9875 TS.diHPCARP_I.14aldHshift.ttmtpmu 7.310e+43 4.96 4.96 1.791e+40 0.241
9876 TS.diHPCARP_I.14aldHshift.mtmtpmu 2.073e+43 4.26 4.26 1.633e+40 0.219
9877 TS.diHPCARP_I.14aldHshift.tpmmpmu 6.358e+42 3.60 3.60 1.522e+40 0.204
9878 TS.diHPCARP_I.14aldHshift.mppppmu 3.310e+43 4.59 4.59 1.503e+40 0.202
9879 TS.diHPCARP_I.14aldHshift.ttmtpmu 2.743e+43 4.55 4.55 1.325e+40 0.178
9880 TS.diHPCARP_I.14aldHshift.tmmmtmu 8.290e+42 3.86 3.86 1.280e+40 0.172
9881 TS.diHPCARP_I.14aldHshift.pmtppmu 1.080e+43 4.03 4.03 1.251e+40 0.168
9882 TS.diHPCARP_I.14aldHshift.ttmppmu 2.029e+43 4.51 4.51 1.055e+40 0.142
9883 TS.diHPCARP_I.14aldHshift.mppptmu 1.162e+43 4.21 4.21 9.986e+39 0.134
9884 TS.diHPCARP_I.14aldHshift.mtmmpmu 2.451e+43 4.66 4.66 9.860e+39 0.132
9885 TS.diHPCARP_I.14aldHshift.tpttmtmu 1.481e+43 4.42 4.42 8.964e+39 0.12
9886 TS.diHPCARP_I.14aldHshift.tpptmtmu 7.963e+43 5.46 5.46 8.344e+39 0.112
9887 TS.diHPCARP_I.14aldHshift.mptmmpu 8.704e+42 4.16 4.16 8.162e+39 0.11
9888 TS.diHPCARP_I.14aldHshift.mtpmmpu 2.486e+43 4.79 4.79 8.003e+39 0.108
9889 TS.diHPCARP_I.14aldHshift.mtppppu 1.798e+44 5.99 5.99 7.720e+39 0.104
9890 TS.diHPCARP_I.14aldHshift.ttmmtmu 6.104e+43 5.35 5.35 7.694e+39 0.103
9891 TS.diHPCARP_I.14aldHshift.mpmmpmu 1.084e+43 4.39 4.39 6.834e+39 0.0918
9892 TS.diHPCARP_I.14aldHshift.tppppmu 1.903e+43 4.75 4.75 6.570e+39 0.0883
9893 TS.diHPCARP_I.14aldHshift.tmpmtmu 6.956e+42 4.20 4.20 6.038e+39 0.0811
9894 TS.diHPCARP_I.14aldHshift.tmmppmu 1.791e+43 4.77 4.77 6.014e+39 0.0808
9895 TS.diHPCARP_I.14aldHshift.mppmtmu 5.485e+43 5.46 5.46 5.820e+39 0.0782
9896 TS.diHPCARP_I.14aldHshift.pmtmmpu 1.919e+43 4.83 4.83 5.788e+39 0.0777
9897 TS.diHPCARP_I.14aldHshift.tptmtmu 2.699e+43 5.07 5.07 5.489e+39 0.0737
9898 TS.diHPCARP_I.14aldHshift.pmttmtmu 2.076e+43 4.93 4.93 5.322e+39 0.0715
9899 TS.diHPCARP_I.14aldHshift.mtmpppu 2.250e+44 6.42 6.42 4.700e+39 0.0631
9900 TS.diHPCARP_I.14aldHshift.mtmtpmu 6.135e+43 5.69 5.69 4.417e+39 0.0593
9901 TS.diHPCARP_I.14aldHshift.mpttmtmu 3.423e+43 5.37 5.37 4.158e+39 0.0559
9902 TS.diHPCARP_I.14aldHshift.ptmmmpu 1.686e+43 4.95 4.95 4.145e+39 0.0557
9903 TS.diHPCARP_I.14aldHshift.ttmmpmu 1.350e+43 4.92 4.92 3.543e+39 0.0476
9904 TS.diHPCARP_I.14aldHshift.mptmmpu 8.453e+42 4.71 4.71 3.145e+39 0.0422
9905 TS.diHPCARP_I.14aldHshift.mppmptmu 8.106e+43 6.06 6.06 3.128e+39 0.042
9906 TS.diHPCARP_I.14aldHshift.mtmmtmu 4.439e+43 5.71 5.71 3.055e+39 0.041
9907 TS.diHPCARP_I.14aldHshift.mtpmmpu 2.486e+43 5.40 5.40 2.897e+39 0.0389
9908 TS.diHPCARP_I.14aldHshift.mmpmtpmu 1.404e+43 5.09 5.09 2.746e+39 0.0369
9909 TS.diHPCARP_I.14aldHshift.mppppmu 3.232e+43 5.59 5.59 2.738e+39 0.0368
9910 TS.diHPCARP_I.14aldHshift.pppppmu 1.922e+43 5.30 5.30 2.655e+39 0.0357
9911 TS.diHPCARP_I.14aldHshift.mtptmtmu 4.067e+43 5.75 5.75 2.642e+39 0.0355
9912 TS.diHPCARP_I.14aldHshift.ttpmtmu 2.154e+43 5.40 5.40 2.521e+39 0.0339

9913	TS.diHPCARP_I.14aldHshift.mtptpmu	1.023e+44	6.34	6.34	2.461e+39	0.0331
9914	TS.diHPCARP_I.14aldHshift.mpmmttu	1.118e+43	5.06	5.06	2.318e+39	0.0311
9915	TS.diHPCARP_I.14aldHshift.pmtttmpu	5.963e+43	6.07	6.07	2.243e+39	0.0301
9916	TS.diHPCARP_I.14aldHshift.tpmmttpu	2.996e+43	5.68	5.68	2.181e+39	0.0293
9917	TS.diHPCARP_I.14aldHshift.mpmtpmu	1.851e+43	5.42	5.42	2.090e+39	0.0281
9918	TS.diHPCARP_I.14aldHshift.ptmmmttu	2.774e+43	5.71	5.71	1.929e+39	0.0259
9919	TS.diHPCARP_I.14aldHshift.tttmttu	5.083e+44	7.45	7.45	1.908e+39	0.0256
9920	TS.diHPCARP_I.14aldHshift.mpmmtmpu	1.014e+44	6.49	6.49	1.896e+39	0.0255
9921	TS.diHPCARP_I.14aldHshift.tptttmpu	5.300e+43	6.12	6.12	1.834e+39	0.0246
9922	TS.diHPCARP_I.14aldHshift.mmmmpmu	9.548e+42	5.13	5.13	1.753e+39	0.0235
9923	TS.diHPCARP_I.14aldHshift.mmpptmu	3.924e+43	6.02	6.02	1.612e+39	0.0217
9924	TS.diHPCARP_I.14aldHshift.mpmmtmu	1.078e+44	6.63	6.63	1.608e+39	0.0216
9925	TS.diHPCARP_I.14aldHshift.tptmpmu	1.834e+43	5.57	5.57	1.600e+39	0.0215
9926	TS.diHPCARP_I.14aldHshift.ppmmtmu	9.341e+42	5.22	5.22	1.470e+39	0.0197
9927	TS.diHPCARP_I.14aldHshift.tmmmttu	1.133e+44	6.79	6.79	1.280e+39	0.0172
9928	TS.diHPCARP_I.14aldHshift.tpmmttu	1.135e+43	5.43	5.43	1.250e+39	0.0168
9929	TS.diHPCARP_I.14aldHshift.ttmmttu	2.532e+44	7.30	7.30	1.209e+39	0.0162
9930	TS.diHPCARP_I.14aldHshift.mmpmtmu	1.406e+43	5.59	5.59	1.199e+39	0.0161
9931	TS.diHPCARP_I.14aldHshift.mpttppu	1.896e+43	5.78	5.78	1.171e+39	0.0157
9932	TS.diHPCARP_I.14aldHshift.tpmmttu	2.111e+43	5.86	5.86	1.133e+39	0.0152
9933	TS.diHPCARP_I.14aldHshift.mmpmttu	3.022e+43	6.08	6.08	1.132e+39	0.0152
9934	TS.diHPCARP_I.14aldHshift.pptttmpu	1.390e+43	5.62	5.62	1.127e+39	0.0151
9935	TS.diHPCARP_I.14aldHshift.tptmttu	2.607e+43	5.99	5.99	1.121e+39	0.0151
9936	TS.diHPCARP_I.14aldHshift.tpmmttu	3.055e+43	6.10	6.10	1.092e+39	0.0147
9937	TS.diHPCARP_I.14aldHshift.pmtmmmu	2.554e+43	6.00	6.00	1.091e+39	0.0147
9938	TS.diHPCARP_I.14aldHshift.ttmmttu	9.866e+43	6.81	6.81	1.077e+39	0.0145
9939	TS.diHPCARP_I.14aldHshift.tptmtpu	2.471e+43	6.00	6.00	1.058e+39	0.0142
9940	TS.diHPCARP_I.14aldHshift.ptmtmpu	2.172e+43	5.93	5.93	1.043e+39	0.014
9941	TS.diHPCARP_I.14aldHshift.mmmpppu	5.549e+43	6.49	6.49	1.031e+39	0.0138
9942	TS.diHPCARP_I.14aldHshift.tptttmpu	1.020e+44	6.91	6.91	9.513e+38	0.0128
9943	TS.diHPCARP_I.14aldHshift.ptmmpmu	3.433e+43	6.29	6.29	8.964e+38	0.012
9944	TS.diHPCARP_I.14aldHshift.tppmpmu	9.541e+42	5.54	5.54	8.722e+38	0.0117
9945	TS.diHPCARP_I.14aldHshift.tpmpppu	4.539e+43	6.48	6.48	8.652e+38	0.0116
9946	TS.diHPCARP_I.14aldHshift.mmpptmu	5.030e+43	6.54	6.54	8.640e+38	0.0116
9947	TS.diHPCARP_I.14aldHshift.pmtmmmu	5.930e+43	6.70	6.70	7.832e+38	0.0105
9948	TS.diHPCARP_I.14aldHshift.ttmmpmu	2.747e+43	6.24	6.24	7.819e+38	0.0105
9949	TS.diHPCARP_I.14aldHshift.tpppppu	3.482e+43	6.38	6.38	7.804e+38	0.0105
9950	TS.diHPCARP_I.14aldHshift.mmpmmmu	3.374e+43	6.39	6.39	7.476e+38	0.01
9951	TS.diHPCARP_I.14aldHshift.ttmmttu	8.330e+43	6.95	6.95	7.151e+38	0.0096
9952	TS.diHPCARP_I.14aldHshift.ptptmpu	8.605e+43	6.99	6.99	6.992e+38	0.00939
9953	TS.diHPCARP_I.14aldHshift.tpmmttu	3.744e+43	6.50	6.50	6.890e+38	0.00926
9954	TS.diHPCARP_I.14aldHshift.tpmmttu	1.135e+44	7.17	7.17	6.837e+38	0.00918
9955	TS.diHPCARP_I.14aldHshift.ttpmmmu	7.646e+43	6.93	6.93	6.801e+38	0.00914
9956	TS.diHPCARP_I.14aldHshift.pmmmttu	1.819e+43	6.08	6.08	6.793e+38	0.00912
9957	TS.diHPCARP_I.14aldHshift.tpmpppu	5.465e+42	5.39	5.39	6.523e+38	0.00876
9958	TS.diHPCARP_I.14aldHshift.mppmttu	7.588e+43	6.97	6.97	6.394e+38	0.00859
9959	TS.diHPCARP_I.14aldHshift.pmpmmmu	1.501e+43	6.07	6.07	5.681e+38	0.00763
9960	TS.diHPCARP_I.14aldHshift.mptttmpu	2.404e+43	6.36	6.36	5.589e+38	0.00751
9961	TS.diHPCARP_I.14aldHshift.ttmmttu	8.926e+43	7.15	7.15	5.484e+38	0.00737
9962	TS.diHPCARP_I.14aldHshift.mppmpmu	6.909e+42	5.64	5.64	5.362e+38	0.0072
9963	TS.diHPCARP_I.14aldHshift.ppptppu	3.215e+43	6.57	6.57	5.261e+38	0.00707
9964	TS.diHPCARP_I.14aldHshift.tmtptmu	1.148e+44	7.36	7.36	4.963e+38	0.00667
9965	TS.diHPCARP_I.14aldHshift.ttptmpu	6.849e+43	7.12	7.12	4.485e+38	0.00602
9966	TS.diHPCARP_I.14aldHshift.pptttmpu	1.424e+43	6.20	6.20	4.302e+38	0.00578
9967	TS.diHPCARP_I.14aldHshift.ptmtmmu	5.219e+43	6.99	6.99	4.227e+38	0.00568
9968	TS.diHPCARP_I.14aldHshift.ppptmmu	3.152e+43	6.71	6.71	4.051e+38	0.00544
9969	TS.diHPCARP_I.14aldHshift.pmtttmpu	8.052e+43	7.29	7.29	3.914e+38	0.00526
9970	TS.diHPCARP_I.14aldHshift.ttmmttu	8.561e+43	7.44	7.44	3.232e+38	0.00434
9971	TS.diHPCARP_I.14aldHshift.ptmtpmu	4.576e+43	7.08	7.08	3.173e+38	0.00426
9972	TS.diHPCARP_I.14aldHshift.ttmmttu	7.654e+43	7.39	7.39	3.152e+38	0.00423
9973	TS.diHPCARP_I.14aldHshift.ptptmpu	3.260e+43	6.88	6.88	3.150e+38	0.00423
9974	TS.diHPCARP_I.14aldHshift.mpppttu	1.622e+43	6.52	6.52	2.878e+38	0.00387
9975	TS.diHPCARP_I.14aldHshift.ttptmpu	4.723e+43	7.17	7.17	2.837e+38	0.00381
9976	TS.diHPCARP_I.14aldHshift.pmmmttu	1.692e+43	6.58	6.58	2.711e+38	0.00364
9977	TS.diHPCARP_I.14aldHshift.tptptmu	1.573e+44	7.93	7.93	2.635e+38	0.00354
9978	TS.diHPCARP_I.14aldHshift.tpmtpmu	2.318e+43	6.81	6.81	2.534e+38	0.0034
9979	TS.diHPCARP_I.14aldHshift.mtpptmu	2.243e+44	8.17	8.17	2.494e+38	0.00335
9980	TS.diHPCARP_I.14aldHshift.tmtptmu	2.578e+44	8.27	8.27	2.444e+38	0.00328
9981	TS.diHPCARP_I.14aldHshift.tpmmpmu	6.095e+42	6.04	6.04	2.411e+38	0.00324
9982	TS.diHPCARP_I.14aldHshift.ttpmpmu	3.988e+43	7.23	7.23	2.158e+38	0.0029
9983	TS.diHPCARP_I.14aldHshift.mtmmttu	7.899e+43	7.69	7.69	1.973e+38	0.00265
9984	TS.diHPCARP_I.14aldHshift.mpmmttu	8.733e+43	7.76	7.76	1.953e+38	0.00262

9985	TS.diHPCARP_I.14aldHshift.mtpptpu	2.013e+44	8.30	8.30	1.804e+38	0.00242
9986	TS.diHPCARP_I.14aldHshift.ptppppmu	2.875e+43	7.15	7.15	1.770e+38	0.00238
9987	TS.diHPCARP_I.14aldHshift.tmmpppu	7.769e+43	7.77	7.77	1.699e+38	0.00228
9988	TS.diHPCARP_I.14aldHshift.tppptmu	6.798e+43	7.69	7.69	1.698e+38	0.00228
9989	TS.diHPCARP_I.14aldHshift.pmtmtmu	1.914e+43	6.94	6.94	1.694e+38	0.00228
9990	TS.diHPCARP_I.14aldHshift.mtmmtmu	6.656e+43	7.69	7.69	1.662e+38	0.00223
9991	TS.diHPCARP_I.14aldHshift.ttpmtpu	1.110e+44	8.02	8.02	1.601e+38	0.00215
9992	TS.diHPCARP_I.14aldHshift.pmtttmu	7.086e+43	7.77	7.77	1.538e+38	0.00207
9993	TS.diHPCARP_I.14aldHshift.mtmptpu	2.236e+44	8.46	8.46	1.529e+38	0.00205
9994	TS.diHPCARP_I.14aldHshift.pptppmu	8.442e+42	6.53	6.53	1.471e+38	0.00198
9995	TS.diHPCARP_I.14aldHshift.pmmpppu	8.147e+43	7.89	7.89	1.462e+38	0.00196
9996	TS.diHPCARP_I.14aldHshift.mtpppmu	9.598e+43	8.00	8.00	1.422e+38	0.00191
9997	TS.diHPCARP_I.14aldHshift.tmmtpmu	5.539e+43	7.68	7.68	1.415e+38	0.0019
9998	TS.diHPCARP_I.14aldHshift.pmtmppu	2.571e+43	7.26	7.26	1.319e+38	0.00177
9999	TS.diHPCARP_I.14aldHshift.mmmtpmu	2.467e+43	7.24	7.24	1.309e+38	0.00176
10000	TS.diHPCARP_I.14aldHshift.tmmmtmu	2.019e+44	8.53	8.53	1.228e+38	0.00165
10001	TS.diHPCARP_I.14aldHshift.pmmtpmu	2.866e+43	7.40	7.40	1.164e+38	0.00156
10002	TS.diHPCARP_I.14aldHshift.mpppmu	2.840e+43	7.40	7.40	1.148e+38	0.00154
10003	TS.diHPCARP_I.14aldHshift.pmmptpu	1.974e+43	7.19	7.19	1.138e+38	0.00153
10004	TS.diHPCARP_I.14aldHshift.ptppmmu	7.773e+43	8.01	8.01	1.127e+38	0.00151
10005	TS.diHPCARP_I.14aldHshift.mmmmtmu	1.049e+44	8.21	8.21	1.098e+38	0.00147
10006	TS.diHPCARP_I.14aldHshift.pmmmtmu	1.445e+44	8.42	8.42	1.061e+38	0.00143
10007	TS.diHPCARP_I.14aldHshift.pmmmmu	3.918e+43	7.65	7.65	1.056e+38	0.00142
10008	TS.diHPCARP_I.14aldHshift.tmmtpmu	1.836e+44	8.57	8.57	1.051e+38	0.00141
10009	TS.diHPCARP_I.14aldHshift.tmmmtmu	1.242e+44	8.39	8.39	9.526e+37	0.00128
10010	TS.diHPCARP_I.14aldHshift.tmppppu	5.745e+43	7.94	7.94	9.392e+37	0.00126
10011	TS.diHPCARP_I.14aldHshift.tmpptpu	1.684e+43	7.21	7.21	9.363e+37	0.00126
10012	TS.diHPCARP_I.14aldHshift.tmmmpmu	4.703e+43	7.83	7.83	9.326e+37	0.00125
10013	TS.diHPCARP_I.14aldHshift.tpmptpu	4.152e+43	7.77	7.77	9.031e+37	0.00121
10014	TS.diHPCARP_I.14aldHshift.tpmmtmu	1.842e+44	8.67	8.67	8.851e+37	0.00119
10015	TS.diHPCARP_I.14aldHshift.mptmtmu	2.380e+43	7.45	7.45	8.836e+37	0.00119
10016	TS.diHPCARP_I.14aldHshift.pmpmtmu	4.818e+43	7.88	7.88	8.794e+37	0.00118
10017	TS.diHPCARP_I.14aldHshift.pmtttpu	7.695e+43	8.19	8.19	8.289e+37	0.00111
10018	TS.diHPCARP_I.14aldHshift.ppmmtmu	4.484e+43	7.88	7.88	8.127e+37	0.00109
10019	TS.diHPCARP_I.14aldHshift.mmpmtmu	4.496e+43	7.93	7.93	7.548e+37	0.00101
10020	TS.diHPCARP_I.14aldHshift.mptttmu	8.356e+43	8.32	8.32	7.296e+37	0.00098
10021	TS.diHPCARP_I.14aldHshift.mtmppmu	1.058e+44	8.53	8.53	6.411e+37	0.000861
10022	TS.diHPCARP_I.14aldHshift.mptttpu	1.485e+44	8.75	8.75	6.319e+37	0.000849
10023	TS.diHPCARP_I.14aldHshift.mmmptmu	6.087e+43	8.25	8.25	5.975e+37	0.000803
10024	TS.diHPCARP_I.14aldHshift.mmmptpu	8.236e+43	8.43	8.43	5.921e+37	0.000795
10025	TS.diHPCARP_I.14aldHshift.pppttpu	4.275e+43	8.06	8.06	5.733e+37	0.00077
10026	TS.diHPCARP_I.14aldHshift.pttmtmu	2.343e+43	7.70	7.70	5.728e+37	0.000769
10027	TS.diHPCARP_I.14aldHshift.pmttppu	6.423e+43	8.31	8.31	5.670e+37	0.000762
10028	TS.diHPCARP_I.14aldHshift.tpppmu	1.047e+43	7.23	7.23	5.641e+37	0.000758
10029	TS.diHPCARP_I.14aldHshift.pmtptmu	4.809e+43	8.16	8.16	5.474e+37	0.000735
10030	TS.diHPCARP_I.14aldHshift.mtpttmu	1.021e+44	8.61	8.61	5.430e+37	0.000729
10031	TS.diHPCARP_I.14aldHshift.mptmmu	9.983e+42	7.24	7.24	5.285e+37	0.00071
10032	TS.diHPCARP_I.14aldHshift.pptmmu	1.876e+43	7.62	7.62	5.249e+37	0.000705
10033	TS.diHPCARP_I.14aldHshift.pmpmtmu	6.889e+43	8.40	8.40	5.208e+37	0.0007
10034	TS.diHPCARP_I.14aldHshift.mppptmu	9.272e+43	8.59	8.59	5.093e+37	0.000684
10035	TS.diHPCARP_I.14aldHshift.pmmtpmu	7.123e+43	8.46	8.46	4.913e+37	0.00066
10036	TS.diHPCARP_I.14aldHshift.ptmmtmu	6.877e+43	8.45	8.45	4.804e+37	0.000645
10037	TS.diHPCARP_I.14aldHshift.ptmmtmu	6.220e+43	8.46	8.46	4.261e+37	0.000572
10038	TS.diHPCARP_I.14aldHshift.mppttmu	9.770e+43	8.74	8.74	4.210e+37	0.000566
10039	TS.diHPCARP_I.14aldHshift.ttmpppu	7.649e+43	8.59	8.59	4.203e+37	0.000565
10040	TS.diHPCARP_I.14aldHshift.ptpmtmu	1.319e+44	8.93	8.93	4.086e+37	0.000549
10041	TS.diHPCARP_I.14aldHshift.tpppppu	5.506e+43	8.42	8.42	4.069e+37	0.000547
10042	TS.diHPCARP_I.14aldHshift.tmmptmu	1.669e+44	9.08	9.08	4.064e+37	0.000546
10043	TS.diHPCARP_I.14aldHshift.mmpptmu	7.050e+43	8.58	8.58	3.989e+37	0.000536
10044	TS.diHPCARP_I.14aldHshift.ttmppmu	4.421e+43	8.30	8.30	3.974e+37	0.000534
10045	TS.diHPCARP_I.14aldHshift.ptppppu	9.451e+43	8.78	8.78	3.822e+37	0.000513
10046	TS.diHPCARP_I.14aldHshift.ptpmtmu	2.262e+43	7.98	7.98	3.455e+37	0.000464
10047	TS.diHPCARP_I.14aldHshift.ptpptmu	3.880e+43	8.32	8.32	3.366e+37	0.000452
10048	TS.diHPCARP_I.14aldHshift.mmmmtmu	3.088e+43	8.19	8.19	3.334e+37	0.000448
10049	TS.diHPCARP_I.14aldHshift.pptmtmu	1.015e+43	7.55	7.55	3.187e+37	0.000428
10050	TS.diHPCARP_I.14aldHshift.pptpptu	1.305e+44	9.09	9.09	3.103e+37	0.000417
10051	TS.diHPCARP_I.14aldHshift.pmmppmu	2.184e+43	8.06	8.06	2.938e+37	0.000395
10052	TS.diHPCARP_I.14aldHshift.pttmttu	2.092e+44	9.49	9.49	2.552e+37	0.000343
10053	TS.diHPCARP_I.14aldHshift.ttttmmu	9.576e+43	9.05	9.05	2.445e+37	0.000328
10054	TS.diHPCARP_I.14aldHshift.tppppmu	2.679e+43	8.31	8.31	2.384e+37	0.00032
10055	TS.diHPCARP_I.14aldHshift.mpmtpmu	3.684e+43	8.55	8.55	2.189e+37	0.000294
10056	TS.diHPCARP_I.14aldHshift.mtmmtmu	1.898e+44	9.53	9.53	2.166e+37	0.000291

10057	TS.diHPCARP_I.14aldHshift.mtptppu	6.302e+43	8.89	8.89	2.088e+37	0.000281
10058	TS.diHPCARP_I.14aldHshift.tmpptmu	1.079e+44	9.25	9.25	1.980e+37	0.000266
10059	TS.diHPCARP_I.14aldHshift.pttpmmu	2.942e+43	8.48	8.48	1.969e+37	0.000264
10060	TS.diHPCARP_I.14aldHshift.ptmmtpu	8.928e+43	9.14	9.14	1.955e+37	0.000263
10061	TS.diHPCARP_I.14aldHshift.pmmmtpu	3.119e+43	8.54	8.54	1.883e+37	0.000253
10062	TS.diHPCARP_I.14aldHshift.ptttmmu	6.797e+43	9.01	9.01	1.848e+37	0.000248
10063	TS.diHPCARP_I.14aldHshift.ptmttmu	9.586e+43	9.22	9.22	1.839e+37	0.000247
10064	TS.diHPCARP_I.14aldHshift.ptpmppu	4.327e+43	8.80	8.80	1.690e+37	0.000227
10065	TS.diHPCARP_I.14aldHshift.mppttmu	1.034e+44	9.32	9.32	1.666e+37	0.000224
10066	TS.diHPCARP_I.14aldHshift.ptmmppu	6.181e+42	7.67	7.67	1.597e+37	0.000215
10067	TS.diHPCARP_I.14aldHshift.pptmtmu	5.135e+43	8.97	8.97	1.489e+37	0.0002
10068	TS.diHPCARP_I.14aldHshift.ttpptmu	1.358e+44	9.59	9.59	1.409e+37	0.000189
10069	TS.diHPCARP_I.14aldHshift.mmmttmu	7.427e+43	9.23	9.23	1.400e+37	0.000188
10070	TS.diHPCARP_I.14aldHshift.mptmtpu	2.611e+43	8.61	8.61	1.388e+37	0.000187
10071	TS.diHPCARP_I.14aldHshift.mtpmtpu	1.414e+44	9.67	9.67	1.284e+37	0.000172
10072	TS.diHPCARP_I.14aldHshift.pmmttmu	1.425e+44	9.68	9.68	1.274e+37	0.000171
10073	TS.diHPCARP_I.14aldHshift.ttmptmu	1.037e+44	9.50	9.50	1.253e+37	0.000168
10074	TS.diHPCARP_I.14aldHshift.pptmttu	8.620e+43	9.41	9.41	1.205e+37	0.000162
10075	TS.diHPCARP_I.14aldHshift.mmmttmu	2.004e+44	9.92	9.92	1.194e+37	0.00016
10076	TS.diHPCARP_I.14aldHshift.mmmmtpu	4.133e+43	8.98	8.98	1.180e+37	0.000158
10077	TS.diHPCARP_I.14aldHshift.pppmmu	4.299e+43	9.01	9.01	1.177e+37	0.000158
10078	TS.diHPCARP_I.14aldHshift.pppttmu	5.172e+43	9.16	9.16	1.100e+37	0.000148
10079	TS.diHPCARP_I.14aldHshift.tpmmtmu	1.166e+44	9.67	9.67	1.056e+37	0.000142
10080	TS.diHPCARP_I.14aldHshift.ttmptpu	3.278e+44	10.31	10.31	1.016e+37	0.000137
10081	TS.diHPCARP_I.14aldHshift.tpmtpu	3.623e+43	9.05	9.05	9.297e+36	0.000125
10082	TS.diHPCARP_I.14aldHshift.mtmmtmu	6.325e+43	9.38	9.38	9.216e+36	0.000124
10083	TS.diHPCARP_I.14aldHshift.pmmttmu	2.093e+44	10.12	10.12	8.864e+36	0.000119
10084	TS.diHPCARP_I.14aldHshift.pppmtmu	3.999e+43	9.14	9.14	8.818e+36	0.000118
10085	TS.diHPCARP_I.14aldHshift.pmmtpu	9.575e+43	9.77	9.77	7.365e+36	9.89e-05
10086	TS.diHPCARP_I.14aldHshift.tmmppmu	2.537e+43	8.98	8.98	7.308e+36	9.82e-05
10087	TS.diHPCARP_I.14aldHshift.tttttmu	1.911e+44	10.21	10.21	6.931e+36	9.31e-05
10088	TS.diHPCARP_I.14aldHshift.pptmtmu	5.057e+43	9.43	9.43	6.796e+36	9.13e-05
10089	TS.diHPCARP_I.14aldHshift.tmpmmu	2.187e+43	9.06	9.06	5.486e+36	7.37e-05
10090	TS.diHPCARP_I.14aldHshift.pmmppu	2.586e+43	9.18	9.18	5.332e+36	7.16e-05
10091	TS.diHPCARP_I.14aldHshift.pptmtmu	3.587e+43	9.42	9.42	4.964e+36	6.67e-05
10092	TS.diHPCARP_I.14aldHshift.tttttmu	2.048e+44	10.55	10.55	4.200e+36	5.64e-05
10093	TS.diHPCARP_I.14aldHshift.ttpptmu	3.024e+44	10.82	10.82	3.953e+36	5.31e-05
10094	TS.diHPCARP_I.14aldHshift.ppmmtmu	1.000e+43	8.82	8.82	3.749e+36	5.04e-05
10095	TS.diHPCARP_I.14aldHshift.pptmtmu	3.993e+43	9.65	9.65	3.726e+36	5.01e-05
10096	TS.diHPCARP_I.14aldHshift.mtpmmu	1.110e+44	10.29	10.29	3.563e+36	4.79e-05
10097	TS.diHPCARP_I.14aldHshift.pptmtmu	4.415e+43	9.74	9.74	3.517e+36	4.72e-05
10098	TS.diHPCARP_I.14aldHshift.pptmpu	4.723e+42	8.42	8.42	3.472e+36	4.66e-05
10099	TS.diHPCARP_I.14aldHshift.mptmpu	1.999e+43	9.54	9.54	2.237e+36	3.01e-05
10100	TS.diHPCARP_I.14aldHshift.ptpttmu	1.587e+44	10.87	10.87	1.928e+36	2.59e-05
10101	TS.diHPCARP_I.14aldHshift.mppmtmu	2.025e+44	11.29	11.29	1.213e+36	1.63e-05
10102	TS.diHPCARP_I.14aldHshift.ptpttmu	1.870e+44	11.26	11.26	1.174e+36	1.58e-05
10103	TS.diHPCARP_I.14aldHshift.ptpptmu	1.493e+44	11.40	11.40	7.348e+35	9.87e-06
10104	TS.diHPCARP_I.14aldHshift.ppmmtmu	3.580e+43	10.56	10.56	7.285e+35	9.79e-06
10105	TS.diHPCARP_I.14aldHshift.ptppmu	5.245e+43	11.02	11.02	4.929e+35	6.62e-06
10106	TS.diHPCARP_I.14aldHshift.ppmmtmu	2.701e+43	11.07	11.07	2.338e+35	3.14e-06
10107	TS.diHPCARP_I.14aldHshift.ppmmmu	2.748e+43	11.33	11.33	1.532e+35	2.06e-06
10108	Total				7.445e+42	100

1,5-aldehyde-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-Ib)

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Note: both enantiomers (R,R and S,S) were calculated at the M06-2X/cc-pVDZ level based on a different template, to check the robustness of the conformer space search. As can be seen, most conformers are found in both enantiomers, though some higher-energy conformers are missing in either the R,R or S,S set. The impact on the rate predictions was found to be negligible. At the M06-02X/aug-cc-pVTZ level of theory, only a single set of enantiomers was calculated.

Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

10129	n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.					
10130	%: contribution to the population (with current data set assumed 100%)					
10131	Compound	Qtot	Erel	Erel2	n*Q*MB	%
10132	-----					
10133	TS.diHPCARP_Ib.15aldHshift.umdmdudd	5.637e+42	0.00	0.00	5.637e+42	17.1
10134	TS.diHPCARP_Ib.15aldHshift.dpupppduu	5.637e+42	0.00	0.00	5.619e+42	17
10135	TS.diHPCARP_Ib.15aldHshift.dmdmduuu	1.402e+43	1.10	1.10	2.228e+42	6.74
10136	TS.diHPCARP_Ib.15aldHshift.upupppudd	1.401e+43	1.10	1.10	2.227e+42	6.74
10137	TS.diHPCARP_Ib.15aldHshift.utupmuuu	8.179e+42	0.86	0.86	1.927e+42	5.83
10138	TS.diHPCARP_Ib.15aldHshift.dtdmpddd	8.179e+42	0.86	0.86	1.927e+42	5.83
10139	TS.diHPCARP_Ib.15aldHshift.dtdmmudd	7.730e+42	0.95	0.95	1.580e+42	4.78
10140	TS.diHPCARP_Ib.15aldHshift.utupppduu	7.730e+42	0.95	0.95	1.580e+42	4.78
10141	TS.diHPCARP_Ib.15aldHshift.utdmmudd	4.438e+42	1.13	1.13	6.679e+41	2.02
10142	TS.diHPCARP_Ib.15aldHshift.dtupppduu	4.438e+42	1.13	1.13	6.679e+41	2.02
10143	TS.diHPCARP_Ib.15aldHshift.dtdppduu	4.295e+42	1.16	1.16	6.169e+41	1.87
10144	TS.diHPCARP_Ib.15aldHshift.utummuudd	4.294e+42	1.16	1.16	6.168e+41	1.87
10145	TS.diHPCARP_Ib.15aldHshift.umdmtddd	4.455e+42	1.42	1.42	4.137e+41	1.25
10146	TS.diHPCARP_Ib.15aldHshift.dpuptuuu	4.455e+42	1.42	1.42	4.136e+41	1.25
10147	TS.diHPCARP_Ib.15aldHshift.dtdmmudd	6.630e+42	2.00	2.00	2.329e+41	0.705
10148	TS.diHPCARP_Ib.15aldHshift.utupppuuu	6.630e+42	2.00	2.00	2.329e+41	0.705
10149	TS.diHPCARP_Ib.15aldHshift.dmdmpduu	7.485e+42	2.09	2.09	2.257e+41	0.683
10150	TS.diHPCARP_Ib.15aldHshift.upupmudd	7.485e+42	2.09	2.09	2.257e+41	0.683
10151	TS.diHPCARP_Ib.15aldHshift.dmuupduu	1.265e+43	2.42	2.42	2.168e+41	0.656
10152	TS.diHPCARP_Ib.15aldHshift.updmmudd	1.258e+43	2.42	2.42	2.154e+41	0.652
10153	TS.diHPCARP_Ib.15aldHshift.umdmppudd	2.287e+43	2.83	2.83	2.001e+41	0.606
10154	TS.diHPCARP_Ib.15aldHshift.dpupmduu	2.287e+43	2.83	2.83	2.001e+41	0.605
10155	TS.diHPCARP_Ib.15aldHshift.dtumduuu	1.362e+43	2.53	2.53	1.967e+41	0.595
10156	TS.diHPCARP_Ib.15aldHshift.utdppudd	1.362e+43	2.53	2.53	1.965e+41	0.595
10157	TS.diHPCARP_Ib.15aldHshift.utummuuu	3.556e+43	3.13	3.13	1.854e+41	0.561
10158	TS.diHPCARP_Ib.15aldHshift.dtdppudd	3.556e+43	3.13	3.13	1.854e+41	0.561
10159	TS.diHPCARP_Ib.15aldHshift.updmtddd	1.731e+43	2.92	2.92	1.285e+41	0.389
10160	TS.diHPCARP_Ib.15aldHshift.dmdmtuuu	1.731e+43	2.92	2.92	1.285e+41	0.389
10161	TS.diHPCARP_Ib.15aldHshift.umdtpddd	1.314e+43	2.79	2.79	1.210e+41	0.366
10162	TS.diHPCARP_Ib.15aldHshift.dputmuuu	1.317e+43	2.80	2.80	1.203e+41	0.364
10163	TS.diHPCARP_Ib.15aldHshift.utdppddd	4.678e+42	2.24	2.24	1.085e+41	0.328
10164	TS.diHPCARP_Ib.15aldHshift.dtummuuu	4.668e+42	2.24	2.24	1.083e+41	0.328
10165	TS.diHPCARP_Ib.15aldHshift.dmdmpuuu	1.938e+43	3.13	3.13	1.023e+41	0.31
10166	TS.diHPCARP_Ib.15aldHshift.uputmudd	4.057e+43	3.59	3.59	9.878e+40	0.299
10167	TS.diHPCARP_Ib.15aldHshift.dtdppudd	2.532e+43	3.31	3.31	9.833e+40	0.298
10168	TS.diHPCARP_Ib.15aldHshift.utdttuudd	2.532e+43	3.31	3.31	9.833e+40	0.298
10169	TS.diHPCARP_Ib.15aldHshift.dmdtpduu	4.022e+43	3.59	3.59	9.771e+40	0.296
10170	TS.diHPCARP_Ib.15aldHshift.umdppduu	7.068e+42	2.58	2.58	9.394e+40	0.284
10171	TS.diHPCARP_Ib.15aldHshift.dpumduuu	7.064e+42	2.58	2.58	9.380e+40	0.284
10172	TS.diHPCARP_Ib.15aldHshift.dputpduu	1.424e+43	3.01	3.01	9.191e+40	0.278
10173	TS.diHPCARP_Ib.15aldHshift.umdtmudd	1.424e+43	3.01	3.01	9.190e+40	0.278
10174	TS.diHPCARP_Ib.15aldHshift.umdtmddd	4.189e+43	3.67	3.67	8.918e+40	0.27
10175	TS.diHPCARP_Ib.15aldHshift.dputpuuu	4.189e+43	3.67	3.67	8.918e+40	0.27
10176	TS.diHPCARP_Ib.15aldHshift.upumpddd	6.046e+42	2.52	2.52	8.826e+40	0.267
10177	TS.diHPCARP_Ib.15aldHshift.dmdmpuuu	6.046e+42	2.52	2.52	8.826e+40	0.267
10178	TS.diHPCARP_Ib.15aldHshift.dtumduudd	7.604e+43	4.04	4.04	8.676e+40	0.263
10179	TS.diHPCARP_Ib.15aldHshift.utdtpduu	7.603e+43	4.04	4.04	8.675e+40	0.263
10180	TS.diHPCARP_Ib.15aldHshift.updmtddd	8.454e+42	2.80	2.80	7.740e+40	0.234
10181	TS.diHPCARP_Ib.15aldHshift.dmuptuuu	8.216e+42	2.82	2.82	7.261e+40	0.22
10182	TS.diHPCARP_Ib.15aldHshift.dpummuuu	1.190e+43	3.08	3.08	6.824e+40	0.206
10183	TS.diHPCARP_Ib.15aldHshift.updppddd	1.189e+43	3.08	3.08	6.823e+40	0.206
10184	TS.diHPCARP_Ib.15aldHshift.upuptuudd	1.925e+43	3.42	3.42	6.179e+40	0.187
10185	TS.diHPCARP_Ib.15aldHshift.dmdmtduu	1.925e+43	3.42	3.42	6.179e+40	0.187
10186	TS.diHPCARP_Ib.15aldHshift.dmdppudd	3.144e+43	3.76	3.76	5.741e+40	0.174
10187	TS.diHPCARP_Ib.15aldHshift.upummuuu	3.127e+43	3.76	3.76	5.705e+40	0.173
10188	TS.diHPCARP_Ib.15aldHshift.dtdppddd	4.591e+42	2.66	2.66	5.272e+40	0.16
10189	TS.diHPCARP_Ib.15aldHshift.utummuuu	4.590e+42	2.66	2.66	5.272e+40	0.16
10190	TS.diHPCARP_Ib.15aldHshift.ututpddd	9.711e+42	3.11	3.11	5.251e+40	0.159
10191	TS.diHPCARP_Ib.15aldHshift.dtdtmuuu	9.711e+42	3.11	3.11	5.251e+40	0.159
10192	TS.diHPCARP_Ib.15aldHshift.uputpduu	5.579e+43	4.22	4.22	4.680e+40	0.142
10193	TS.diHPCARP_Ib.15aldHshift.dmdtmudd	5.579e+43	4.22	4.22	4.680e+40	0.142
10194	TS.diHPCARP_Ib.15aldHshift.dtdtpddd	1.822e+43	3.60	3.60	4.337e+40	0.131
10195	TS.diHPCARP_Ib.15aldHshift.ututmuuu	1.822e+43	3.60	3.60	4.337e+40	0.131
10196	TS.diHPCARP_Ib.15aldHshift.utdtpuuu	8.781e+43	4.57	4.57	4.133e+40	0.125
10197	TS.diHPCARP_Ib.15aldHshift.dtumtddd	8.781e+43	4.57	4.57	4.133e+40	0.125
10198	TS.diHPCARP_Ib.15aldHshift.dtumtuuu	2.117e+43	3.73	3.73	4.094e+40	0.124
10199	TS.diHPCARP_Ib.15aldHshift.utdtpddd	2.117e+43	3.73	3.73	4.093e+40	0.124
10200	TS.diHPCARP_Ib.15aldHshift.ututmudd	1.422e+43	3.53	3.53	3.841e+40	0.116

10201	TS.diHPCARP_Ib.15aldHshift.dtdtpduu	1.421e+43	3.53	3.53	3.840e+40	0.116
10202	TS.diHPCARP_Ib.15aldHshift.dmdmmuuu	1.152e+43	3.44	3.44	3.587e+40	0.109
10203	TS.diHPCARP_Ib.15aldHshift.upuppddd	1.152e+43	3.44	3.44	3.587e+40	0.109
10204	TS.diHPCARP_Ib.15aldHshift.uputmuuu	2.484e+43	3.95	3.95	3.272e+40	0.099
10205	TS.diHPCARP_Ib.15aldHshift.dmdtpddd	2.484e+43	3.95	3.95	3.269e+40	0.0989
10206	TS.diHPCARP_Ib.15aldHshift.utdtmuuu	1.742e+43	3.77	3.77	3.104e+40	0.0939
10207	TS.diHPCARP_Ib.15aldHshift.dtutpddd	1.737e+43	3.78	3.78	3.088e+40	0.0934
10208	TS.diHPCARP_Ib.15aldHshift.dmdtmddd	7.081e+43	4.62	4.62	3.046e+40	0.0922
10209	TS.diHPCARP_Ib.15aldHshift.uputpuuu	7.080e+43	4.62	4.62	3.043e+40	0.0921
10210	TS.diHPCARP_Ib.15aldHshift.ututmddd	2.799e+43	4.08	4.08	2.974e+40	0.09
10211	TS.diHPCARP_Ib.15aldHshift.dtdtpuuu	2.799e+43	4.08	4.08	2.974e+40	0.09
10212	TS.diHPCARP_Ib.15aldHshift.dpumpduu	1.536e+43	3.76	3.76	2.784e+40	0.0843
10213	TS.diHPCARP_Ib.15aldHshift.umdpmudd	1.535e+43	3.76	3.76	2.780e+40	0.0841
10214	TS.diHPCARP_Ib.15aldHshift.dpummduu	3.684e+43	4.35	4.35	2.489e+40	0.0753
10215	TS.diHPCARP_Ib.15aldHshift.umdppudd	3.683e+43	4.35	4.35	2.489e+40	0.0753
10216	TS.diHPCARP_Ib.15aldHshift.dmdmmudd	2.387e+43	4.13	4.13	2.334e+40	0.0706
10217	TS.diHPCARP_Ib.15aldHshift.upuppduu	2.387e+43	4.13	4.13	2.334e+40	0.0706
10218	TS.diHPCARP_Ib.15aldHshift.utuptduu	2.423e+43	4.14	4.14	2.320e+40	0.0702
10219	TS.diHPCARP_Ib.15aldHshift.dtdmtudd	2.422e+43	4.14	4.14	2.319e+40	0.0702
10220	TS.diHPCARP_Ib.15aldHshift.updmmduu	6.698e+43	4.82	4.82	2.060e+40	0.0623
10221	TS.diHPCARP_Ib.15aldHshift.dmuppduu	6.694e+43	4.82	4.82	2.057e+40	0.0622
10222	TS.diHPCARP_Ib.15aldHshift.ututpduu	1.574e+43	3.99	3.99	1.963e+40	0.0594
10223	TS.diHPCARP_Ib.15aldHshift.dtdtmduu	1.574e+43	3.99	3.99	1.963e+40	0.0594
10224	TS.diHPCARP_Ib.15aldHshift.updppduu	1.461e+43	4.04	4.04	1.678e+40	0.0508
10225	TS.diHPCARP_Ib.15aldHshift.dmummduu	1.461e+43	4.04	4.04	1.678e+40	0.0508
10226	TS.diHPCARP_Ib.15aldHshift.dputmduu	5.172e+43	4.82	4.82	1.597e+40	0.0483
10227	TS.diHPCARP_Ib.15aldHshift.umdtpudd	5.170e+43	4.82	4.82	1.597e+40	0.0483
10228	TS.diHPCARP_Ib.15aldHshift.dtdptuuu	3.501e+42	3.22	3.22	1.588e+40	0.048
10229	TS.diHPCARP_Ib.15aldHshift.utumtddd	3.501e+42	3.22	3.22	1.588e+40	0.048
10230	TS.diHPCARP_Ib.15aldHshift.umdttddd	5.153e+43	4.87	4.87	1.453e+40	0.044
10231	TS.diHPCARP_Ib.15aldHshift.dputtuu	5.147e+43	4.87	4.87	1.447e+40	0.0438
10232	TS.diHPCARP_Ib.15aldHshift.umdmddd	1.103e+43	4.05	4.05	1.241e+40	0.0376
10233	TS.diHPCARP_Ib.15aldHshift.dpuppuuu	1.103e+43	4.05	4.05	1.241e+40	0.0376
10234	TS.diHPCARP_Ib.15aldHshift.dtuuptduu	1.123e+43	4.13	4.13	1.096e+40	0.0332
10235	TS.diHPCARP_Ib.15aldHshift.utdmtduu	1.123e+43	4.13	4.13	1.096e+40	0.0332
10236	TS.diHPCARP_Ib.15aldHshift.utumtuu	6.018e+43	5.15	5.15	1.071e+40	0.0324
10237	TS.diHPCARP_Ib.15aldHshift.dtdptddd	5.995e+43	5.15	5.15	1.064e+40	0.0322
10238	TS.diHPCARP_Ib.15aldHshift.upupmuuu	1.719e+43	4.41	4.41	1.058e+40	0.032
10239	TS.diHPCARP_Ib.15aldHshift.dmdmpddd	1.714e+43	4.41	4.41	1.051e+40	0.0318
10240	TS.diHPCARP_Ib.15aldHshift.dmutmddd	1.942e+44	5.91	5.91	9.652e+39	0.0292
10241	TS.diHPCARP_Ib.15aldHshift.updtpuuu	1.942e+44	5.91	5.91	9.639e+39	0.0292
10242	TS.diHPCARP_Ib.15aldHshift.dmummuuu	1.474e+43	4.39	4.39	9.300e+39	0.0281
10243	TS.diHPCARP_Ib.15aldHshift.updpddd	1.474e+43	4.39	4.39	9.298e+39	0.0281
10244	TS.diHPCARP_Ib.15aldHshift.umdmpddd	5.648e+42	3.85	3.85	8.886e+39	0.0269
10245	TS.diHPCARP_Ib.15aldHshift.dpupmuuu	5.648e+42	3.85	3.85	8.885e+39	0.0269
10246	TS.diHPCARP_Ib.15aldHshift.dtdptudd	7.032e+43	5.43	5.43	7.794e+39	0.0236
10247	TS.diHPCARP_Ib.15aldHshift.utumtduu	7.025e+43	5.43	5.43	7.785e+39	0.0236
10248	TS.diHPCARP_Ib.15aldHshift.dtdmtduu	5.787e+42	4.00	4.00	7.025e+39	0.0213
10249	TS.diHPCARP_Ib.15aldHshift.utuptduu	5.787e+42	4.00	4.00	7.025e+39	0.0213
10250	TS.diHPCARP_Ib.15aldHshift.dmutmuuu	3.074e+43	5.00	5.00	6.964e+39	0.0211
10251	TS.diHPCARP_Ib.15aldHshift.updtpddd	3.073e+43	5.00	5.00	6.963e+39	0.0211
10252	TS.diHPCARP_Ib.15aldHshift.dtuupddd	8.672e+42	4.29	4.29	6.466e+39	0.0196
10253	TS.diHPCARP_Ib.15aldHshift.dpdptuuu	9.736e+42	4.37	4.37	6.382e+39	0.0193
10254	TS.diHPCARP_Ib.15aldHshift.umumtddd	9.734e+42	4.37	4.37	6.381e+39	0.0193
10255	TS.diHPCARP_Ib.15aldHshift.upumpuuu	1.709e+43	4.76	4.76	5.777e+39	0.0175
10256	TS.diHPCARP_Ib.15aldHshift.dmdptudd	1.225e+43	4.57	4.57	5.766e+39	0.0174
10257	TS.diHPCARP_Ib.15aldHshift.upumtduu	1.225e+43	4.57	4.57	5.766e+39	0.0174
10258	TS.diHPCARP_Ib.15aldHshift.dputtduu	6.329e+43	5.60	5.60	5.296e+39	0.016
10259	TS.diHPCARP_Ib.15aldHshift.umdttddd	6.328e+43	5.60	5.60	5.295e+39	0.016
10260	TS.diHPCARP_Ib.15aldHshift.dmutpddd	4.315e+43	5.38	5.38	5.200e+39	0.0157
10261	TS.diHPCARP_Ib.15aldHshift.dtdptduu	7.219e+42	4.32	4.32	5.106e+39	0.0154
10262	TS.diHPCARP_Ib.15aldHshift.utumtuu	7.219e+42	4.32	4.32	5.105e+39	0.0154
10263	TS.diHPCARP_Ib.15aldHshift.ututtuuu	7.351e+43	5.73	5.73	4.890e+39	0.0148
10264	TS.diHPCARP_Ib.15aldHshift.dtdttddd	7.350e+43	5.73	5.73	4.890e+39	0.0148
10265	TS.diHPCARP_Ib.15aldHshift.dtuttddd	6.691e+43	5.71	5.71	4.649e+39	0.0141
10266	TS.diHPCARP_Ib.15aldHshift.ututtddd	3.534e+43	5.34	5.34	4.544e+39	0.0138
10267	TS.diHPCARP_Ib.15aldHshift.dtdttuuu	3.533e+43	5.34	5.34	4.544e+39	0.0137
10268	TS.diHPCARP_Ib.15aldHshift.umdptudd	4.699e+43	5.54	5.54	4.327e+39	0.0131
10269	TS.diHPCARP_Ib.15aldHshift.dpumtduu	4.699e+43	5.54	5.54	4.327e+39	0.0131
10270	TS.diHPCARP_Ib.15aldHshift.uputtuuu	6.969e+43	5.78	5.78	4.320e+39	0.0131
10271	TS.diHPCARP_Ib.15aldHshift.dmdttddd	6.969e+43	5.78	5.78	4.319e+39	0.0131
10272	TS.diHPCARP_Ib.15aldHshift.dmutpduu	6.504e+43	5.76	5.76	4.166e+39	0.0126

10273	TS.diHPCARP_Ib.15aldHshift.updmtudd	6.504e+43	5.76	5.76	4.162e+39	0.0126
10274	TS.diHPCARP_Ib.15aldHshift.dtdmduu	2.370e+43	5.17	5.17	4.064e+39	0.0123
10275	TS.diHPCARP_Ib.15aldHshift.utuppudd	2.348e+43	5.17	5.17	3.997e+39	0.0121
10276	TS.diHPCARP_Ib.15aldHshift.utupppdd	2.041e+43	5.12	5.12	3.778e+39	0.0114
10277	TS.diHPCARP_Ib.15aldHshift.dtdmmuuu	2.041e+43	5.12	5.12	3.778e+39	0.0114
10278	TS.diHPCARP_Ib.15aldHshift.updtmudd	2.461e+43	5.26	5.26	3.634e+39	0.011
10279	TS.diHPCARP_Ib.15aldHshift.dmutpduu	2.461e+43	5.26	5.26	3.631e+39	0.011
10280	TS.diHPCARP_Ib.15aldHshift.dtutpudd	5.078e+43	5.71	5.71	3.501e+39	0.0106
10281	TS.diHPCARP_Ib.15aldHshift.dpdmmduu	2.570e+43	5.40	5.40	3.017e+39	0.00913
10282	TS.diHPCARP_Ib.15aldHshift.umuppudd	2.568e+43	5.40	5.40	3.011e+39	0.00911
10283	TS.diHPCARP_Ib.15aldHshift.ututpudd	2.504e+43	5.40	5.40	2.924e+39	0.00885
10284	TS.diHPCARP_Ib.15aldHshift.dtdtmduu	2.503e+43	5.40	5.40	2.924e+39	0.00885
10285	TS.diHPCARP_Ib.15aldHshift.dmutpuuu	8.613e+43	6.20	6.20	2.643e+39	0.008
10286	TS.diHPCARP_Ib.15aldHshift.updtmddd	8.612e+43	6.20	6.20	2.643e+39	0.008
10287	TS.diHPCARP_Ib.15aldHshift.dtuptddd	4.596e+43	5.87	5.87	2.452e+39	0.00742
10288	TS.diHPCARP_Ib.15aldHshift.umdptddd	5.579e+43	6.07	6.07	2.119e+39	0.00641
10289	TS.diHPCARP_Ib.15aldHshift.dpumtuuu	5.579e+43	6.07	6.07	2.118e+39	0.00641
10290	TS.diHPCARP_Ib.15aldHshift.uputmduu	5.146e+43	6.03	6.03	2.083e+39	0.0063
10291	TS.diHPCARP_Ib.15aldHshift.dmutpduu	5.151e+43	6.03	6.03	2.083e+39	0.0063
10292	TS.diHPCARP_Ib.15aldHshift.dmdpmduu	8.404e+42	5.01	5.01	1.895e+39	0.00574
10293	TS.diHPCARP_Ib.15aldHshift.upumpudd	8.404e+42	5.01	5.01	1.895e+39	0.00574
10294	TS.diHPCARP_Ib.15aldHshift.dtdmpuuu	5.732e+42	4.82	4.82	1.757e+39	0.00532
10295	TS.diHPCARP_Ib.15aldHshift.updtpduu	5.946e+43	6.22	6.22	1.747e+39	0.00529
10296	TS.diHPCARP_Ib.15aldHshift.dmutmudd	5.944e+43	6.22	6.22	1.747e+39	0.00529
10297	TS.diHPCARP_Ib.15aldHshift.dtuttudd	1.003e+44	6.53	6.53	1.746e+39	0.00528
10298	TS.diHPCARP_Ib.15aldHshift.dmdpmddd	6.945e+42	4.96	4.96	1.681e+39	0.00509
10299	TS.diHPCARP_Ib.15aldHshift.utdptudd	1.931e+43	5.59	5.59	1.646e+39	0.00498
10300	TS.diHPCARP_Ib.15aldHshift.dtuutduu	1.925e+43	5.59	5.59	1.636e+39	0.00495
10301	TS.diHPCARP_Ib.15aldHshift.dpuppudd	2.163e+43	5.67	5.67	1.613e+39	0.00488
10302	TS.diHPCARP_Ib.15aldHshift.umdmmduu	2.163e+43	5.67	5.67	1.612e+39	0.00488
10303	TS.diHPCARP_Ib.15aldHshift.dmdttudd	8.782e+43	6.51	6.51	1.586e+39	0.0048
10304	TS.diHPCARP_Ib.15aldHshift.uputtduu	8.779e+43	6.51	6.51	1.585e+39	0.0048
10305	TS.diHPCARP_Ib.15aldHshift.dtdttduu	3.950e+43	6.04	6.04	1.571e+39	0.00475
10306	TS.diHPCARP_Ib.15aldHshift.ututtudd	3.950e+43	6.04	6.04	1.571e+39	0.00475
10307	TS.diHPCARP_Ib.15aldHshift.dmutpddd	2.166e+44	7.10	7.10	1.459e+39	0.00442
10308	TS.diHPCARP_Ib.15aldHshift.updmtuuu	2.166e+44	7.10	7.10	1.459e+39	0.00441
10309	TS.diHPCARP_Ib.15aldHshift.dmdptddd	6.129e+43	6.42	6.42	1.298e+39	0.00393
10310	TS.diHPCARP_Ib.15aldHshift.upumtuuu	6.128e+43	6.42	6.42	1.298e+39	0.00393
10311	TS.diHPCARP_Ib.15aldHshift.dpdppudd	5.693e+43	6.40	6.40	1.233e+39	0.00373
10312	TS.diHPCARP_Ib.15aldHshift.updptudd	1.513e+43	5.65	5.65	1.166e+39	0.00353
10313	TS.diHPCARP_Ib.15aldHshift.dmutpduu	1.513e+43	5.65	5.65	1.166e+39	0.00353
10314	TS.diHPCARP_Ib.15aldHshift.dtuptduu	1.455e+43	5.73	5.73	9.769e+38	0.00296
10315	TS.diHPCARP_Ib.15aldHshift.dpdtpduu	3.847e+43	6.31	6.31	9.744e+38	0.00295
10316	TS.diHPCARP_Ib.15aldHshift.umutmudd	3.845e+43	6.31	6.31	9.740e+38	0.00295
10317	TS.diHPCARP_Ib.15aldHshift.dpumtudd	4.129e+43	6.38	6.38	9.317e+38	0.00282
10318	TS.diHPCARP_Ib.15aldHshift.umutpduu	1.286e+44	7.07	7.07	9.069e+38	0.00274
10319	TS.diHPCARP_Ib.15aldHshift.dpdmtudd	1.285e+44	7.07	7.07	9.069e+38	0.00274
10320	TS.diHPCARP_Ib.15aldHshift.uputpddd	3.151e+43	6.24	6.24	9.027e+38	0.00273
10321	TS.diHPCARP_Ib.15aldHshift.dpdmtuuu	3.151e+43	6.24	6.24	9.025e+38	0.00273
10322	TS.diHPCARP_Ib.15aldHshift.upumddd	3.259e+42	4.94	4.94	8.171e+38	0.00247
10323	TS.diHPCARP_Ib.15aldHshift.umutuuu	5.134e+43	6.60	6.60	7.972e+38	0.00241
10324	TS.diHPCARP_Ib.15aldHshift.dpdtpddd	5.132e+43	6.60	6.60	7.969e+38	0.00241
10325	TS.diHPCARP_Ib.15aldHshift.utdtmudd	2.786e+43	6.30	6.30	7.119e+38	0.00215
10326	TS.diHPCARP_Ib.15aldHshift.utdmpddd	4.878e+42	5.27	5.27	7.114e+38	0.00215
10327	TS.diHPCARP_Ib.15aldHshift.dmutpduu	4.852e+42	5.27	5.27	7.052e+38	0.00213
10328	TS.diHPCARP_Ib.15aldHshift.dtuupduu	2.766e+43	6.31	6.31	7.048e+38	0.00213
10329	TS.diHPCARP_Ib.15aldHshift.utumpddd	3.926e+42	5.21	5.21	6.236e+38	0.00189
10330	TS.diHPCARP_Ib.15aldHshift.dtdpmuuu	3.926e+42	5.21	5.21	6.236e+38	0.00189
10331	TS.diHPCARP_Ib.15aldHshift.dmutmduu	9.787e+43	7.22	7.22	5.368e+38	0.00162
10332	TS.diHPCARP_Ib.15aldHshift.updtpudd	9.786e+43	7.22	7.22	5.368e+38	0.00162
10333	TS.diHPCARP_Ib.15aldHshift.umdpmddd	4.881e+42	5.45	5.45	5.259e+38	0.00159
10334	TS.diHPCARP_Ib.15aldHshift.dpumpuuu	4.870e+42	5.45	5.45	5.236e+38	0.00158
10335	TS.diHPCARP_Ib.15aldHshift.dmutuuu	9.307e+43	7.21	7.21	5.177e+38	0.00157
10336	TS.diHPCARP_Ib.15aldHshift.updttddd	9.307e+43	7.21	7.21	5.177e+38	0.00157
10337	TS.diHPCARP_Ib.15aldHshift.utumddd	8.468e+42	5.82	5.82	4.880e+38	0.00148
10338	TS.diHPCARP_Ib.15aldHshift.dtdppuuu	8.457e+42	5.82	5.82	4.868e+38	0.00147
10339	TS.diHPCARP_Ib.15aldHshift.updpmduu	1.497e+43	6.21	6.21	4.481e+38	0.00136
10340	TS.diHPCARP_Ib.15aldHshift.dpdmtddd	1.900e+44	7.73	7.73	4.426e+38	0.00134
10341	TS.diHPCARP_Ib.15aldHshift.umdtpduu	3.998e+43	6.82	6.82	4.288e+38	0.0013
10342	TS.diHPCARP_Ib.15aldHshift.dputpudd	3.998e+43	6.82	6.82	4.288e+38	0.0013
10343	TS.diHPCARP_Ib.15aldHshift.dmutpduu	1.549e+44	7.67	7.67	4.017e+38	0.00122
10344	TS.diHPCARP_Ib.15aldHshift.updmtduu	1.549e+44	7.67	7.67	4.016e+38	0.00122

10345	TS.diHPCARP_Ib.15aldHshift.dmuttddd	1.201e+44	7.53	7.53	3.953e+38	0.0012
10346	TS.diHPCARP_Ib.15aldHshift.dpdtpuuu	6.719e+43	7.28	7.28	3.364e+38	0.00102
10347	TS.diHPCARP_Ib.15aldHshift.umutmddd	6.719e+43	7.28	7.28	3.364e+38	0.00102
10348	TS.diHPCARP_Ib.15aldHshift.dputmudd	4.307e+43	7.02	7.02	3.296e+38	0.000997
10349	TS.diHPCARP_Ib.15aldHshift.umdtmduu	4.285e+43	7.02	7.02	3.275e+38	0.000991
10350	TS.diHPCARP_Ib.15aldHshift.dtuppddd	1.305e+43	6.33	6.33	3.193e+38	0.000966
10351	TS.diHPCARP_Ib.15aldHshift.utdmmuuu	1.305e+43	6.33	6.33	3.189e+38	0.000965
10352	TS.diHPCARP_Ib.15aldHshift.dmuupddd	1.491e+43	6.42	6.42	3.128e+38	0.000947
10353	TS.diHPCARP_Ib.15aldHshift.updpmuuu	1.491e+43	6.42	6.42	3.128e+38	0.000947
10354	TS.diHPCARP_Ib.15aldHshift.updmddd	2.008e+43	6.62	6.62	3.027e+38	0.000916
10355	TS.diHPCARP_Ib.15aldHshift.dmuupuuu	1.997e+43	6.62	6.62	3.005e+38	0.000909
10356	TS.diHPCARP_Ib.15aldHshift.dmuupddd	1.875e+43	6.60	6.60	2.928e+38	0.000886
10357	TS.diHPCARP_Ib.15aldHshift.updmpuuu	1.875e+43	6.60	6.60	2.928e+38	0.000886
10358	TS.diHPCARP_Ib.15aldHshift.dmutpudd	1.134e+44	7.72	7.72	2.673e+38	0.000809
10359	TS.diHPCARP_Ib.15aldHshift.updttudd	1.512e+44	7.90	7.90	2.645e+38	0.0008
10360	TS.diHPCARP_Ib.15aldHshift.dmuttduu	1.509e+44	7.90	7.90	2.637e+38	0.000798
10361	TS.diHPCARP_Ib.15aldHshift.updtmduu	1.120e+44	7.73	7.73	2.618e+38	0.000792
10362	TS.diHPCARP_Ib.15aldHshift.updppudd	4.084e+43	7.17	7.17	2.455e+38	0.000743
10363	TS.diHPCARP_Ib.15aldHshift.dmuupuuu	4.084e+43	7.17	7.17	2.455e+38	0.000743
10364	TS.diHPCARP_Ib.15aldHshift.dpdmpduu	1.856e+43	6.80	6.80	2.062e+38	0.000624
10365	TS.diHPCARP_Ib.15aldHshift.umupmudd	1.854e+43	6.80	6.80	2.058e+38	0.000623
10366	TS.diHPCARP_Ib.15aldHshift.dmdmtddd	9.724e+42	6.49	6.49	1.825e+38	0.000552
10367	TS.diHPCARP_Ib.15aldHshift.umumtudd	5.348e+43	7.52	7.52	1.776e+38	0.000537
10368	TS.diHPCARP_Ib.15aldHshift.dpdptduu	5.347e+43	7.52	7.52	1.776e+38	0.000537
10369	TS.diHPCARP_Ib.15aldHshift.dtdmtuuu	2.502e+43	7.09	7.09	1.702e+38	0.000515
10370	TS.diHPCARP_Ib.15aldHshift.utuptddd	2.501e+43	7.09	7.09	1.702e+38	0.000515
10371	TS.diHPCARP_Ib.15aldHshift.dtumpddd	1.761e+43	6.89	6.89	1.698e+38	0.000514
10372	TS.diHPCARP_Ib.15aldHshift.utdpmuuu	1.761e+43	6.89	6.89	1.697e+38	0.000514
10373	TS.diHPCARP_Ib.15aldHshift.dmuupuuu	8.988e+42	6.50	6.50	1.657e+38	0.000501
10374	TS.diHPCARP_Ib.15aldHshift.updmpddd	8.988e+42	6.50	6.50	1.657e+38	0.000501
10375	TS.diHPCARP_Ib.15aldHshift.dputpddd	2.007e+43	6.98	6.98	1.656e+38	0.000501
10376	TS.diHPCARP_Ib.15aldHshift.umdtmuuu	2.007e+43	6.98	6.98	1.656e+38	0.000501
10377	TS.diHPCARP_Ib.15aldHshift.dpdmpuuu	2.492e+43	7.20	7.20	1.428e+38	0.000432
10378	TS.diHPCARP_Ib.15aldHshift.utdttddd	9.057e+43	8.00	8.00	1.342e+38	0.000406
10379	TS.diHPCARP_Ib.15aldHshift.upumtudd	7.240e+43	7.89	7.89	1.285e+38	0.000389
10380	TS.diHPCARP_Ib.15aldHshift.dpumddd	4.665e+43	7.66	7.66	1.229e+38	0.000372
10381	TS.diHPCARP_Ib.15aldHshift.dmuupduu	5.702e+42	6.43	6.43	1.182e+38	0.000358
10382	TS.diHPCARP_Ib.15aldHshift.updmpuud	5.702e+42	6.43	6.43	1.182e+38	0.000358
10383	TS.diHPCARP_Ib.15aldHshift.dputpuuu	7.000e+42	6.57	6.57	1.148e+38	0.000347
10384	TS.diHPCARP_Ib.15aldHshift.umumtuu	6.545e+43	7.93	7.93	1.091e+38	0.00033
10385	TS.diHPCARP_Ib.15aldHshift.dpdptudd	1.735e+43	7.17	7.17	1.033e+38	0.000313
10386	TS.diHPCARP_Ib.15aldHshift.umdmtuu	3.469e+43	7.62	7.62	9.765e+37	0.000295
10387	TS.diHPCARP_Ib.15aldHshift.dputpddd	3.469e+43	7.62	7.62	9.764e+37	0.000295
10388	TS.diHPCARP_Ib.15aldHshift.umummudd	6.985e+42	6.69	6.69	9.391e+37	0.000284
10389	TS.diHPCARP_Ib.15aldHshift.dpdttuuu	1.029e+44	8.37	8.37	8.196e+37	0.000248
10390	TS.diHPCARP_Ib.15aldHshift.umuttddd	1.029e+44	8.37	8.37	8.196e+37	0.000248
10391	TS.diHPCARP_Ib.15aldHshift.utumpudd	2.594e+42	6.22	6.22	7.673e+37	0.000232
10392	TS.diHPCARP_Ib.15aldHshift.dtdpmduu	2.593e+42	6.22	6.22	7.673e+37	0.000232
10393	TS.diHPCARP_Ib.15aldHshift.umutpudd	8.191e+43	8.33	8.33	7.032e+37	0.000213
10394	TS.diHPCARP_Ib.15aldHshift.dpdmtduu	8.191e+43	8.33	8.33	7.032e+37	0.000213
10395	TS.diHPCARP_Ib.15aldHshift.umuppudd	2.361e+43	7.60	7.60	6.876e+37	0.000208
10396	TS.diHPCARP_Ib.15aldHshift.dpdmmuuu	2.360e+43	7.60	7.60	6.872e+37	0.000208
10397	TS.diHPCARP_Ib.15aldHshift.umuptudd	1.007e+44	8.53	8.53	6.135e+37	0.000186
10398	TS.diHPCARP_Ib.15aldHshift.dpdmtduu	1.007e+44	8.53	8.53	6.135e+37	0.000186
10399	TS.diHPCARP_Ib.15aldHshift.utdmddd	4.366e+42	6.70	6.70	5.740e+37	0.000174
10400	TS.diHPCARP_Ib.15aldHshift.utdmtuu	8.382e+42	7.11	7.11	5.552e+37	0.000168
10401	TS.diHPCARP_Ib.15aldHshift.dputtddd	8.172e+43	8.58	8.58	4.612e+37	0.00014
10402	TS.diHPCARP_Ib.15aldHshift.umdttuu	8.164e+43	8.58	8.58	4.608e+37	0.000139
10403	TS.diHPCARP_Ib.15aldHshift.dpdmtuuu	1.715e+44	9.03	9.03	4.565e+37	0.000138
10404	TS.diHPCARP_Ib.15aldHshift.umuptddd	1.715e+44	9.03	9.03	4.564e+37	0.000138
10405	TS.diHPCARP_Ib.15aldHshift.dpdttddd	1.054e+44	8.78	8.78	4.258e+37	0.000129
10406	TS.diHPCARP_Ib.15aldHshift.updptddd	1.024e+44	8.79	8.79	4.017e+37	0.000122
10407	TS.diHPCARP_Ib.15aldHshift.dmuumtuu	1.024e+44	8.79	8.79	4.017e+37	0.000122
10408	TS.diHPCARP_Ib.15aldHshift.dpdptddd	1.019e+44	8.89	8.89	3.400e+37	0.000103
10409	TS.diHPCARP_Ib.15aldHshift.utdmduu	1.526e+44	9.21	9.21	3.001e+37	9.08e-05
10410	TS.diHPCARP_Ib.15aldHshift.dpumtddd	6.510e+43	8.76	8.76	2.720e+37	8.23e-05
10411	TS.diHPCARP_Ib.15aldHshift.dpdtpudd	1.278e+44	9.17	9.17	2.668e+37	8.07e-05
10412	TS.diHPCARP_Ib.15aldHshift.dpdttduu	1.451e+44	9.28	9.28	2.522e+37	7.63e-05
10413	TS.diHPCARP_Ib.15aldHshift.umuttudd	1.442e+44	9.28	9.28	2.502e+37	7.57e-05
10414	TS.diHPCARP_Ib.15aldHshift.umumddd	2.318e+43	8.29	8.29	2.115e+37	6.4e-05
10415	TS.diHPCARP_Ib.15aldHshift.dpdttudd	1.833e+44	9.56	9.56	1.980e+37	5.99e-05
10416	TS.diHPCARP_Ib.15aldHshift.dmdmtudd	1.500e+44	9.51	9.51	1.785e+37	5.4e-05

10417	TS.diHPCARP_Ib.15aldHshift.upuptduu	1.497e+44	9.51	9.51	1.780e+37	5.39e-05
10418	TS.diHPCARP_Ib.15aldHshift.dpdppuuu	1.948e+43	8.40	8.40	1.488e+37	4.5e-05
10419	TS.diHPCARP_Ib.15aldHshift.umumtduu	2.868e+43	8.66	8.66	1.407e+37	4.26e-05
10420	TS.diHPCARP_Ib.15aldHshift.dpdpmuuu	9.948e+42	8.11	8.11	1.229e+37	3.72e-05
10421	TS.diHPCARP_Ib.15aldHshift.umumpddd	9.947e+42	8.11	8.11	1.229e+37	3.72e-05
10422	TS.diHPCARP_Ib.15aldHshift.dmumpudd	1.029e+43	8.26	8.26	9.829e+36	2.97e-05
10423	TS.diHPCARP_Ib.15aldHshift.dmumtudd	9.495e+43	9.61	9.61	9.433e+36	2.85e-05
10424	TS.diHPCARP_Ib.15aldHshift.updptduu	9.494e+43	9.61	9.61	9.432e+36	2.85e-05
10425	TS.diHPCARP_Ib.15aldHshift.umumpuuu	8.308e+43	9.55	9.55	9.113e+36	2.76e-05
10426	TS.diHPCARP_Ib.15aldHshift.dpdpmddd	8.306e+43	9.55	9.55	9.110e+36	2.76e-05
10427	TS.diHPCARP_Ib.15aldHshift.dmdmdudd	5.187e+43	9.32	9.32	8.442e+36	2.55e-05
10428	TS.diHPCARP_Ib.15aldHshift.upuppuuu	5.184e+43	9.32	9.32	8.437e+36	2.55e-05
10429	TS.diHPCARP_Ib.15aldHshift.umdptduu	2.287e+43	8.94	8.94	7.046e+36	2.13e-05
10430	TS.diHPCARP_Ib.15aldHshift.dpdpmduu	7.185e+42	8.28	8.28	6.627e+36	2.01e-05
10431	TS.diHPCARP_Ib.15aldHshift.umumpudd	7.182e+42	8.29	8.29	6.617e+36	2e-05
10432	TS.diHPCARP_Ib.15aldHshift.umuppduu	3.769e+43	9.33	9.33	6.049e+36	1.83e-05
10433	TS.diHPCARP_Ib.15aldHshift.dpdmmudd	3.752e+43	9.33	9.33	6.021e+36	1.82e-05
10434	TS.diHPCARP_Ib.15aldHshift.umumduu	4.903e+43	9.49	9.49	5.965e+36	1.8e-05
10435	TS.diHPCARP_Ib.15aldHshift.dmdmpudd	5.022e+43	9.57	9.57	5.389e+36	1.55e-05
10436	TS.diHPCARP_Ib.15aldHshift.upupmduu	5.021e+43	9.57	9.57	5.382e+36	1.63e-05
10437	TS.diHPCARP_Ib.15aldHshift.updppuuu	4.268e+43	9.50	9.50	5.107e+36	1.55e-05
10438	TS.diHPCARP_Ib.15aldHshift.dmuumddd	4.268e+43	9.50	9.50	5.107e+36	1.55e-05
10439	TS.diHPCARP_Ib.15aldHshift.dtumtudd	8.013e+43	10.49	10.49	1.823e+36	5.52e-06
10440	TS.diHPCARP_Ib.15aldHshift.utdptduu	8.012e+43	10.49	10.49	1.823e+36	5.52e-06
10441	TS.diHPCARP_Ib.15aldHshift.umupmddd	1.256e+43	9.67	9.67	1.127e+36	3.41e-06
10442	TS.diHPCARP_Ib.15aldHshift.utdttuuu	3.777e+43	10.37	10.37	1.045e+36	3.16e-06
10443	TS.diHPCARP_Ib.15aldHshift.utdppuuu	3.517e+43	10.70	10.70	5.683e+35	1.72e-06
10444	TS.diHPCARP_Ib.15aldHshift.dtumddd	3.301e+43	10.71	10.71	5.223e+35	1.58e-06
10445	TS.diHPCARP_Ib.15aldHshift.utdttduu	4.161e+43	10.94	10.94	4.453e+35	1.35e-06
10446	TS.diHPCARP_Ib.15aldHshift.dpdmtddd	1.489e+43	10.38	10.38	4.067e+35	1.23e-06
10447	TS.diHPCARP_Ib.15aldHshift.umdpuuu	1.463e+43	11.16	11.16	1.085e+35	3.28e-07
10448	TS.diHPCARP_Ib.15aldHshift.umdmpuuu	5.757e+42	10.70	10.70	9.221e+34	2.79e-07
10449	TS.diHPCARP_Ib.15aldHshift.dpdmtudd	1.125e+44	12.65	12.65	6.854e+34	2.07e-07
10450	Total				3.305e+43	100

10451
10452
10453

1,6-aldehyde-H-shift in (2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-Ic)

10455
10456

=====
=

10457
10458

Population analysis at 300K. Vibrational scaling: 0.971.

10459

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

10460

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

10461

#: contribution to the population (with current data set assumed 100%)

10462

Compound Qtot Erel Erel2 n*Q*MB %

10463

10464

TS.diHPCARP_Ic.16aldHshift.a.pmtmud 4.549e+42 0.00 0.00 4.549e+42 32.8

10465

TS.diHPCARP_Ic.16aldHshift.a.pmmpdu 1.227e+43 1.07 1.07 2.049e+42 14.8

10466

TS.diHPCARP_Ic.16aldHshift.b.pmtmud 5.365e+42 0.62 0.62 1.884e+42 13.6

10467

TS.diHPCARP_Ic.16aldHshift.a.mptmud 5.446e+42 0.88 0.88 1.253e+42 9.03

10468

TS.diHPCARP_Ic.16aldHshift.b.mptmud 5.619e+42 1.24 1.24 7.028e+41 5.06

10469

TS.diHPCARP_Ic.16aldHshift.a.ppmpdu 9.533e+42 1.60 1.60 6.551e+41 4.72

10470

TS.diHPCARP_Ic.16aldHshift.e.pptmud 5.236e+42 1.42 1.42 4.855e+41 3.5

10471

TS.diHPCARP_Ic.16aldHshift.a.tmpmdu 1.113e+43 1.96 1.96 4.139e+41 2.98

10472

TS.diHPCARP_Ic.16aldHshift.a.pmmud 1.852e+43 2.35 2.35 3.578e+41 2.58

10473

TS.diHPCARP_Ic.16aldHshift.b.pmppud 3.550e+42 1.50 1.50 2.866e+41 2.06

10474

TS.diHPCARP_Ic.16aldHshift.a.pptmud 4.092e+42 1.99 1.99 1.465e+41 1.06

10475

TS.diHPCARP_Ic.16aldHshift.a.mppmdu 7.855e+42 2.51 2.51 1.169e+41 0.842

10476

TS.diHPCARP_Ic.16aldHshift.b.pppud 3.233e+42 2.05 2.05 1.032e+41 0.743

10477

TS.diHPCARP_Ic.16aldHshift.e.pptud 7.180e+42 2.54 2.54 1.014e+41 0.73

10478

TS.diHPCARP_Ic.16aldHshift.a.pmpmdu 2.981e+43 3.46 3.46 9.040e+40 0.651

10479

TS.diHPCARP_Ic.16aldHshift.a.pmpmdu 1.907e+43 3.26 3.26 8.059e+40 0.581

10480

TS.diHPCARP_Ic.16aldHshift.a.pmppud 4.230e+42 2.62 2.62 5.209e+40 0.375

10481

TS.diHPCARP_Ic.16aldHshift.e.pmmpdu 1.184e+43 3.30 3.30 4.706e+40 0.339

10482

TS.diHPCARP_Ic.16aldHshift.b.mppud 3.768e+42 2.63 2.63 4.561e+40 0.329

10483

TS.diHPCARP_Ic.16aldHshift.a.pmmdu 2.492e+43 3.80 3.80 4.242e+40 0.306

10484

TS.diHPCARP_Ic.16aldHshift.a.mppmdu 1.632e+43 3.65 3.65 3.572e+40 0.257

10485

TS.diHPCARP_Ic.16aldHshift.e.mppmdu 4.763e+42 2.94 2.94 3.453e+40 0.249

10486

TS.diHPCARP_Ic.16aldHshift.a.pppmdu 1.826e+43 3.83 3.83 2.979e+40 0.215

10487

TS.diHPCARP_Ic.16aldHshift.a.pptud 6.722e+42 3.25 3.25 2.893e+40 0.208

10488

10489	TS.diHPCARP_Ic.16aldHshift.a.pmp pdu	4.823e+43	4.57	4.57	2.274e+40	0.164
10490	TS.diHPCARP_Ic.16aldHshift.b.mmm pdu	3.058e+42	3.00	3.00	1.985e+40	0.143
10491	TS.diHPCARP_Ic.16aldHshift.b.pmm mud	2.504e+43	4.30	4.30	1.858e+40	0.134
10492	TS.diHPCARP_Ic.16aldHshift.e.pmp pdu	5.220e+42	3.37	3.37	1.824e+40	0.131
10493	TS.diHPCARP_Ic.16aldHshift.a.pmt pdu	1.285e+43	3.95	3.95	1.698e+40	0.122
10494	TS.diHPCARP_Ic.16aldHshift.e.ppp pdu	7.446e+42	3.65	3.65	1.640e+40	0.118
10495	TS.diHPCARP_Ic.16aldHshift.b.tmm pdu	8.513e+42	3.75	3.75	1.576e+40	0.114
10496	TS.diHPCARP_Ic.16aldHshift.e.mpp pdu	3.835e+42	3.38	3.38	1.316e+40	0.0948
10497	TS.diHPCARP_Ic.16aldHshift.a.pmt pdu	4.433e+43	5.02	5.02	9.831e+39	0.0708
10498	TS.diHPCARP_Ic.16aldHshift.a.tmp pdu	1.402e+43	4.37	4.37	9.169e+39	0.0661
10499	TS.diHPCARP_Ic.16aldHshift.b.ppp pdu	8.950e+42	4.11	4.11	9.082e+39	0.0654
10500	TS.diHPCARP_Ic.16aldHshift.b.mmp pdu	2.657e+42	3.41	3.41	8.758e+39	0.0631
10501	TS.diHPCARP_Ic.16aldHshift.a.ppp pdu	3.716e+42	3.68	3.68	7.750e+39	0.0558
10502	TS.diHPCARP_Ic.16aldHshift.a.ppp pdu	3.457e+43	5.06	5.06	7.121e+39	0.0513
10503	TS.diHPCARP_Ic.16aldHshift.a.mpp pdu	4.356e+42	3.85	3.85	6.836e+39	0.0493
10504	TS.diHPCARP_Ic.16aldHshift.c.pmm mud	1.272e+43	4.54	4.54	6.280e+39	0.0452
10505	TS.diHPCARP_Ic.16aldHshift.b.pmt pdu	1.474e+43	4.68	4.68	5.731e+39	0.0413
10506	TS.diHPCARP_Ic.16aldHshift.a.ppp pdu	1.584e+43	4.74	4.74	5.542e+39	0.0399
10507	TS.diHPCARP_Ic.16aldHshift.e.ppp pdu	1.671e+43	4.84	4.84	4.977e+39	0.0359
10508	TS.diHPCARP_Ic.16aldHshift.e.tmp pdu	8.464e+42	4.54	4.54	4.144e+39	0.0299
10509	TS.diHPCARP_Ic.16aldHshift.a.ppp mud	9.980e+42	4.66	4.66	4.030e+39	0.029
10510	TS.diHPCARP_Ic.16aldHshift.a.mpp pdu	1.814e+43	5.05	5.05	3.799e+39	0.0274
10511	TS.diHPCARP_Ic.16aldHshift.a.pmt pdu	1.613e+42	4.60	4.60	3.643e+39	0.0262
10512	TS.diHPCARP_Ic.16aldHshift.a.ppt pdu	7.147e+43	5.99	5.99	3.095e+39	0.0223
10513	TS.diHPCARP_Ic.16aldHshift.c.pmm pdu	1.613e+43	5.14	5.14	2.889e+39	0.0208
10514	TS.diHPCARP_Ic.16aldHshift.b.mpp pdu	1.456e+43	5.08	5.08	2.885e+39	0.0208
10515	TS.diHPCARP_Ic.16aldHshift.b.ppp pdu	8.846e+42	4.83	4.83	2.660e+39	0.0192
10516	TS.diHPCARP_Ic.16aldHshift.c.pmt pdu	9.617e+42	4.91	4.91	2.558e+39	0.0184
10517	TS.diHPCARP_Ic.16aldHshift.b.pmt pdu	1.104e+43	5.00	5.00	2.536e+39	0.0183
10518	TS.diHPCARP_Ic.16aldHshift.e.tmp pdu	5.664e+42	4.71	4.71	2.105e+39	0.0152
10519	TS.diHPCARP_Ic.16aldHshift.a.mpt pdu	1.606e+43	5.42	5.42	1.815e+39	0.0131
10520	TS.diHPCARP_Ic.16aldHshift.b.mmm pdu	8.233e+42	5.02	5.02	1.804e+39	0.013
10521	TS.diHPCARP_Ic.16aldHshift.e.tpt mud	9.097e+42	5.16	5.16	1.597e+39	0.0115
10522	TS.diHPCARP_Ic.16aldHshift.a.ppt mud	4.614e+43	6.12	6.12	1.596e+39	0.0115
10523	TS.diHPCARP_Ic.16aldHshift.b.mpp mud	2.117e+43	5.68	5.68	1.531e+39	0.011
10524	TS.diHPCARP_Ic.16aldHshift.c.ppp mud	6.715e+42	5.08	5.08	1.328e+39	0.00957
10525	TS.diHPCARP_Ic.16aldHshift.e.ppp mud	1.816e+43	5.72	5.72	1.236e+39	0.00891
10526	TS.diHPCARP_Ic.16aldHshift.a.mpp pdu	1.397e+43	5.57	5.57	1.229e+39	0.00886
10527	TS.diHPCARP_Ic.16aldHshift.a.mmt pdu	8.622e+42	5.30	5.30	1.191e+39	0.00858
10528	TS.diHPCARP_Ic.16aldHshift.c.ppp pdu	1.052e+43	5.43	5.43	1.159e+39	0.00835
10529	TS.diHPCARP_Ic.16aldHshift.e.pmt pdu	1.997e+43	5.84	5.84	1.117e+39	0.00805
10530	TS.diHPCARP_Ic.16aldHshift.a.tmm pdu	2.226e+43	5.92	5.92	1.079e+39	0.00778
10531	TS.diHPCARP_Ic.16aldHshift.b.pmm mud	4.172e+43	6.42	6.42	8.753e+38	0.00631
10532	TS.diHPCARP_Ic.16aldHshift.c.pmm pdu	3.455e+43	6.32	6.32	8.537e+38	0.00615
10533	TS.diHPCARP_Ic.16aldHshift.e.tpp pdu	4.800e+42	5.20	5.20	7.774e+38	0.0056
10534	TS.diHPCARP_Ic.16aldHshift.a.tpp pdu	4.876e+43	6.61	6.61	7.509e+38	0.00541
10535	TS.diHPCARP_Ic.16aldHshift.c.tpm pdu	1.440e+43	5.91	5.91	7.076e+38	0.0051
10536	TS.diHPCARP_Ic.16aldHshift.e.tmt pdu	5.819e+43	6.75	6.75	7.051e+38	0.00508
10537	TS.diHPCARP_Ic.16aldHshift.a.tmp pdu	5.225e+42	5.32	5.32	6.915e+38	0.00498
10538	TS.diHPCARP_Ic.16aldHshift.b.mmt pdu	1.217e+43	5.88	5.88	6.305e+38	0.00454
10539	TS.diHPCARP_Ic.16aldHshift.e.mpt pdu	8.579e+42	5.68	5.68	6.292e+38	0.00453
10540	TS.diHPCARP_Ic.16aldHshift.e.tmt pdu	9.482e+42	5.75	5.75	6.110e+38	0.0044
10541	TS.diHPCARP_Ic.16aldHshift.a.tmt pdu	6.349e+43	6.89	6.89	6.101e+38	0.0044
10542	TS.diHPCARP_Ic.16aldHshift.c.mpp mud	1.384e+43	6.01	6.01	5.754e+38	0.00415
10543	TS.diHPCARP_Ic.16aldHshift.b.mpt pdu	1.244e+43	6.12	6.12	4.317e+38	0.00311
10544	TS.diHPCARP_Ic.16aldHshift.c.pmt pdu	1.282e+43	6.25	6.25	3.565e+38	0.00257
10545	TS.diHPCARP_Ic.16aldHshift.c.pmm pdu	2.185e+43	6.58	6.58	3.508e+38	0.00253
10546	TS.diHPCARP_Ic.16aldHshift.c.mpp pdu	1.708e+43	6.47	6.47	3.331e+38	0.0024
10547	TS.diHPCARP_Ic.16aldHshift.b.ppt pdu	5.788e+43	7.24	7.24	3.054e+38	0.0022
10548	TS.diHPCARP_Ic.16aldHshift.a.tpp mud	8.590e+42	6.26	6.26	2.352e+38	0.0017
10549	TS.diHPCARP_Ic.16aldHshift.e.pmp pdu	2.457e+43	6.91	6.91	2.265e+38	0.00163
10550	TS.diHPCARP_Ic.16aldHshift.e.tpp mud	7.504e+42	6.23	6.23	2.166e+38	0.00156
10551	TS.diHPCARP_Ic.16aldHshift.a.tmm pdu	1.192e+43	6.51	6.51	2.151e+38	0.00155
10552	TS.diHPCARP_Ic.16aldHshift.a.tpp pdu	5.110e+42	6.15	6.15	1.685e+38	0.00121
10553	TS.diHPCARP_Ic.16aldHshift.a.mmm mud	2.209e+43	7.09	7.09	1.514e+38	0.00109
10554	TS.diHPCARP_Ic.16aldHshift.a.tmm mud	1.086e+43	6.69	6.69	1.453e+38	0.00105
10555	TS.diHPCARP_Ic.16aldHshift.c.mpp pdu	8.187e+42	6.57	6.57	1.351e+38	0.000973
10556	TS.diHPCARP_Ic.16aldHshift.b.tmm pdu	4.524e+43	7.66	7.66	1.190e+38	0.000857
10557	TS.diHPCARP_Ic.16aldHshift.e.tpp pdu	4.377e+43	7.66	7.66	1.152e+38	0.00083
10558	TS.diHPCARP_Ic.16aldHshift.a.tmt pdu	1.865e+43	7.16	7.16	1.143e+38	0.000824
10559	TS.diHPCARP_Ic.16aldHshift.e.mpp pdu	1.320e+43	6.97	6.97	1.109e+38	0.000799
10560	TS.diHPCARP_Ic.16aldHshift.b.pmm pdu	4.801e+43	7.76	7.76	1.076e+38	0.000775

10561	TS.diHPCARP_Ic.16aldHshift.c.mpppud	7.190e+42	6.70	6.70	9.496e+37	0.000684
10562	TS.diHPCARP_Ic.16aldHshift.b.ppppdu	6.373e+43	8.05	8.05	8.653e+37	0.000623
10563	TS.diHPCARP_Ic.16aldHshift.a.mpppdu	1.310e+43	7.20	7.20	7.469e+37	0.000538
10564	TS.diHPCARP_Ic.16aldHshift.e.tmmppud	1.729e+43	7.38	7.38	7.251e+37	0.000522
10565	TS.diHPCARP_Ic.16aldHshift.b.tppmdu	2.024e+43	7.49	7.49	7.019e+37	0.000506
10566	TS.diHPCARP_Ic.16aldHshift.b.tptmdu	5.187e+43	8.12	8.12	6.266e+37	0.000451
10567	TS.diHPCARP_Ic.16aldHshift.e.tmmud	1.444e+43	7.44	7.44	5.517e+37	0.000398
10568	TS.diHPCARP_Ic.16aldHshift.a.mmmppud	3.738e+43	8.02	8.02	5.333e+37	0.000384
10569	TS.diHPCARP_Ic.16aldHshift.c.pppmdu	3.128e+43	8.06	8.06	4.185e+37	0.000302
10570	TS.diHPCARP_Ic.16aldHshift.c.ppppud	2.913e+43	8.11	8.11	3.599e+37	0.000259
10571	TS.diHPCARP_Ic.16aldHshift.b.pptpdu	1.535e+43	7.74	7.74	3.533e+37	0.000255
10572	TS.diHPCARP_Ic.16aldHshift.c.ppppdu	2.077e+43	7.97	7.97	3.225e+37	0.000232
10573	TS.diHPCARP_Ic.16aldHshift.a.mmpmud	2.517e+43	8.09	8.09	3.223e+37	0.000232
10574	TS.diHPCARP_Ic.16aldHshift.b.mpppud	8.101e+42	7.47	7.47	2.924e+37	0.000211
10575	TS.diHPCARP_Ic.16aldHshift.b.tpppud	1.226e+43	7.99	7.99	2.598e+37	0.000187
10576	TS.diHPCARP_Ic.16aldHshift.e.mmmud	5.519e+43	8.69	8.69	2.591e+37	0.000187
10577	TS.diHPCARP_Ic.16aldHshift.a.mptmdu	1.420e+43	7.96	7.96	2.259e+37	0.000163
10578	TS.diHPCARP_Ic.16aldHshift.a.mmtpud	2.450e+43	8.32	8.32	2.141e+37	0.000154
10579	TS.diHPCARP_Ic.16aldHshift.e.mmpmud	4.248e+43	8.65	8.65	2.137e+37	0.000154
10580	TS.diHPCARP_Ic.16aldHshift.a.mpppud	1.536e+43	8.18	8.18	1.700e+37	0.000122
10581	TS.diHPCARP_Ic.16aldHshift.b.tmtmud	5.748e+42	7.61	7.61	1.640e+37	0.000118
10582	TS.diHPCARP_Ic.16aldHshift.c.pppmdu	6.072e+43	9.07	9.07	1.491e+37	0.000107
10583	TS.diHPCARP_Ic.16aldHshift.e.mmtpud	4.750e+43	8.98	8.98	1.368e+37	9.86e-05
10584	TS.diHPCARP_Ic.16aldHshift.a.tppmud	2.978e+43	8.72	8.72	1.333e+37	9.61e-05
10585	TS.diHPCARP_Ic.16aldHshift.c.pmtmdu	3.748e+43	8.90	8.90	1.242e+37	8.95e-05
10586	TS.diHPCARP_Ic.16aldHshift.b.tptpdu	4.445e+42	7.66	7.66	1.162e+37	8.37e-05
10587	TS.diHPCARP_Ic.16aldHshift.c.ppppud	4.923e+43	9.13	9.13	1.095e+37	7.89e-05
10588	TS.diHPCARP_Ic.16aldHshift.c.pmtpdu	3.018e+43	8.84	8.84	1.089e+37	7.85e-05
10589	TS.diHPCARP_Ic.16aldHshift.c.pppmud	1.552e+43	8.47	8.47	1.044e+37	7.52e-05
10590	TS.diHPCARP_Ic.16aldHshift.e.mmpmud	6.662e+43	9.62	9.62	6.571e+36	4.73e-05
10591	TS.diHPCARP_Ic.16aldHshift.c.ppppud	1.927e+43	8.88	8.88	6.546e+36	4.72e-05
10592	TS.diHPCARP_Ic.16aldHshift.c.mmtpud	1.890e+43	9.00	9.00	5.222e+36	3.76e-05
10593	TS.diHPCARP_Ic.16aldHshift.c.mmmud	1.942e+43	9.24	9.24	3.608e+36	2.6e-05
10594	TS.diHPCARP_Ic.16aldHshift.c.mmpmud	2.339e+43	9.47	9.47	2.933e+36	2.11e-05
10595	TS.diHPCARP_Ic.16aldHshift.c.tmmppud	2.171e+43	9.52	9.52	2.529e+36	1.82e-05
10596	TS.diHPCARP_Ic.16aldHshift.c.pppmdu	8.318e+43	10.46	10.46	1.995e+36	1.44e-05
10597	TS.diHPCARP_Ic.16aldHshift.c.pptpdu	5.148e+43	10.21	10.21	1.880e+36	1.35e-05
10598	TS.diHPCARP_Ic.16aldHshift.e.tppmud	3.497e+43	10.04	10.04	1.691e+36	1.22e-05
10599	TS.diHPCARP_Ic.16aldHshift.c.pptmdu	4.050e+43	10.13	10.13	1.686e+36	1.21e-05
10600	TS.diHPCARP_Ic.16aldHshift.c.ppppud	8.350e+43	10.64	10.64	1.482e+36	1.07e-05
10601	TS.diHPCARP_Ic.16aldHshift.c.mmpmud	1.142e+43	9.61	9.61	1.139e+36	8.21e-06
10602	TS.diHPCARP_Ic.16aldHshift.c.tppmud	4.826e+43	10.67	10.67	8.109e+35	5.84e-06
10603	TS.diHPCARP_Ic.16aldHshift.c.mpppud	1.350e+43	10.17	10.17	5.275e+35	3.8e-06
10604	TS.diHPCARP_Ic.16aldHshift.c.tpppud	7.767e+43	11.49	11.49	3.314e+35	2.39e-06
10605	TS.diHPCARP_Ic.16aldHshift.e.tptpud	3.108e+43	11.13	11.13	2.441e+35	1.76e-06
10606	TS.diHPCARP_Ic.16aldHshift.c.tmtpud	6.385e+43	11.69	11.69	1.932e+35	1.39e-06
10607	TS.diHPCARP_Ic.16aldHshift.a.tptpud	3.012e+43	11.29	11.29	1.799e+35	1.3e-06
10608	TS.diHPCARP_Ic.16aldHshift.a.tmtmdu	3.973e+43	11.48	11.48	1.710e+35	1.23e-06
10609	TS.diHPCARP_Ic.16aldHshift.c.tppmud	3.523e+43	11.79	11.79	9.098e+34	6.56e-07
10610	TS.diHPCARP_Ic.16aldHshift.c.tpppud	4.571e+43	12.20	12.20	5.929e+34	4.27e-07
10611	Total				1.388e+43	100

1,6-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia), forming B' (di-HPCARP-Ib)

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Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
10626	TS.diHPCARP_I.1600HHshift.b.lmmpud	3.576e+42	0.00	0.00	3.576e+42	90.2
10627	TS.diHPCARP_I.1600HHshift.b.hppmud	2.850e+42	1.50	1.50	2.293e+41	5.79
10628	TS.diHPCARP_I.1600HHshift.a.tpppud	2.488e+43	3.67	3.67	5.239e+40	1.32
10629	TS.diHPCARP_I.1600HHshift.b.tppmdu	5.837e+42	2.85	2.85	4.910e+40	1.24
10630	TS.diHPCARP_I.1600HHshift.b.lppmdu	1.060e+43	3.83	3.83	1.707e+40	0.431
10631	TS.diHPCARP_I.1600HHshift.b.tpppud	1.530e+43	4.34	4.34	1.048e+40	0.264
10632	TS.diHPCARP_I.1600HHshift.b.lpppud	1.190e+43	4.67	4.67	4.708e+39	0.119

10633	TS.diHPCARP_I.1600HHshift.a.lmmpdu	6.386e+42	4.41	4.41	3.895e+39	0.0983
10634	TS.diHPCARP_I.1600HHshift.a.tttmpud	8.838e+42	4.65	4.65	3.618e+39	0.0913
10635	TS.diHPCARP_I.1600HHshift.a.tptmpud	2.969e+43	5.50	5.50	2.912e+39	0.0735
10636	TS.diHPCARP_I.1600HHshift.b.lptmdu	3.285e+43	5.78	5.78	2.013e+39	0.0508
10637	TS.diHPCARP_I.1600HHshift.b.hpppud	1.714e+43	5.60	5.60	1.430e+39	0.0361
10638	TS.diHPCARP_I.1600HHshift.a.tptpud	3.361e+43	6.14	6.14	1.138e+39	0.0287
10639	TS.diHPCARP_I.1600HHshift.a.ttptdu	5.140e+43	6.53	6.53	8.937e+38	0.0226
10640	TS.diHPCARP_I.1600HHshift.a.lppmdu	1.361e+43	5.79	5.79	8.290e+38	0.0209
10641	TS.diHPCARP_I.1600HHshift.b.lmmdu	1.792e+43	6.00	6.00	7.685e+38	0.0194
10642	TS.diHPCARP_I.1600HHshift.a.ttpmud	8.989e+42	5.65	5.65	6.866e+38	0.0173
10643	TS.diHPCARP_I.1600HHshift.b.lmttdu	2.705e+43	6.34	6.34	6.557e+38	0.0165
10644	TS.diHPCARP_I.1600HHshift.a.ltmpdu	1.648e+43	6.13	6.13	5.612e+38	0.0142
10645	TS.diHPCARP_I.1600HHshift.a.hmpmdu	5.390e+42	5.51	5.51	5.229e+38	0.0132
10646	TS.diHPCARP_I.1600HHshift.b.lptpdu	3.259e+43	6.65	6.65	4.696e+38	0.0118
10647	TS.diHPCARP_I.1600HHshift.a.ttpmdu	3.429e+43	6.81	6.81	3.752e+38	0.00947
10648	TS.diHPCARP_I.1600HHshift.a.lpppdu	1.294e+43	6.26	6.26	3.591e+38	0.00906
10649	TS.diHPCARP_I.1600HHshift.a.tmtpud	2.116e+43	6.57	6.57	3.455e+38	0.00872
10650	TS.diHPCARP_I.1600HHshift.b.htmpud	2.173e+43	6.61	6.61	3.343e+38	0.00844
10651	TS.diHPCARP_I.1600HHshift.b.ltmpdu	1.600e+43	6.77	6.77	3.197e+38	0.00807
10652	TS.diHPCARP_I.1600HHshift.a.hmmtdu	6.147e+42	6.01	6.01	2.558e+38	0.00646
10653	TS.diHPCARP_I.1600HHshift.b.hptmud	2.861e+43	6.95	6.95	2.483e+38	0.00627
10654	TS.diHPCARP_I.1600HHshift.b.hmptdu	2.217e+43	7.14	7.14	1.388e+38	0.0035
10655	TS.diHPCARP_I.1600HHshift.b.cmmdu	1.586e+43	7.03	7.03	1.191e+38	0.00301
10656	TS.diHPCARP_I.1600HHshift.b.hmpmdu	2.128e+43	7.26	7.26	1.090e+38	0.00275
10657	TS.diHPCARP_I.1600HHshift.b.hmttdu	4.671e+43	7.75	7.75	1.056e+38	0.00266
10658	TS.diHPCARP_I.1600HHshift.a.lptmdu	5.306e+43	7.85	7.85	1.021e+38	0.00258
10659	TS.diHPCARP_I.1600HHshift.a.ltpmdu	1.348e+43	7.19	7.19	7.787e+37	0.00197
10660	TS.diHPCARP_I.1600HHshift.b.hptpud	2.480e+43	7.60	7.60	7.174e+37	0.00181
10661	TS.diHPCARP_I.1600HHshift.a.tptpud	9.590e+42	7.29	7.29	4.663e+37	0.00118
10662	TS.diHPCARP_I.1600HHshift.b.hmtpud	1.549e+43	7.59	7.59	4.544e+37	0.00115
10663	TS.diHPCARP_I.1600HHshift.a.tttmdu	6.714e+43	8.49	8.49	4.423e+37	0.00112
10664	TS.diHPCARP_I.1600HHshift.a.tttmdu	3.449e+43	8.11	8.11	4.271e+37	0.00108
10665	TS.diHPCARP_I.1600HHshift.a.tttpdu	4.332e+43	8.28	8.28	4.012e+37	0.00101
10666	TS.diHPCARP_I.1600HHshift.a.lttmdu	6.394e+43	8.58	8.58	3.603e+37	0.000909
10667	TS.diHPCARP_I.1600HHshift.b.htmpud	2.923e+43	8.26	8.26	2.801e+37	0.000707
10668	TS.diHPCARP_I.1600HHshift.b.lptpud	5.227e+43	8.80	8.80	2.041e+37	0.000515
10669	TS.diHPCARP_I.1600HHshift.a.mmmdu	2.072e+43	8.34	8.34	1.741e+37	0.000439
10670	TS.diHPCARP_I.1600HHshift.b.ltpmdu	1.915e+43	8.52	8.52	1.188e+37	0.0003
10671	TS.diHPCARP_I.1600HHshift.b.cmpmdu	3.994e+43	9.05	9.05	1.014e+37	0.000256
10672	TS.diHPCARP_I.1600HHshift.a.mmtpdu	3.284e+43	8.97	8.97	9.649e+36	0.000244
10673	TS.diHPCARP_I.1600HHshift.b.ctpud	4.036e+43	9.15	9.15	8.649e+36	0.000218
10674	TS.diHPCARP_I.1600HHshift.a.hmttdu	5.417e+43	9.38	9.38	7.973e+36	0.000201
10675	TS.diHPCARP_I.1600HHshift.b.cmpmdu	2.773e+43	9.03	9.03	7.290e+36	0.000184
10676	TS.diHPCARP_I.1600HHshift.b.cpppud	2.216e+43	9.26	9.26	3.947e+36	9.96e-05
10677	TS.diHPCARP_I.1600HHshift.b.cmtmdu	3.292e+43	9.62	9.62	3.233e+36	8.16e-05
10678	TS.diHPCARP_I.1600HHshift.a.pmpmdu	1.345e+43	9.24	9.24	2.517e+36	6.35e-05
10679	TS.diHPCARP_I.1600HHshift.a.mmpmdu	2.495e+43	9.75	9.75	1.967e+36	4.96e-05
10680	TS.diHPCARP_I.1600HHshift.b.ctmpud	1.770e+43	9.57	9.57	1.884e+36	4.75e-05
10681	TS.diHPCARP_I.1600HHshift.b.cppmdu	1.199e+43	9.38	9.38	1.763e+36	4.45e-05
10682	TS.diHPCARP_I.1600HHshift.b.hmttud	1.132e+43	9.49	9.49	1.383e+36	3.49e-05
10683	TS.diHPCARP_I.1600HHshift.a.cpppdu	1.287e+43	9.79	9.79	9.573e+35	2.42e-05
10684	TS.diHPCARP_I.1600HHshift.b.ctttdu	4.069e+43	10.85	10.85	5.039e+35	1.27e-05
10685	TS.diHPCARP_I.1600HHshift.b.cpppdu	1.757e+43	10.52	10.52	3.833e+35	9.67e-06
10686	TS.diHPCARP_I.1600HHshift.a.cptmdu	3.258e+43	10.95	10.95	3.450e+35	8.71e-06
10687	TS.diHPCARP_I.1600HHshift.b.ctmtud	2.798e+43	10.88	10.88	3.337e+35	8.42e-06
10688	TS.diHPCARP_I.1600HHshift.b.cptmdu	3.074e+43	11.11	11.11	2.478e+35	6.25e-06
10689	TS.diHPCARP_I.1600HHshift.b.cptmdu	3.592e+43	11.21	11.21	2.459e+35	6.2e-06
10690	TS.diHPCARP_I.1600HHshift.b.ctmmdu	3.547e+43	11.41	11.41	1.723e+35	4.35e-06
10691	TS.diHPCARP_I.1600HHshift.b.mppmdu	6.228e+43	11.92	11.92	1.297e+35	3.27e-06
10692	TS.diHPCARP_I.1600HHshift.b.lppmdu	9.578e+42	10.84	10.84	1.206e+35	3.04e-06
10693	TS.diHPCARP_I.1600HHshift.b.cptpud	2.860e+43	11.55	11.55	1.103e+35	2.78e-06
10694	TS.diHPCARP_I.1600HHshift.b.cppmdu	1.406e+43	11.55	11.55	5.444e+34	1.37e-06
10695	TS.diHPCARP_I.1600HHshift.b.ctpmdu	1.098e+43	11.78	11.78	2.895e+34	7.31e-07
10696	TS.diHPCARP_I.1600HHshift.b.ctttud	3.403e+43	12.45	12.45	2.882e+34	7.27e-07
10697	TS.diHPCARP_I.1600HHshift.b.cmtpud	2.587e+43	12.63	12.63	1.635e+34	4.13e-07
10698	TS.diHPCARP_I.1600HHshift.b.cmmtud	2.281e+43	14.41	14.41	7.261e+32	1.83e-08
10699	TS.diHPCARP_I.1600HHshift.a.hpmtdu	1.850e+43	14.45	14.45	5.543e+32	1.4e-08
10700	Total				3.963e+42	100
10701						
10702						
10703						

10704 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-
 10705 HPCARP-Ia), forming C' (di-HPCARP-Ic)
 10706 =====
 10707 =====
 10708 =====

10709 Population analysis at 300K. Vibrational scaling: 0.971.

10710 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

10711 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

10712 %: contribution to the population (with current data set assumed 100%)

10713	Compound	Qtot	Erel	Erel2	n*Q*MB	%
10714	-----	-----	-----	-----	-----	-----
10715	TS.diHPCARP_I.1700HHshift.BB.tmuud	4.607e+42	0.00	0.00	4.607e+42	71.2
10716	TS.diHPCARP_I.1700HHshift.BB.ttddu	4.032e+42	1.05	1.05	6.950e+41	10.7
10717	TS.diHPCARP_I.1700HHshift.BB.ttudu	1.440e+43	2.10	2.10	4.221e+41	6.53
10718	TS.diHPCARP_I.1700HHshift.BB.tmudu	1.948e+42	1.53	1.53	1.491e+41	2.31
10719	TS.diHPCARP_I.1700HHshift.CR.hpddu	4.451e+42	2.31	2.31	9.271e+40	1.43
10720	TS.diHPCARP_I.1700HHshift.BB.mmdud	7.302e+42	2.60	2.60	9.269e+40	1.43
10721	TS.diHPCARP_I.1700HHshift.BB.tpdu	5.152e+42	2.44	2.44	8.660e+40	1.34
10722	TS.diHPCARP_I.1700HHshift.BB.htdu	2.329e+43	3.53	3.53	6.265e+40	0.969
10723	TS.diHPCARP_I.1700HHshift.BB.ttuud	2.586e+43	3.64	3.64	5.768e+40	0.892
10724	TS.diHPCARP_I.1700HHshift.BB.lmddu	1.566e+43	3.48	3.48	4.565e+40	0.706
10725	TS.diHPCARP_I.1700HHshift.BB.ltuud	1.368e+43	3.42	3.42	4.445e+40	0.687
10726	TS.diHPCARP_I.1700HHshift.BB.lpuud	1.413e+43	3.72	3.72	2.776e+40	0.429
10727	TS.diHPCARP_I.1700HHshift.BB.ltdud	1.873e+43	3.89	3.89	2.736e+40	0.423
10728	TS.diHPCARP_I.1700HHshift.BB.cmudu	1.851e+42	3.20	3.20	8.671e+39	0.134
10729	TS.diHPCARP_I.1700HHshift.CR.tmdud	4.916e+42	3.94	3.94	6.666e+39	0.103
10730	TS.diHPCARP_I.1700HHshift.BB.tmuud	2.668e+43	5.01	5.01	5.967e+39	0.0923
10731	TS.diHPCARP_I.1700HHshift.BB.lpddu	4.336e+42	3.94	3.94	5.813e+39	0.0899
10732	TS.diHPCARP_I.1700HHshift.BB.ctdud	2.458e+43	5.00	5.00	5.634e+39	0.0871
10733	TS.diHPCARP_I.1700HHshift.CR.tmuud	4.870e+42	4.06	4.06	5.366e+39	0.083
10734	TS.diHPCARP_I.1700HHshift.BB.mpuud	2.195e+43	5.01	5.01	4.924e+39	0.0761
10735	TS.diHPCARP_I.1700HHshift.BB.lmdu	3.934e+42	4.14	4.14	3.779e+39	0.0584
10736	TS.diHPCARP_I.1700HHshift.BB.tpudu	3.347e+42	4.28	4.28	2.562e+39	0.0396
10737	TS.diHPCARP_I.1700HHshift.BB.ctddu	3.324e+42	4.40	4.40	2.081e+39	0.0322
10738	TS.diHPCARP_I.1700HHshift.BC.lpddu	7.719e+42	5.23	5.23	1.190e+39	0.0184
10739	TS.diHPCARP_I.1700HHshift.CR.lpddu	6.111e+42	5.12	5.12	1.131e+39	0.0175
10740	TS.diHPCARP_I.1700HHshift.BC.htuud	5.615e+42	5.17	5.17	9.632e+38	0.0149
10741	TS.diHPCARP_I.1700HHshift.CR.tpdu	2.682e+42	4.76	4.76	9.120e+38	0.0141
10742	TS.diHPCARP_I.1700HHshift.BB.cpddu	4.521e+42	6.01	6.01	1.891e+38	0.00292
10743	TS.diHPCARP_I.1700HHshift.CR.cmuud	4.020e+42	6.04	6.04	1.612e+38	0.00249
10744	TS.diHPCARP_I.1700HHshift.BC.pmuud	7.683e+42	6.56	6.56	1.277e+38	0.00197
10745	TS.diHPCARP_I.1700HHshift.BC.ppudu	1.213e+43	6.95	6.95	1.049e+38	0.00162
10746	TS.diHPCARP_I.1700HHshift.BB.hpddu	5.606e+42	6.70	6.70	7.339e+37	0.00113
10747	TS.diHPCARP_I.1700HHshift.BB.ppddu	2.194e+42	6.30	6.30	5.624e+37	0.00087
10748	TS.diHPCARP_I.1700HHshift.BC.ttdud	1.775e+43	7.76	7.76	3.931e+37	0.000608
10749	TS.diHPCARP_I.1700HHshift.CR.ltuud	1.609e+43	7.76	7.76	3.590e+37	0.000555
10750	TS.diHPCARP_I.1700HHshift.BC.htdu	1.235e+43	7.66	7.66	3.229e+37	0.000499
10751	TS.diHPCARP_I.1700HHshift.BC.htddu	1.601e+43	8.16	8.16	1.830e+37	0.000283
10752	TS.diHPCARP_I.1700HHshift.CR.pmdud	4.101e+42	7.36	7.36	1.789e+37	0.000277
10753	TS.diHPCARP_I.1700HHshift.CR.lmudu	1.937e+43	8.37	8.37	1.545e+37	0.000239
10754	TS.diHPCARP_I.1700HHshift.BC.ptudu	1.508e+43	8.25	8.25	1.484e+37	0.000229
10755	TS.diHPCARP_I.1700HHshift.BB.mpuud	2.371e+42	7.18	7.18	1.403e+37	0.000217
10756	TS.diHPCARP_I.1700HHshift.CR.lmddu	1.773e+43	8.66	8.66	8.729e+36	0.000135
10757	TS.diHPCARP_I.1700HHshift.BC.pmddu	2.216e+43	8.95	8.95	6.699e+36	0.000104
10758	TS.diHPCARP_I.1700HHshift.BC.hpdu	1.142e+43	8.58	8.58	6.404e+36	9.9e-05
10759	TS.diHPCARP_I.1700HHshift.BC.ctuud	5.575e+42	8.45	8.45	3.896e+36	6.02e-05
10760	TS.diHPCARP_I.1700HHshift.BC.tpdu	6.022e+42	8.56	8.56	3.500e+36	5.41e-05
10761	TS.diHPCARP_I.1700HHshift.BC.tpddu	3.401e+42	8.38	8.38	2.655e+36	4.1e-05
10762	TS.diHPCARP_I.1700HHshift.BC.hmuud	7.979e+42	9.73	9.73	6.470e+35	1e-05
10763	TS.diHPCARP_I.1700HHshift.BC.tmuud	1.265e+43	10.55	10.55	2.629e+35	4.06e-06
10764	TS.diHPCARP_I.1700HHshift.BC.ttddu	8.314e+42	10.63	10.63	1.500e+35	2.32e-06
10765	TS.diHPCARP_I.1700HHshift.BC.ltuud	2.357e+43	11.36	11.36	1.253e+35	1.94e-06
10766	TS.diHPCARP_I.1700HHshift.BC.tpudu	6.263e+42	10.66	10.66	1.067e+35	1.65e-06
10767	TS.diHPCARP_I.1700HHshift.BC.ttudu	7.137e+42	10.86	10.86	8.722e+34	1.35e-06
10768	TS.diHPCARP_I.1700HHshift.BC.cpdu	4.456e+42	10.76	10.76	6.430e+34	9.94e-07
10769	TS.diHPCARP_I.1700HHshift.BC.tpuud	8.698e+42	11.34	11.34	4.791e+34	7.41e-07
10770	TS.diHPCARP_I.1700HHshift.BC.tmdud	3.915e+42	10.97	10.97	3.989e+34	6.17e-07
10771	TS.diHPCARP_I.1700HHshift.BC.tmddu	8.271e+42	11.73	11.73	2.358e+34	3.65e-07
10772	TS.diHPCARP_I.1700HHshift.BC.tmuud	9.224e+42	11.82	11.82	2.260e+34	3.49e-07
10773	TS.diHPCARP_I.1700HHshift.BC.ctudu	2.535e+43	13.47	13.47	3.916e+33	6.05e-08
10774	TS.diHPCARP_I.1700HHshift.BC.ctddu	3.065e+43	13.81	13.81	2.671e+33	4.13e-08
10775	Total				6.468e+42	100

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10779 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-
10780 HPCARP-Ib), forming C' (di-HPCARP-Ic)
10781 =====
10782 =====
10783
10784 Population analysis at 300K. Vibrational scaling: 0.971.
10785 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
10786 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
10787 %: contribution to the population (with current data set assumed 100%)
10788 Compound Qtot Erel Erel2 n*Q*MB %
10789 -----
10790 TS.diHPCARP_Ib.1600HHshift.b.pmpmud 6.274e+42 0.00 0.00 6.274e+42 21.8
10791 TS.diHPCARP_Ib.1600HHshift.b.cppmud 5.372e+43 1.44 1.44 4.823e+42 16.8
10792 TS.diHPCARP_Ib.1600HHshift.a.httpdu 3.980e+42 0.01 0.01 3.934e+42 13.7
10793 TS.diHPCARP_Ib.1600HHshift.a.cmpmdu 4.972e+42 0.43 0.43 2.435e+42 8.46
10794 TS.diHPCARP_Ib.1600HHshift.a.lttmud 1.365e+43 1.22 1.22 1.764e+42 6.13
10795 TS.diHPCARP_Ib.1600HHshift.b.lttmud 1.409e+43 1.33 1.33 1.524e+42 5.29
10796 TS.diHPCARP_Ib.1600HHshift.b.ltpmud 8.673e+42 1.09 1.09 1.405e+42 4.88
10797 TS.diHPCARP_Ib.1600HHshift.a.cppmud 1.193e+43 1.30 1.30 1.346e+42 4.68
10798 TS.diHPCARP_Ib.1600HHshift.b.cmpmud 1.276e+43 1.48 1.48 1.067e+42 3.71
10799 TS.diHPCARP_Ib.1600HHshift.a.lmpmud 5.203e+42 1.09 1.09 8.331e+41 2.89
10800 TS.diHPCARP_Ib.1600HHshift.a.ltpmud 9.574e+42 1.47 1.47 8.179e+41 2.84
10801 TS.diHPCARP_Ib.1600HHshift.b.lmpmud 7.926e+42 1.62 1.62 5.237e+41 1.82
10802 TS.diHPCARP_Ib.1600HHshift.b.pmpmud 1.212e+43 2.28 2.28 2.843e+41 0.988
10803 TS.diHPCARP_Ib.1600HHshift.a.cmpmud 8.858e+42 2.09 2.09 2.664e+41 0.926
10804 TS.diHPCARP_Ib.1600HHshift.a.ltmud 8.695e+42 2.41 2.41 1.522e+41 0.529
10805 TS.diHPCARP_Ib.1600HHshift.a.ltpmud 1.830e+43 3.05 3.05 1.100e+41 0.382
10806 TS.diHPCARP_Ib.1600HHshift.b.ltmud 1.212e+43 2.84 2.84 1.036e+41 0.36
10807 TS.diHPCARP_Ib.1600HHshift.a.mtpmud 1.429e+43 3.07 3.07 8.324e+40 0.289
10808 TS.diHPCARP_Ib.1600HHshift.a.cmpmud 1.024e+43 2.92 2.92 7.634e+40 0.265
10809 TS.diHPCARP_Ib.1600HHshift.a.pmtmud 2.808e+43 3.53 3.53 7.569e+40 0.263
10810 TS.diHPCARP_Ib.1600HHshift.b.pmtmud 3.114e+43 3.62 3.62 7.215e+40 0.251
10811 TS.diHPCARP_Ib.1600HHshift.a.lttmud 9.291e+42 3.04 3.04 5.640e+40 0.196
10812 TS.diHPCARP_Ib.1600HHshift.b.pmpmud 5.254e+43 4.08 4.08 5.600e+40 0.195
10813 TS.diHPCARP_Ib.1600HHshift.b.ctmmd 3.024e+43 3.79 3.79 5.223e+40 0.182
10814 TS.diHPCARP_Ib.1600HHshift.b.ltpmud 2.596e+43 3.76 3.76 4.732e+40 0.164
10815 TS.diHPCARP_Ib.1600HHshift.b.ptpmud 3.128e+43 3.94 3.94 4.193e+40 0.146
10816 TS.diHPCARP_Ib.1600HHshift.b.pmtmud 3.333e+43 4.04 4.04 3.777e+40 0.131
10817 TS.diHPCARP_Ib.1600HHshift.a.httpmud 4.071e+43 4.17 4.17 3.753e+40 0.13
10818 TS.diHPCARP_Ib.1600HHshift.a.pmtmud 2.518e+43 3.89 3.89 3.694e+40 0.128
10819 TS.diHPCARP_Ib.1600HHshift.a.pmpmud 2.270e+43 3.84 3.84 3.608e+40 0.125
10820 TS.diHPCARP_Ib.1600HHshift.b.ctpmud 1.842e+43 3.73 3.73 3.559e+40 0.124
10821 TS.diHPCARP_Ib.1600HHshift.b.htpmud 1.239e+43 3.52 3.52 3.364e+40 0.117
10822 TS.diHPCARP_Ib.1600HHshift.a.ltmud 4.809e+43 4.48 4.48 2.606e+40 0.0905
10823 TS.diHPCARP_Ib.1600HHshift.b.ltmud 4.256e+43 4.43 4.43 2.538e+40 0.0882
10824 TS.diHPCARP_Ib.1600HHshift.a.ctpmud 1.996e+43 3.99 3.99 2.457e+40 0.0854
10825 TS.diHPCARP_Ib.1600HHshift.b.htmud 5.955e+43 4.67 4.67 2.358e+40 0.0819
10826 TS.diHPCARP_Ib.1600HHshift.a.ltpmud 1.112e+43 3.73 3.73 2.128e+40 0.074
10827 TS.diHPCARP_Ib.1600HHshift.b.ptpmud 4.851e+43 4.61 4.61 2.110e+40 0.0733
10828 TS.diHPCARP_Ib.1600HHshift.a.htmud 2.230e+43 4.22 4.22 1.895e+40 0.0658
10829 TS.diHPCARP_Ib.1600HHshift.b.mtmud 2.828e+43 4.40 4.40 1.765e+40 0.0613
10830 TS.diHPCARP_Ib.1600HHshift.a.ptpmud 1.928e+43 4.24 4.24 1.562e+40 0.0543
10831 TS.diHPCARP_Ib.1600HHshift.a.httpmud 5.805e+43 4.90 4.90 1.552e+40 0.0539
10832 TS.diHPCARP_Ib.1600HHshift.b.ltpmud 2.787e+43 4.49 4.49 1.501e+40 0.0521
10833 TS.diHPCARP_Ib.1600HHshift.a.ctmud 3.012e+43 4.62 4.62 1.304e+40 0.0453
10834 TS.diHPCARP_Ib.1600HHshift.a.mmpmud 5.403e+42 3.72 3.72 1.050e+40 0.0365
10835 TS.diHPCARP_Ib.1600HHshift.a.ptpmud 3.262e+43 4.83 4.83 9.934e+39 0.0345
10836 TS.diHPCARP_Ib.1600HHshift.a.pmpmud 8.786e+42 4.14 4.14 8.509e+39 0.0296
10837 TS.diHPCARP_Ib.1600HHshift.b.httpmud 3.557e+43 4.98 4.98 8.439e+39 0.0293
10838 TS.diHPCARP_Ib.1600HHshift.a.ctpmud 2.288e+43 5.01 5.01 7.375e+39 0.0256
10839 TS.diHPCARP_Ib.1600HHshift.a.pmmud 2.327e+43 4.91 4.91 6.120e+39 0.0213
10840 TS.diHPCARP_Ib.1600HHshift.b.htmud 5.515e+43 5.65 5.65 4.250e+39 0.0148
10841 TS.diHPCARP_Ib.1600HHshift.b.pmmud 5.893e+43 5.69 5.69 4.222e+39 0.0147
10842 TS.diHPCARP_Ib.1600HHshift.b.lppmud 9.052e+42 4.58 4.58 4.145e+39 0.0144
10843 TS.diHPCARP_Ib.1600HHshift.a.lppmud 1.403e+43 4.99 4.99 3.262e+39 0.0113
10844 TS.diHPCARP_Ib.1600HHshift.a.mtpmud 2.510e+43 5.41 5.41 2.869e+39 0.00997
10845 TS.diHPCARP_Ib.1600HHshift.b.ctmud 2.672e+43 5.45 5.45 2.842e+39 0.00988
10846 TS.diHPCARP_Ib.1600HHshift.b.hmmud 5.772e+42 4.57 4.57 2.693e+39 0.00936
10847 TS.diHPCARP_Ib.1600HHshift.b.mtpmud 2.094e+43 5.38 5.38 2.530e+39 0.00879

10848	TS.diHPCARP_Ib.1600HHshift.a.ltmmdu	1.313e+43	5.18	5.18	2.225e+39	0.00773
10849	TS.diHPCARP_Ib.1600HHshift.b.lttmdu	9.249e+42	5.01	5.01	2.060e+39	0.00716
10850	TS.diHPCARP_Ib.1600HHshift.a.cttpud	2.434e+43	5.62	5.62	1.966e+39	0.00683
10851	TS.diHPCARP_Ib.1600HHshift.b.ctmpud	3.552e+43	5.87	5.87	1.880e+39	0.00653
10852	TS.diHPCARP_Ib.1600HHshift.a.mmtmdu	1.166e+43	5.29	5.29	1.624e+39	0.00564
10853	TS.diHPCARP_Ib.1600HHshift.a.hmpmud	2.092e+43	5.71	5.71	1.443e+39	0.00501
10854	TS.diHPCARP_Ib.1600HHshift.b.mppmud	4.987e+43	6.27	6.27	1.348e+39	0.00469
10855	TS.diHPCARP_Ib.1600HHshift.a.cttmud	3.358e+43	6.08	6.08	1.257e+39	0.00437
10856	TS.diHPCARP_Ib.1600HHshift.b.lttmdu	1.378e+43	5.66	5.66	1.037e+39	0.0036
10857	TS.diHPCARP_Ib.1600HHshift.a.cmtmdu	1.865e+43	5.86	5.86	1.012e+39	0.00352
10858	TS.diHPCARP_Ib.1600HHshift.b.lptmud	1.195e+43	5.64	5.64	9.244e+38	0.00321
10859	TS.diHPCARP_Ib.1600HHshift.b.cmpmdu	3.063e+43	6.30	6.30	7.858e+38	0.00273
10860	TS.diHPCARP_Ib.1600HHshift.b.pppmud	2.527e+43	6.23	6.23	7.295e+38	0.00253
10861	TS.diHPCARP_Ib.1600HHshift.b.hmtmdu	9.566e+42	5.68	5.68	6.975e+38	0.00242
10862	TS.diHPCARP_Ib.1600HHshift.a.lptmud	1.554e+43	6.14	6.14	5.234e+38	0.00182
10863	TS.diHPCARP_Ib.1600HHshift.a.lptmdu	1.377e+43	6.07	6.07	5.206e+38	0.00181
10864	TS.diHPCARP_Ib.1600HHshift.b.cttpud	2.623e+43	6.47	6.47	5.059e+38	0.00176
10865	TS.diHPCARP_Ib.1600HHshift.b.cpmud	1.564e+43	6.24	6.24	4.482e+38	0.00156
10866	TS.diHPCARP_Ib.1600HHshift.a.cttmud	3.517e+43	6.84	6.84	3.639e+38	0.00126
10867	TS.diHPCARP_Ib.1600HHshift.b.lmmpud	1.242e+43	6.37	6.37	2.845e+38	0.000989
10868	TS.diHPCARP_Ib.1600HHshift.b.mppmdu	1.964e+43	6.76	6.76	2.324e+38	0.000807
10869	TS.diHPCARP_Ib.1600HHshift.a.pppmud	3.175e+43	7.27	7.27	1.615e+38	0.000561
10870	TS.diHPCARP_Ib.1600HHshift.a.lmmpud	2.571e+43	7.18	7.18	1.520e+38	0.000528
10871	TS.diHPCARP_Ib.1600HHshift.a.cpmud	2.581e+43	7.39	7.39	1.071e+38	0.000372
10872	TS.diHPCARP_Ib.1600HHshift.a.cmpmdu	8.894e+42	6.83	6.83	9.431e+37	0.000328
10873	TS.diHPCARP_Ib.1600HHshift.b.lppmud	4.056e+43	7.93	7.93	6.750e+37	0.000235
10874	TS.diHPCARP_Ib.1600HHshift.a.lppmud	1.862e+43	7.70	7.70	4.606e+37	0.00016
10875	TS.diHPCARP_Ib.1600HHshift.b.tmmud	3.191e+43	8.05	8.05	4.341e+37	0.000151
10876	TS.diHPCARP_Ib.1600HHshift.a.tppmud	5.909e+42	7.28	7.28	2.958e+37	0.000103
10877	TS.diHPCARP_Ib.1600HHshift.a.hmmpud	8.349e+42	7.63	7.63	2.316e+37	8.05e-05
10878	TS.diHPCARP_Ib.1600HHshift.b.hmmpud	1.388e+43	8.10	8.10	1.740e+37	6.05e-05
10879	TS.diHPCARP_Ib.1600HHshift.a.lmtpud	2.004e+43	8.57	8.57	1.140e+37	3.96e-05
10880	TS.diHPCARP_Ib.1600HHshift.a.lmmpud	1.171e+43	8.26	8.26	1.130e+37	3.93e-05
10881	TS.diHPCARP_Ib.1600HHshift.b.lmtpud	3.345e+43	8.94	8.94	1.035e+37	3.59e-05
10882	TS.diHPCARP_Ib.1600HHshift.a.mppmdu	3.220e+43	9.08	9.08	7.871e+36	2.73e-05
10883	TS.diHPCARP_Ib.1600HHshift.b.lppmud	3.698e+43	9.44	9.44	4.920e+36	1.71e-05
10884	TS.diHPCARP_Ib.1600HHshift.b.hptmdu	2.859e+43	9.68	9.68	2.521e+36	8.76e-06
10885	TS.diHPCARP_Ib.1600HHshift.b.tppmud	1.361e+43	9.60	9.60	1.387e+36	4.82e-06
10886	TS.diHPCARP_Ib.1600HHshift.b.lppmud	5.730e+43	10.52	10.52	1.234e+36	4.29e-06
10887	TS.diHPCARP_Ib.1600HHshift.a.lppmud	3.451e+43	11.14	11.14	2.628e+35	9.13e-07
10888	TS.diHPCARP_Ib.1600HHshift.a.hptmdu	1.719e+43	11.48	11.48	7.431e+34	2.58e-07
10889	Total				2.878e+43	100

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1,4-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde

10895
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Population analysis at 300K. Vibrational scaling: 0.971.

10899 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

10900 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

10901 %: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
10904	TS.diHPCARP_I.14HPHshift.mtppptd	4.166e+42	0.00	0.00	4.166e+42	98.5
10905	TS.diHPCARP_I.14HPHshift.mttmtd	2.751e+43	4.17	4.17	2.540e+40	0.601
10906	TS.diHPCARP_I.14HPHshift.mptmtd	2.412e+43	4.62	4.62	1.046e+40	0.247
10907	TS.diHPCARP_I.14HPHshift.mppmtd	1.821e+43	4.71	4.71	6.767e+39	0.16
10908	TS.diHPCARP_I.14HPHshift.mptptd	1.217e+43	4.68	4.68	4.767e+39	0.113
10909	TS.diHPCARP_I.14HPHshift.mmpmtd	8.921e+42	4.53	4.53	4.438e+39	0.105
10910	TS.diHPCARP_I.14HPHshift.mmmptd	6.690e+42	4.77	4.77	2.236e+39	0.0529
10911	TS.diHPCARP_I.14HPHshift.ptpppd	3.712e+43	5.88	5.88	1.934e+39	0.0457
10912	TS.diHPCARP_I.14HPHshift.ptppptd	4.109e+43	6.13	6.13	1.407e+39	0.0333
10913	TS.diHPCARP_I.14HPHshift.mtmtpd	5.240e+43	6.87	6.87	5.159e+38	0.0122
10914	TS.diHPCARP_I.14HPHshift.mttmtd	1.985e+43	6.32	6.32	4.968e+38	0.0117
10915	TS.diHPCARP_I.14HPHshift.mtmtpd	8.237e+43	7.35	7.35	3.672e+38	0.00868
10916	TS.diHPCARP_I.14HPHshift.mmpmtd	5.456e+42	5.77	5.77	3.434e+38	0.00812
10917	TS.diHPCARP_I.14HPHshift.pmpptd	8.272e+42	6.04	6.04	3.313e+38	0.00784
10918	TS.diHPCARP_I.14HPHshift.ptppmtd	9.925e+42	6.26	6.26	2.728e+38	0.00645
10919	TS.diHPCARP_I.14HPHshift.mmpmtd	9.083e+42	6.21	6.21	2.725e+38	0.00644

10920	TS.diHPCARP_I.14HPHshift.mmmmtmd	5.574e+43	7.37	7.37	2.367e+38	0.0056
10921	TS.diHPCARP_I.14HPHshift.mmmtpdp	7.136e+43	7.57	7.57	2.176e+38	0.00515
10922	TS.diHPCARP_I.14HPHshift.mtppmtd	1.897e+43	6.80	6.80	2.108e+38	0.00499
10923	TS.diHPCARP_I.14HPHshift.mmpppmd	1.520e+43	6.71	6.71	1.968e+38	0.00465
10924	TS.diHPCARP_I.14HPHshift.mtptptd	1.814e+43	6.92	6.92	1.637e+38	0.00387
10925	TS.diHPCARP_I.14HPHshift.mtpptmd	7.381e+43	7.87	7.87	1.367e+38	0.00323
10926	TS.diHPCARP_I.14HPHshift.mmmmtmd	6.843e+43	8.11	8.11	8.394e+37	0.00199
10927	TS.diHPCARP_I.14HPHshift.pmmmtmd	6.138e+43	8.08	8.08	8.037e+37	0.0019
10928	TS.diHPCARP_I.14HPHshift.tmmmtmd	4.156e+43	7.87	7.87	7.660e+37	0.00181
10929	TS.diHPCARP_I.14HPHshift.mmttmd	5.611e+43	8.09	8.09	7.127e+37	0.00169
10930	TS.diHPCARP_I.14HPHshift.mtmptmd	4.978e+43	8.09	8.09	6.415e+37	0.00152
10931	TS.diHPCARP_I.14HPHshift.mmmtptd	4.892e+43	8.12	8.12	5.956e+37	0.00141
10932	TS.diHPCARP_I.14HPHshift.mmttmd	4.829e+43	8.17	8.17	5.372e+37	0.00127
10933	TS.diHPCARP_I.14HPHshift.pmmtpdp	4.413e+43	8.17	8.17	4.931e+37	0.00117
10934	TS.diHPCARP_I.14HPHshift.pmpmtd	6.653e+43	8.47	8.47	4.470e+37	0.00106
10935	TS.diHPCARP_I.14HPHshift.mmmtttd	1.377e+44	8.95	8.95	4.152e+37	0.000982
10936	TS.diHPCARP_I.14HPHshift.mtptppd	4.154e+43	8.32	8.32	3.612e+37	0.000854
10937	TS.diHPCARP_I.14HPHshift.mtttptd	6.448e+43	8.73	8.73	2.817e+37	0.000666
10938	TS.diHPCARP_I.14HPHshift.tmmptmd	4.958e+43	8.61	8.61	2.634e+37	0.000623
10939	TS.diHPCARP_I.14HPHshift.mtptmmd	4.572e+43	8.57	8.57	2.617e+37	0.000619
10940	TS.diHPCARP_I.14HPHshift.tpmtpdp	1.814e+44	9.41	9.41	2.547e+37	0.000602
10941	TS.diHPCARP_I.14HPHshift.mmppppd	1.628e+43	8.02	8.02	2.359e+37	0.000558
10942	TS.diHPCARP_I.14HPHshift.mtmtpdp	8.899e+43	9.04	9.04	2.325e+37	0.00055
10943	TS.diHPCARP_I.14HPHshift.mmpmtd	3.582e+43	8.50	8.50	2.296e+37	0.000543
10944	TS.diHPCARP_I.14HPHshift.mppmtd	8.132e+43	9.00	9.00	2.276e+37	0.000538
10945	TS.diHPCARP_I.14HPHshift.mptptmd	1.889e+44	9.51	9.51	2.232e+37	0.000528
10946	TS.diHPCARP_I.14HPHshift.mptmtd	1.388e+43	7.98	7.98	2.145e+37	0.000507
10947	TS.diHPCARP_I.14HPHshift.mppmtd	1.450e+43	8.01	8.01	2.104e+37	0.000497
10948	TS.diHPCARP_I.14HPHshift.tpmptmd	1.455e+44	9.45	9.45	1.914e+37	0.000453
10949	TS.diHPCARP_I.14HPHshift.tppmtd	3.070e+43	8.60	8.60	1.661e+37	0.000393
10950	TS.diHPCARP_I.14HPHshift.mttmmd	1.285e+44	9.51	9.51	1.507e+37	0.000356
10951	TS.diHPCARP_I.14HPHshift.mmpmtd	3.092e+43	8.72	8.72	1.385e+37	0.000328
10952	TS.diHPCARP_I.14HPHshift.mmtttd	4.291e+44	10.38	10.38	1.182e+37	0.00028
10953	TS.diHPCARP_I.14HPHshift.ptptptd	4.536e+43	9.12	9.12	1.038e+37	0.000246
10954	TS.diHPCARP_I.14HPHshift.ptmtpdp	4.064e+43	9.67	9.67	9.583e+36	0.000227
10955	TS.diHPCARP_I.14HPHshift.mmpmmd	7.528e+42	8.10	8.10	9.497e+36	0.000225
10956	TS.diHPCARP_I.14HPHshift.mmpmtd	4.899e+43	9.27	9.27	8.597e+36	0.000203
10957	TS.diHPCARP_I.14HPHshift.mmpmtd	2.219e+43	8.81	8.81	8.478e+36	0.000201
10958	TS.diHPCARP_I.14HPHshift.mtmmtmd	6.465e+43	9.46	9.46	8.268e+36	0.000196
10959	TS.diHPCARP_I.14HPHshift.mpmtd	7.039e+43	9.52	9.52	8.151e+36	0.000193
10960	TS.diHPCARP_I.14HPHshift.mmpmtd	1.842e+43	8.91	8.91	5.920e+36	0.00014
10961	TS.diHPCARP_I.14HPHshift.mtmtpmd	4.834e+43	9.52	9.52	5.627e+36	0.000133
10962	TS.diHPCARP_I.14HPHshift.ttttmd	8.990e+43	9.89	9.89	5.581e+36	0.000132
10963	TS.diHPCARP_I.14HPHshift.mptmmd	4.310e+43	9.47	9.47	5.482e+36	0.00013
10964	TS.diHPCARP_I.14HPHshift.ttttmd	6.272e+43	9.69	9.69	5.459e+36	0.000129
10965	TS.diHPCARP_I.14HPHshift.mmpmtd	4.806e+43	9.57	9.57	5.115e+36	0.000121
10966	TS.diHPCARP_I.14HPHshift.mttttd	1.634e+44	10.33	10.33	4.901e+36	0.000116
10967	TS.diHPCARP_I.14HPHshift.mtmppd	6.295e+43	9.81	9.81	4.457e+36	0.000105
10968	TS.diHPCARP_I.14HPHshift.mtpttd	8.787e+43	10.02	10.02	4.400e+36	0.000104
10969	TS.diHPCARP_I.14HPHshift.ptptmd	5.461e+43	9.75	9.75	4.281e+36	0.000101
10970	TS.diHPCARP_I.14HPHshift.mtmtpdp	1.177e+44	10.31	10.31	3.633e+36	8.59e-05
10971	TS.diHPCARP_I.14HPHshift.tppmtd	1.021e+43	8.87	8.87	3.547e+36	8.39e-05
10972	TS.diHPCARP_I.14HPHshift.mppmmd	4.161e+43	9.76	9.76	3.236e+36	7.65e-05
10973	TS.diHPCARP_I.14HPHshift.mtmtpmd	7.804e+43	10.14	10.14	3.222e+36	7.62e-05
10974	TS.diHPCARP_I.14HPHshift.ppttpd	8.383e+43	10.19	10.19	3.180e+36	7.52e-05
10975	TS.diHPCARP_I.14HPHshift.mttmtd	1.099e+44	10.40	10.40	2.934e+36	6.94e-05
10976	TS.diHPCARP_I.14HPHshift.mmpmtd	8.774e+42	8.90	8.90	2.881e+36	6.81e-05
10977	TS.diHPCARP_I.14HPHshift.pmtmtd	4.735e+43	9.93	9.93	2.780e+36	6.57e-05
10978	TS.diHPCARP_I.14HPHshift.ptmppd	3.059e+43	9.67	9.67	2.767e+36	6.54e-05
10979	TS.diHPCARP_I.14HPHshift.mmpmtd	3.808e+43	9.85	9.85	2.524e+36	5.97e-05
10980	TS.diHPCARP_I.14HPHshift.mppmtd	1.413e+44	10.65	10.65	2.470e+36	5.84e-05
10981	TS.diHPCARP_I.14HPHshift.ptptmd	4.772e+43	10.05	10.05	2.269e+36	5.37e-05
10982	TS.diHPCARP_I.14HPHshift.mppmtd	2.158e+44	10.95	10.95	2.261e+36	5.35e-05
10983	TS.diHPCARP_I.14HPHshift.tpttmd	1.456e+44	10.73	10.73	2.205e+36	5.21e-05
10984	TS.diHPCARP_I.14HPHshift.mttmtd	1.394e+44	10.71	10.71	2.185e+36	5.17e-05
10985	TS.diHPCARP_I.14HPHshift.mppmtd	5.400e+43	10.27	10.27	1.794e+36	4.24e-05
10986	TS.diHPCARP_I.14HPHshift.tptmtd	6.583e+43	10.39	10.39	1.767e+36	4.18e-05
10987	TS.diHPCARP_I.14HPHshift.mpmtd	1.571e+44	10.97	10.97	1.592e+36	3.76e-05
10988	TS.diHPCARP_I.14HPHshift.mpmtd	2.805e+44	11.32	11.32	1.583e+36	3.74e-05
10989	TS.diHPCARP_I.14HPHshift.ttttmd	4.973e+44	11.67	11.67	1.577e+36	3.73e-05
10990	TS.diHPCARP_I.14HPHshift.mtmppd	3.936e+43	10.17	10.17	1.537e+36	3.63e-05
10991	TS.diHPCARP_I.14HPHshift.tptppd	8.818e+43	10.69	10.69	1.442e+36	3.41e-05

10992	TS.diHPCARP_I.14HPHshift.mtmmtpd	4.249e+43	10.25	10.25	1.440e+36	3.4e-05
10993	TS.diHPCARP_I.14HPHshift.mptttmd	5.377e+44	11.84	11.84	1.284e+36	3.04e-05
10994	TS.diHPCARP_I.14HPHshift.mttttpd	2.130e+44	11.31	11.31	1.220e+36	2.89e-05
10995	TS.diHPCARP_I.14HPHshift.ppppppd	3.740e+43	10.31	10.31	1.147e+36	2.71e-05
10996	TS.diHPCARP_I.14HPHshift.mppmtd	1.313e+44	11.07	11.07	1.127e+36	2.67e-05
10997	TS.diHPCARP_I.14HPHshift.mpptmd	1.470e+44	11.15	11.15	1.104e+36	2.61e-05
10998	TS.diHPCARP_I.14HPHshift.tpptpd	2.450e+44	11.50	11.50	1.036e+36	2.45e-05
10999	TS.diHPCARP_I.14HPHshift.mttmppd	3.444e+43	10.36	10.36	9.742e+35	2.3e-05
11000	TS.diHPCARP_I.14HPHshift.mttttmd	2.454e+44	11.54	11.54	9.660e+35	2.28e-05
11001	TS.diHPCARP_I.14HPHshift.pppmptd	3.015e+43	10.31	10.31	9.310e+35	2.2e-05
11002	TS.diHPCARP_I.14HPHshift.mptmtpd	2.728e+43	10.28	10.28	8.786e+35	2.08e-05
11003	TS.diHPCARP_I.14HPHshift.ppttptd	2.283e+44	11.56	11.56	8.725e+35	2.06e-05
11004	TS.diHPCARP_I.14HPHshift.ptmptmd	1.638e+44	11.37	11.37	8.489e+35	2.01e-05
11005	TS.diHPCARP_I.14HPHshift.mptmtd	6.746e+43	10.89	10.89	7.826e+35	1.85e-05
11006	TS.diHPCARP_I.14HPHshift.mmpmtd	7.161e+43	10.94	10.94	7.656e+35	1.81e-05
11007	TS.diHPCARP_I.14HPHshift.mppmtpd	2.318e+43	10.30	10.30	7.249e+35	1.71e-05
11008	TS.diHPCARP_I.14HPHshift.mtptmd	8.973e+43	11.21	11.21	6.154e+35	1.46e-05
11009	TS.diHPCARP_I.14HPHshift.mmpmtmd	6.323e+43	11.02	11.02	5.919e+35	1.4e-05
11010	TS.diHPCARP_I.14HPHshift.ptptpd	1.172e+44	11.44	11.44	5.403e+35	1.28e-05
11011	TS.diHPCARP_I.14HPHshift.mmpmtpd	9.234e+43	11.36	11.36	4.930e+35	1.17e-05
11012	TS.diHPCARP_I.14HPHshift.ppptmmd	1.431e+44	11.62	11.62	4.891e+35	1.16e-05
11013	TS.diHPCARP_I.14HPHshift.pppptmd	2.212e+44	11.97	11.97	4.196e+35	9.92e-06
11014	TS.diHPCARP_I.14HPHshift.mptpmd	6.850e+43	11.28	11.28	4.162e+35	9.84e-06
11015	TS.diHPCARP_I.14HPHshift.mppmmd	8.851e+42	10.15	10.15	3.562e+35	8.42e-06
11016	TS.diHPCARP_I.14HPHshift.pptmmd	7.428e+43	11.51	11.51	3.042e+35	7.19e-06
11017	TS.diHPCARP_I.14HPHshift.ptmpmd	2.263e+43	10.84	10.84	2.864e+35	6.77e-06
11018	TS.diHPCARP_I.14HPHshift.pptpmd	1.472e+44	12.15	12.15	2.077e+35	4.91e-06
11019	TS.diHPCARP_I.14HPHshift.ptttptd	7.396e+43	11.80	11.80	1.874e+35	4.43e-06
11020	TS.diHPCARP_I.14HPHshift.ptmtmmd	7.857e+43	11.89	11.89	1.704e+35	4.03e-06
11021	TS.diHPCARP_I.14HPHshift.ppptmpd	5.267e+43	11.66	11.66	1.681e+35	3.97e-06
11022	TS.diHPCARP_I.14HPHshift.pttptd	3.559e+43	11.48	11.48	1.552e+35	3.67e-06
11023	TS.diHPCARP_I.14HPHshift.ppttptd	1.009e+44	12.21	12.21	1.279e+35	3.02e-06
11024	TS.diHPCARP_I.14HPHshift.mptmppd	2.438e+43	11.47	11.47	1.083e+35	2.56e-06
11025	TS.diHPCARP_I.14HPHshift.ppptmmd	1.285e+44	12.68	12.68	7.397e+34	1.75e-06
11026	TS.diHPCARP_I.14HPHshift.mppmppd	2.201e+43	11.65	11.65	7.121e+34	1.68e-06
11027	TS.diHPCARP_I.14HPHshift.ppppmd	1.798e+43	11.74	11.74	5.041e+34	1.19e-06
11028	TS.diHPCARP_I.14HPHshift.tptmtd	2.126e+44	15.70	15.70	7.796e+32	1.84e-08
11029	TS.diHPCARP_I.14HPHshift.ttmppd	5.023e+43	15.01	15.01	5.881e+32	1.39e-08
11030	TS.diHPCARP_I.14HPHshift.tppmppd	4.343e+43	16.85	16.85	2.304e+31	5.45e-10
11031	TS.diHPCARP_I.14HPHshift.tptmppd	4.145e+43	16.85	16.85	2.187e+31	5.17e-10
11032	Total				4.228e+42	100

11033
11034
11035
11036 1,5-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,R-
11037 di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde
11038 =====
11039 =====

11040
11041 Population analysis at 300K. Vibrational scaling: 0.971.
11042 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
11043 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
11044 %: contribution to the population (with current data set assumed 100%)
11045

Compound	Qtot	Erel	Erel2	n*Q*MB	%
11046					
11047	TS.diHPCARP_I.15HPHshift.dmtduuu	2.645e+42	0.00	0.00	2.645e+42 42.7
11048	TS.diHPCARP_I.15HPHshift.dmmdudu	8.890e+43	2.43	2.43	1.511e+42 24.4
11049	TS.diHPCARP_I.15HPHshift.dmmtddu	5.929e+42	1.42	1.42	5.464e+41 8.81
11050	TS.diHPCARP_I.15HPHshift.dcmumu	1.664e+44	4.05	4.05	1.850e+41 2.98
11051	TS.diHPCARP_I.15HPHshift.dmmdupu	1.206e+43	2.55	2.55	1.668e+41 2.69
11052	TS.diHPCARP_I.15HPHshift.dmmupdu	7.771e+43	3.73	3.73	1.493e+41 2.41
11053	TS.diHPCARP_I.15HPHshift.dmpumu	2.205e+44	4.53	4.53	1.112e+41 1.79
11054	TS.diHPCARP_I.15HPHshift.dmpdmu	2.084e+44	4.56	4.56	9.926e+40 1.6
11055	TS.diHPCARP_I.15HPHshift.dmmduddu	2.367e+43	3.27	3.27	9.886e+40 1.59
11056	TS.diHPCARP_I.15HPHshift.dmpupuu	2.793e+42	2.04	2.04	9.049e+40 1.46
11057	TS.diHPCARP_I.15HPHshift.dmpdupu	2.940e+43	3.64	3.64	6.524e+40 1.05
11058	TS.diHPCARP_I.15HPHshift.dmmupuu	1.464e+43	3.35	3.35	5.324e+40 0.859
11059	TS.diHPCARP_I.15HPHshift.dmmupuu	5.131e+42	2.78	2.78	4.838e+40 0.78
11060	TS.diHPCARP_I.15HPHshift.dmmutdu	1.108e+43	3.28	3.28	4.555e+40 0.735
11061	TS.diHPCARP_I.15HPHshift.dmpupu	2.080e+43	3.69	3.69	4.275e+40 0.689
11062	TS.diHPCARP_I.15HPHshift.dcmudu	2.811e+42	2.59	2.59	3.634e+40 0.586
11063	TS.diHPCARP_I.15HPHshift.dmpdtdu	1.884e+43	3.78	3.78	3.348e+40 0.54

11064	TS.diHPCARP_I.15HPHshift.dmpu	4.733e+42	3.08	3.08	2.679e+40	0.432
11065	TS.diHPCARP_I.15HPHshift.dmpu	1.739e+43	3.99	3.99	2.155e+40	0.348
11066	TS.diHPCARP_I.15HPHshift.dctu	5.957e+44	6.19	6.19	1.831e+40	0.295
11067	TS.diHPCARP_I.15HPHshift.dctu	1.114e+44	5.29	5.29	1.561e+40	0.252
11068	TS.diHPCARP_I.15HPHshift.dmt	1.142e+43	4.01	4.01	1.376e+40	0.222
11069	TS.diHPCARP_I.15HPHshift.dmt	5.945e+43	5.03	5.03	1.291e+40	0.208
11070	TS.diHPCARP_I.15HPHshift.dcp	1.366e+43	4.16	4.16	1.270e+40	0.205
11071	TS.diHPCARP_I.15HPHshift.dcm	2.978e+43	4.72	4.72	1.092e+40	0.176
11072	TS.diHPCARP_I.15HPHshift.dcp	4.431e+43	4.97	4.97	1.066e+40	0.172
11073	TS.diHPCARP_I.15HPHshift.dcm	1.311e+43	4.29	4.29	9.880e+39	0.159
11074	TS.diHPCARP_I.15HPHshift.dmd	9.171e+42	4.24	4.24	7.528e+39	0.121
11075	TS.diHPCARP_I.15HPHshift.dmt	1.766e+44	6.02	6.02	7.326e+39	0.118
11076	TS.diHPCARP_I.15HPHshift.dmt	1.328e+44	5.85	5.85	7.277e+39	0.117
11077	TS.diHPCARP_I.15HPHshift.umt	1.002e+44	5.75	5.75	6.442e+39	0.104
11078	TS.diHPCARP_I.15HPHshift.umt	4.053e+43	5.23	5.23	6.253e+39	0.101
11079	TS.diHPCARP_I.15HPHshift.dmt	1.336e+43	4.70	4.70	5.066e+39	0.0817
11080	TS.diHPCARP_I.15HPHshift.dmt	3.942e+42	3.98	3.98	4.986e+39	0.0804
11081	TS.diHPCARP_I.15HPHshift.umt	7.438e+43	5.79	5.79	4.484e+39	0.0723
11082	TS.diHPCARP_I.15HPHshift.dmt	8.536e+42	4.51	4.51	4.435e+39	0.0715
11083	TS.diHPCARP_I.15HPHshift.dpt	1.185e+43	4.73	4.73	4.212e+39	0.0679
11084	TS.diHPCARP_I.15HPHshift.dmt	2.157e+43	5.11	5.11	4.074e+39	0.0657
11085	TS.diHPCARP_I.15HPHshift.umt	5.470e+43	5.67	5.67	4.039e+39	0.0652
11086	TS.diHPCARP_I.15HPHshift.dcp	1.502e+43	5.10	5.10	2.906e+39	0.0469
11087	TS.diHPCARP_I.15HPHshift.dmm	1.598e+44	6.59	6.59	2.529e+39	0.0408
11088	TS.diHPCARP_I.15HPHshift.dmp	1.887e+43	5.33	5.33	2.481e+39	0.04
11089	TS.diHPCARP_I.15HPHshift.dct	1.207e+43	5.09	5.09	2.377e+39	0.0383
11090	TS.diHPCARP_I.15HPHshift.dmm	8.169e+43	6.23	6.23	2.365e+39	0.0382
11091	TS.diHPCARP_I.15HPHshift.dmt	2.387e+43	5.51	5.51	2.297e+39	0.0371
11092	TS.diHPCARP_I.15HPHshift.ucp	4.667e+43	5.93	5.93	2.223e+39	0.0359
11093	TS.diHPCARP_I.15HPHshift.dcm	3.961e+42	4.51	4.51	2.037e+39	0.0329
11094	TS.diHPCARP_I.15HPHshift.dmt	2.528e+43	5.68	5.68	1.832e+39	0.0295
11095	TS.diHPCARP_I.15HPHshift.uct	1.262e+43	5.30	5.30	1.725e+39	0.0278
11096	TS.diHPCARP_I.15HPHshift.ucp	2.695e+44	7.17	7.17	1.614e+39	0.026
11097	TS.diHPCARP_I.15HPHshift.dmp	2.065e+44	7.08	7.08	1.444e+39	0.0233
11098	TS.diHPCARP_I.15HPHshift.uct	6.473e+43	6.42	6.42	1.364e+39	0.022
11099	TS.diHPCARP_I.15HPHshift.ucm	3.281e+43	6.04	6.04	1.299e+39	0.0209
11100	TS.diHPCARP_I.15HPHshift.dmp	2.156e+43	5.80	5.80	1.284e+39	0.0207
11101	TS.diHPCARP_I.15HPHshift.dcp	1.884e+43	5.72	5.72	1.276e+39	0.0206
11102	TS.diHPCARP_I.15HPHshift.dmt	9.105e+42	5.34	5.34	1.173e+39	0.0189
11103	TS.diHPCARP_I.15HPHshift.umt	3.489e+42	4.80	4.80	1.118e+39	0.018
11104	TS.diHPCARP_I.15HPHshift.dhm	4.357e+42	4.94	4.94	1.097e+39	0.0177
11105	TS.diHPCARP_I.15HPHshift.dmm	5.582e+43	6.50	6.50	1.035e+39	0.0167
11106	TS.diHPCARP_I.15HPHshift.uct	1.441e+43	5.69	5.69	1.025e+39	0.0165
11107	TS.diHPCARP_I.15HPHshift.ulp	4.943e+43	6.54	6.54	8.553e+38	0.0138
11108	TS.diHPCARP_I.15HPHshift.ucm	1.570e+43	5.86	5.86	8.435e+38	0.0136
11109	TS.diHPCARP_I.15HPHshift.ulp	5.829e+44	8.02	8.02	8.354e+38	0.0135
11110	TS.diHPCARP_I.15HPHshift.dhm	5.681e+42	5.32	5.32	7.611e+38	0.0123
11111	TS.diHPCARP_I.15HPHshift.dcm	3.256e+43	6.37	6.37	7.450e+38	0.012
11112	TS.diHPCARP_I.15HPHshift.ult	2.499e+43	6.27	6.27	6.744e+38	0.0109
11113	TS.diHPCARP_I.15HPHshift.dhm	4.857e+42	5.30	5.30	6.728e+38	0.0109
11114	TS.diHPCARP_I.15HPHshift.ult	1.083e+44	7.18	7.18	6.404e+38	0.0103
11115	TS.diHPCARP_I.15HPHshift.dlmut	4.903e+43	6.72	6.72	6.248e+38	0.0101
11116	TS.diHPCARP_I.15HPHshift.ulp	3.375e+44	7.91	7.91	5.849e+38	0.00943
11117	TS.diHPCARP_I.15HPHshift.dmm	1.009e+43	5.84	5.84	5.644e+38	0.0091
11118	TS.diHPCARP_I.15HPHshift.ulp	2.804e+44	7.84	7.84	5.423e+38	0.00875
11119	TS.diHPCARP_I.15HPHshift.upp	1.224e+44	7.37	7.37	5.242e+38	0.00846
11120	TS.diHPCARP_I.15HPHshift.umm	7.022e+43	7.05	7.05	5.130e+38	0.00827
11121	TS.diHPCARP_I.15HPHshift.uct	3.275e+43	6.73	6.73	4.104e+38	0.00662
11122	TS.diHPCARP_I.15HPHshift.dhm	4.969e+43	7.06	7.06	3.583e+38	0.00578
11123	TS.diHPCARP_I.15HPHshift.dhp	1.155e+43	6.27	6.27	3.153e+38	0.00509
11124	TS.diHPCARP_I.15HPHshift.dhp	9.935e+42	6.25	6.25	2.773e+38	0.00447
11125	TS.diHPCARP_I.15HPHshift.dlmd	5.940e+43	7.35	7.35	2.635e+38	0.00425
11126	TS.diHPCARP_I.15HPHshift.ucp	2.650e+44	8.28	8.28	2.476e+38	0.00399
11127	TS.diHPCARP_I.15HPHshift.ucp	1.239e+43	6.46	6.46	2.441e+38	0.00394
11128	TS.diHPCARP_I.15HPHshift.dhm	5.885e+42	6.11	6.11	2.092e+38	0.00337
11129	TS.diHPCARP_I.15HPHshift.ump	1.376e+43	6.71	6.71	1.785e+38	0.00288
11130	TS.diHPCARP_I.15HPHshift.dlp	2.325e+43	7.04	7.04	1.738e+38	0.0028
11131	TS.diHPCARP_I.15HPHshift.dmd	1.853e+44	8.29	8.29	1.686e+38	0.00272
11132	TS.diHPCARP_I.15HPHshift.dpp	3.967e+42	6.05	6.05	1.542e+38	0.00249
11133	TS.diHPCARP_I.15HPHshift.ulp	2.739e+43	7.21	7.21	1.529e+38	0.00247
11134	TS.diHPCARP_I.15HPHshift.dmp	7.401e+42	6.45	6.45	1.485e+38	0.0024
11135	TS.diHPCARP_I.15HPHshift.dmt	1.356e+44	8.20	8.20	1.435e+38	0.00231

11136	TS.diHPCARP_I.15HPHshift.ummdpuuu	2.452e+43	7.22	7.22	1.352e+38	0.00218
11137	TS.diHPCARP_I.15HPHshift.umpumuuu	4.630e+43	7.63	7.63	1.282e+38	0.00207
11138	TS.diHPCARP_I.15HPHshift.ulmupduu	1.276e+43	6.88	6.88	1.250e+38	0.00202
11139	TS.diHPCARP_I.15HPHshift.ummupduu	2.269e+43	7.29	7.29	1.111e+38	0.00179
11140	TS.diHPCARP_I.15HPHshift.ulpdmuuu	4.960e+43	7.76	7.76	1.110e+38	0.00179
11141	TS.diHPCARP_I.15HPHshift.ulpdmduu	4.147e+43	7.66	7.66	1.083e+38	0.00175
11142	TS.diHPCARP_I.15HPHshift.dmpdpduu	4.335e+42	6.33	6.33	1.064e+38	0.00172
11143	TS.diHPCARP_I.15HPHshift.ummumduu	7.121e+43	8.03	8.03	1.007e+38	0.00162
11144	TS.diHPCARP_I.15HPHshift.ucmdtudu	7.710e+42	6.73	6.73	9.608e+37	0.00155
11145	TS.diHPCARP_I.15HPHshift.utmdpduu	1.143e+43	6.97	6.97	9.509e+37	0.00153
11146	TS.diHPCARP_I.15HPHshift.dmpupduu	4.552e+42	6.46	6.46	8.884e+37	0.00143
11147	TS.diHPCARP_I.15HPHshift.ucputddu	2.495e+43	7.48	7.48	8.867e+37	0.00143
11148	TS.diHPCARP_I.15HPHshift.ulpupudu	4.384e+43	7.86	7.86	8.306e+37	0.00134
11149	TS.diHPCARP_I.15HPHshift.dcpdmuuu	2.039e+43	7.41	7.41	8.110e+37	0.00131
11150	TS.diHPCARP_I.15HPHshift.umpdtduu	6.086e+42	6.72	6.72	7.774e+37	0.00125
11151	TS.diHPCARP_I.15HPHshift.dhmutduu	8.491e+43	8.34	8.34	7.140e+37	0.00115
11152	TS.diHPCARP_I.15HPHshift.ulmdpddu	3.621e+43	7.89	7.89	6.488e+37	0.00105
11153	TS.diHPCARP_I.15HPHshift.ulmumudu	1.284e+44	8.66	8.66	6.297e+37	0.00102
11154	TS.diHPCARP_I.15HPHshift.umpdpduu	2.558e+42	6.35	6.35	6.095e+37	0.000983
11155	TS.diHPCARP_I.15HPHshift.dhmdtudu	3.473e+43	7.92	7.92	5.884e+37	0.000949
11156	TS.diHPCARP_I.15HPHshift.dhpdmudu	4.065e+43	8.04	8.04	5.660e+37	0.000913
11157	TS.diHPCARP_I.15HPHshift.dpmumuuu	1.279e+43	7.37	7.37	5.478e+37	0.000884
11158	TS.diHPCARP_I.15HPHshift.dhmutuuu	3.117e+43	7.91	7.91	5.398e+37	0.000871
11159	TS.diHPCARP_I.15HPHshift.umpupduu	4.091e+43	8.08	8.08	5.324e+37	0.000859
11160	TS.diHPCARP_I.15HPHshift.ulputddu	3.817e+43	8.12	8.12	4.660e+37	0.000752
11161	TS.diHPCARP_I.15HPHshift.ummnutuu	4.633e+43	8.26	8.26	4.488e+37	0.000724
11162	TS.diHPCARP_I.15HPHshift.dhpumudu	5.003e+43	8.35	8.35	4.164e+37	0.000672
11163	TS.diHPCARP_I.15HPHshift.ummdmduu	2.992e+43	8.07	8.07	3.940e+37	0.000635
11164	TS.diHPCARP_I.15HPHshift.dppdpduu	3.889e+42	6.86	6.86	3.925e+37	0.000633
11165	TS.diHPCARP_I.15HPHshift.uctdtudu	1.094e+43	7.51	7.51	3.729e+37	0.000602
11166	TS.diHPCARP_I.15HPHshift.ummupduu	3.171e+43	8.15	8.15	3.681e+37	0.000594
11167	TS.diHPCARP_I.15HPHshift.dmtumduu	1.683e+44	9.14	9.14	3.665e+37	0.000591
11168	TS.diHPCARP_I.15HPHshift.ucpdpudu	1.683e+43	7.77	7.77	3.655e+37	0.00059
11169	TS.diHPCARP_I.15HPHshift.dhmumudu	2.472e+43	8.02	8.02	3.549e+37	0.000572
11170	TS.diHPCARP_I.15HPHshift.upmdpduu	8.538e+42	7.42	7.42	3.370e+37	0.000544
11171	TS.diHPCARP_I.15HPHshift.ulmupddu	2.726e+43	8.15	8.15	3.159e+37	0.000509
11172	TS.diHPCARP_I.15HPHshift.uppumuuu	3.645e+43	8.34	8.34	3.052e+37	0.000492
11173	TS.diHPCARP_I.15HPHshift.uhmdpddu	7.558e+42	7.44	7.44	2.883e+37	0.000465
11174	TS.diHPCARP_I.15HPHshift.dhtupduu	1.214e+43	7.72	7.72	2.883e+37	0.000465
11175	TS.diHPCARP_I.15HPHshift.ulpdtuuu	6.118e+43	8.70	8.70	2.806e+37	0.000453
11176	TS.diHPCARP_I.15HPHshift.dhtdpduu	7.243e+42	7.43	7.43	2.784e+37	0.000449
11177	TS.diHPCARP_I.15HPHshift.ummtdduu	3.784e+43	8.45	8.45	2.628e+37	0.000424
11178	TS.diHPCARP_I.15HPHshift.ummupduu	1.530e+43	7.92	7.92	2.618e+37	0.000422
11179	TS.diHPCARP_I.15HPHshift.dlpdtuuu	1.219e+43	7.82	7.82	2.431e+37	0.000392
11180	TS.diHPCARP_I.15HPHshift.ultumuuu	2.064e+44	9.56	9.56	2.240e+37	0.000361
11181	TS.diHPCARP_I.15HPHshift.uhpdmudu	2.354e+44	9.64	9.64	2.238e+37	0.000361
11182	TS.diHPCARP_I.15HPHshift.dmmtdduu	1.573e+43	8.07	8.07	2.073e+37	0.000334
11183	TS.diHPCARP_I.15HPHshift.ucmupudu	7.848e+43	9.07	9.07	1.932e+37	0.000312
11184	TS.diHPCARP_I.15HPHshift.ultupuuu	3.931e+43	8.67	8.67	1.895e+37	0.000306
11185	TS.diHPCARP_I.15HPHshift.uctdmuuu	4.596e+43	8.81	8.81	1.766e+37	0.000285
11186	TS.diHPCARP_I.15HPHshift.ultdpuuu	3.849e+43	8.75	8.75	1.636e+37	0.000264
11187	TS.diHPCARP_I.15HPHshift.uhpdpduu	6.477e+43	9.10	9.10	1.512e+37	0.000244
11188	TS.diHPCARP_I.15HPHshift.uhpupduu	3.759e+43	8.78	8.78	1.511e+37	0.000244
11189	TS.diHPCARP_I.15HPHshift.dhmupuuu	5.880e+42	7.70	7.70	1.443e+37	0.000233
11190	TS.diHPCARP_I.15HPHshift.ulpdtudu	7.139e+43	9.19	9.19	1.430e+37	0.000231
11191	TS.diHPCARP_I.15HPHshift.dhpdpduu	4.506e+42	7.59	7.59	1.338e+37	0.000216
11192	TS.diHPCARP_I.15HPHshift.ummdpddu	1.208e+43	8.18	8.18	1.335e+37	0.000215
11193	TS.diHPCARP_I.15HPHshift.uhmupduu	6.173e+42	7.84	7.84	1.194e+37	0.000193
11194	TS.diHPCARP_I.15HPHshift.dmtutduu	1.004e+43	8.14	8.14	1.172e+37	0.000189
11195	TS.diHPCARP_I.15HPHshift.dhmdpduu	1.137e+43	8.25	8.25	1.120e+37	0.000181
11196	TS.diHPCARP_I.15HPHshift.ultdmuuu	1.293e+44	9.84	9.84	8.843e+36	0.000143
11197	TS.diHPCARP_I.15HPHshift.dhtupduu	1.505e+43	8.59	8.59	8.378e+36	0.000135
11198	TS.diHPCARP_I.15HPHshift.dhtdmudu	1.760e+43	8.69	8.69	8.259e+36	0.000133
11199	TS.diHPCARP_I.15HPHshift.dhmdmuuu	4.141e+43	9.21	9.21	8.107e+36	0.000131
11200	TS.diHPCARP_I.15HPHshift.uhpumudu	1.662e+44	10.06	10.06	7.784e+36	0.000126
11201	TS.diHPCARP_I.15HPHshift.upputduu	6.876e+42	8.22	8.22	7.115e+36	0.000115
11202	TS.diHPCARP_I.15HPHshift.ucpupuuu	1.926e+43	8.94	8.94	5.894e+36	9.51e-05
11203	TS.diHPCARP_I.15HPHshift.dhtumuuu	3.582e+43	9.35	9.35	5.501e+36	8.87e-05
11204	TS.diHPCARP_I.15HPHshift.uppupuuu	6.463e+42	8.44	8.44	4.569e+36	7.37e-05
11205	TS.diHPCARP_I.15HPHshift.dhmdpduu	1.236e+43	8.85	8.85	4.435e+36	7.15e-05
11206	TS.diHPCARP_I.15HPHshift.ultdpduu	2.388e+43	9.29	9.29	4.108e+36	6.63e-05
11207	TS.diHPCARP_I.15HPHshift.ultdtduu	4.363e+43	9.68	9.68	3.877e+36	6.25e-05

11208	TS.diHPCARP_I.15HPHshift.uctdtudu	6.981e+43	9.98	9.98	3.749e+36	6.05e-05
11209	TS.diHPCARP_I.15HPHshift.ucpdtudu	5.361e+43	9.84	9.84	3.612e+36	5.83e-05
11210	TS.diHPCARP_I.15HPHshift.uhpdpuu	3.002e+43	9.58	9.58	3.167e+36	5.11e-05
11211	TS.diHPCARP_I.15HPHshift.dlpdpduu	1.260e+43	9.08	9.08	3.044e+36	4.91e-05
11212	TS.diHPCARP_I.15HPHshift.dhpdtudu	1.683e+44	10.65	10.65	2.936e+36	4.74e-05
11213	TS.diHPCARP_I.15HPHshift.uhmumudu	1.132e+44	10.43	10.43	2.834e+36	4.57e-05
11214	TS.diHPCARP_I.15HPHshift.uhmumuuu	6.945e+43	10.22	10.22	2.505e+36	4.04e-05
11215	TS.diHPCARP_I.15HPHshift.ultdtudu	1.097e+44	10.51	10.51	2.413e+36	3.89e-05
11216	TS.diHPCARP_I.15HPHshift.umpupuuu	2.237e+43	9.57	9.57	2.404e+36	3.88e-05
11217	TS.diHPCARP_I.15HPHshift.dhtupuuu	2.112e+43	9.54	9.54	2.379e+36	3.84e-05
11218	TS.diHPCARP_I.15HPHshift.uctdtduu	6.539e+43	10.29	10.29	2.083e+36	3.36e-05
11219	TS.diHPCARP_I.15HPHshift.uctdmuuu	2.472e+43	9.79	9.79	1.833e+36	2.96e-05
11220	TS.diHPCARP_I.15HPHshift.dmpdpduu	1.238e+43	9.48	9.48	1.525e+36	2.46e-05
11221	TS.diHPCARP_I.15HPHshift.uhmupduu	2.404e+43	9.90	9.90	1.480e+36	2.39e-05
11222	TS.diHPCARP_I.15HPHshift.dhputudu	1.131e+44	10.84	10.84	1.437e+36	2.32e-05
11223	TS.diHPCARP_I.15HPHshift.uhpdtduu	1.537e+44	11.08	11.08	1.307e+36	2.11e-05
11224	TS.diHPCARP_I.15HPHshift.uhtdpuuu	2.086e+43	9.90	9.90	1.285e+36	2.07e-05
11225	TS.diHPCARP_I.15HPHshift.dhpdtduu	5.952e+42	9.18	9.18	1.229e+36	1.98e-05
11226	TS.diHPCARP_I.15HPHshift.utpdpduu	3.097e+42	8.92	8.92	9.889e+35	1.6e-05
11227	TS.diHPCARP_I.15HPHshift.uhpupudu	5.075e+43	10.59	10.59	9.774e+35	1.58e-05
11228	TS.diHPCARP_I.15HPHshift.uhpdtduu	6.365e+43	10.73	10.73	9.633e+35	1.55e-05
11229	TS.diHPCARP_I.15HPHshift.dhpdtduu	1.790e+43	9.99	9.99	9.378e+35	1.51e-05
11230	TS.diHPCARP_I.15HPHshift.dhmutduu	7.976e+43	10.93	10.93	8.650e+35	1.4e-05
11231	TS.diHPCARP_I.15HPHshift.uhputduu	3.522e+43	10.57	10.57	7.047e+35	1.14e-05
11232	TS.diHPCARP_I.15HPHshift.uhtdmuuu	7.823e+43	11.16	11.16	5.785e+35	9.33e-06
11233	TS.diHPCARP_I.15HPHshift.utpdpduu	6.886e+42	9.76	9.76	5.390e+35	8.69e-06
11234	TS.diHPCARP_I.15HPHshift.uhpupduu	1.540e+43	10.24	10.24	5.390e+35	8.69e-06
11235	TS.diHPCARP_I.15HPHshift.uppupduu	9.783e+42	9.99	9.99	5.145e+35	8.3e-06
11236	TS.diHPCARP_I.15HPHshift.umtdtduu	7.641e+42	9.90	9.90	4.684e+35	7.56e-06
11237	TS.diHPCARP_I.15HPHshift.uhmdpudu	1.888e+44	11.89	11.89	4.143e+35	6.68e-06
11238	TS.diHPCARP_I.15HPHshift.uhmumduu	7.233e+43	11.32	11.32	4.115e+35	6.64e-06
11239	TS.diHPCARP_I.15HPHshift.umtutduu	1.892e+43	10.55	10.55	3.923e+35	6.33e-06
11240	TS.diHPCARP_I.15HPHshift.dhtutudu	1.039e+44	11.66	11.66	3.349e+35	5.4e-06
11241	TS.diHPCARP_I.15HPHshift.uhmutuuu	5.058e+43	11.29	11.29	3.005e+35	4.85e-06
11242	TS.diHPCARP_I.15HPHshift.uhtdtudu	2.488e+43	10.87	10.87	2.983e+35	4.81e-06
11243	TS.diHPCARP_I.15HPHshift.dhtdtudu	7.118e+43	11.52	11.52	2.878e+35	4.64e-06
11244	TS.diHPCARP_I.15HPHshift.ulmutduu	3.462e+43	11.14	11.14	2.655e+35	4.28e-06
11245	TS.diHPCARP_I.15HPHshift.utpdtduu	1.125e+43	10.47	10.47	2.646e+35	4.27e-06
11246	TS.diHPCARP_I.15HPHshift.uhpdtduu	3.916e+44	12.61	12.61	2.570e+35	4.14e-06
11247	TS.diHPCARP_I.15HPHshift.dlpdtduu	1.107e+43	10.52	10.52	2.400e+35	3.87e-06
11248	TS.diHPCARP_I.15HPHshift.dhpdpuuu	6.426e+42	10.26	10.26	2.154e+35	3.47e-06
11249	TS.diHPCARP_I.15HPHshift.uhpdmuuu	6.376e+43	11.65	11.65	2.075e+35	3.35e-06
11250	TS.diHPCARP_I.15HPHshift.uhmutduu	1.816e+43	11.04	11.04	1.658e+35	2.67e-06
11251	TS.diHPCARP_I.15HPHshift.uhmdpuuu	1.912e+43	11.08	11.08	1.618e+35	2.61e-06
11252	TS.diHPCARP_I.15HPHshift.uhpdmduu	6.200e+43	11.82	11.82	1.527e+35	2.46e-06
11253	TS.diHPCARP_I.15HPHshift.ucmutduu	2.607e+43	11.35	11.35	1.399e+35	2.26e-06
11254	TS.diHPCARP_I.15HPHshift.uhtupuuu	8.683e+43	12.28	12.28	9.920e+34	1.6e-06
11255	TS.diHPCARP_I.15HPHshift.dhtutduu	2.917e+43	11.70	11.70	8.767e+34	1.41e-06
11256	TS.diHPCARP_I.15HPHshift.dhputduu	1.802e+43	11.88	11.88	4.005e+34	6.46e-07
11257	TS.diHPCARP_I.15HPHshift.uhmutduu	3.385e+43	12.74	12.74	1.784e+34	2.88e-07
11258	TS.diHPCARP_I.15HPHshift.uhtdpduu	5.554e+43	13.70	13.70	5.821e+33	9.39e-08
11259	TS.diHPCARP_I.15HPHshift.uhmdtudu	8.108e+44	15.46	15.46	4.466e+33	7.2e-08
11260	TS.diHPCARP_I.15HPHshift.uhtupduu	1.387e+43	13.13	13.13	3.763e+33	6.07e-08
11261	TS.diHPCARP_I.15HPHshift.uhtutduu	2.911e+43	14.65	14.65	6.223e+32	1e-08
11262	Total				6.200e+42	100
11263						
11264						
11265						
11266	#####					
11267	M06-2X/cc-pVDZ data for tri-HPACYL-I					
11268	#####					
11269						
11270	(2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)					
11271	=====					
11272						
11273	Population analysis at 300K. Vibrational scaling: 0.971.					
11274	Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)					
11275	n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.					
11276	#: contribution to the population (with current data set assumed 100%)					
11277	Compound Qtot Erel Erel2 n*Q*MB %					
11278	-----					
11279	triHPacyl.ppmptmppd 9.894e+42 0.00 0.00 9.894e+42 10.9					

11280	triHPacyl.tmmmtmtpd	2.051e+43	0.49	0.49	9.083e+42	9.98
11281	triHPacyl.pmmptmtpd	1.909e+43	1.08	1.08	3.141e+42	3.45
11282	triHPacyl.pppmptmtpd	1.273e+43	0.90	0.90	2.795e+42	3.07
11283	triHPacyl.pppmptmtpd	1.940e+43	1.22	1.22	2.518e+42	2.77
11284	triHPacyl.pppmptmtpd	3.583e+43	1.61	1.61	2.426e+42	2.67
11285	triHPacyl.pppmptmtpd	2.119e+43	1.42	1.42	1.954e+42	2.15
11286	triHPacyl.tmmmtmtpd	2.024e+43	1.39	1.39	1.954e+42	2.15
11287	triHPacyl.pmmmtmtpd	1.128e+43	1.18	1.18	1.565e+42	1.72
11288	triHPacyl.ppppptmtpd	2.731e+43	1.75	1.75	1.439e+42	1.58
11289	triHPacyl.ppppptmtpd	3.808e+43	1.99	1.99	1.347e+42	1.48
11290	triHPacyl.ptmmtmtpd	4.351e+43	2.07	2.07	1.346e+42	1.48
11291	triHPacyl.pppmptmtpd	1.542e+43	1.46	1.46	1.321e+42	1.45
11292	triHPacyl.pptmptmtpd	4.406e+43	2.09	2.09	1.320e+42	1.45
11293	triHPacyl.pppmptmtpd	7.786e+43	2.45	2.45	1.275e+42	1.4
11294	triHPacyl.mtppmptmtpd	9.542e+43	3.98	3.98	1.209e+42	1.33
11295	triHPacyl.ppppptmtpd	1.495e+43	1.52	1.52	1.175e+42	1.29
11296	triHPacyl.ppppptmtpd	1.082e+44	2.72	2.72	1.127e+42	1.24
11297	triHPacyl.tppmmtmtpd	2.078e+43	1.88	1.88	8.848e+41	0.972
11298	triHPacyl.mmtmptmtpd	3.222e+43	2.15	2.15	8.701e+41	0.956
11299	triHPacyl.pppmptmtpd	2.288e+43	1.97	1.97	8.384e+41	0.921
11300	triHPacyl.pmmptmtpd	1.476e+43	1.81	1.81	7.143e+41	0.785
11301	triHPacyl.ppppptmtpd	6.153e+42	1.30	1.30	6.986e+41	0.768
11302	triHPacyl.pppmptmtpd	7.837e+43	2.83	2.83	6.779e+41	0.745
11303	triHPacyl.tmtmmtmtpd	4.028e+43	2.45	2.45	6.645e+41	0.73
11304	triHPacyl.pptmptmtpd	2.559e+43	2.18	2.18	6.587e+41	0.724
11305	triHPacyl.tmmmtmtpd	4.599e+43	2.53	2.53	6.575e+41	0.722
11306	triHPacyl.ppppptmtpd	7.697e+43	2.85	2.85	6.481e+41	0.712
11307	triHPacyl.pmtmmtmtpd	1.655e+43	1.93	1.93	6.462e+41	0.71
11308	triHPacyl.pmmptmtpd	1.027e+44	3.08	3.08	5.851e+41	0.643
11309	triHPacyl.ppppptmtpd	1.829e+44	3.44	3.44	5.669e+41	0.623
11310	triHPacyl.tmtmmtmtpd	2.549e+43	2.28	2.28	5.595e+41	0.615
11311	triHPacyl.tmmmtmtpd	5.387e+43	2.72	2.72	5.588e+41	0.614
11312	triHPacyl.tppmptmtpd	2.692e+43	2.34	2.34	5.337e+41	0.586
11313	triHPacyl.ppppptmtpd	4.556e+43	2.67	2.67	5.212e+41	0.573
11314	triHPacyl.tppmmtmtpd	1.029e+43	1.80	1.80	5.035e+41	0.553
11315	triHPacyl.pmtmptmtpd	2.324e+43	2.30	2.30	4.918e+41	0.54
11316	triHPacyl.ptmmtmtpd	3.871e+43	2.61	2.61	4.875e+41	0.536
11317	triHPacyl.tppmmtmtpd	1.190e+43	1.91	1.91	4.840e+41	0.532
11318	triHPacyl.ptmptmtpd	3.207e+43	2.52	2.52	4.678e+41	0.514
11319	triHPacyl.pppppptmtpd	5.461e+43	2.85	2.85	4.569e+41	0.502
11320	triHPacyl.pptpptmtpd	3.822e+43	2.66	2.66	4.386e+41	0.482
11321	triHPacyl.ppppptmtpd	4.999e+42	1.51	1.51	3.991e+41	0.439
11322	triHPacyl.tppmmtmtpd	1.761e+43	2.29	2.29	3.770e+41	0.414
11323	triHPacyl.pptmptmtpd	1.037e+44	3.37	3.37	3.621e+41	0.398
11324	triHPacyl.pmmptmtpd	3.924e+43	2.81	2.81	3.501e+41	0.385
11325	triHPacyl.pptmptmtpd	7.594e+43	3.22	3.22	3.440e+41	0.378
11326	triHPacyl.pptpptmtpd	4.261e+43	2.88	2.88	3.380e+41	0.371
11327	triHPacyl.ppppptmtpd	1.251e+43	2.16	2.16	3.344e+41	0.367
11328	triHPacyl.pppmptmtpd	1.612e+43	2.33	2.33	3.242e+41	0.356
11329	triHPacyl.mtmptmtpd	2.427e+43	2.60	2.60	3.085e+41	0.339
11330	triHPacyl.tppmptmtpd	1.079e+43	2.13	2.13	3.031e+41	0.333
11331	triHPacyl.mmpmptmtpd	1.343e+43	2.31	2.31	2.771e+41	0.305
11332	triHPacyl.mmtmptmtpd	4.054e+43	2.97	2.97	2.770e+41	0.304
11333	triHPacyl.pptpptmtpd	7.592e+43	3.35	3.35	2.757e+41	0.303
11334	triHPacyl.tmmmtmtpd	4.591e+43	3.06	3.06	2.701e+41	0.297
11335	triHPacyl.tppmmtmtpd	2.280e+43	2.66	2.66	2.631e+41	0.289
11336	triHPacyl.pptmptmtpd	1.166e+44	3.65	3.65	2.574e+41	0.283
11337	triHPacyl.mpppptmtpd	6.432e+42	1.93	1.93	2.517e+41	0.277
11338	triHPacyl.pptpptmtpd	2.593e+43	2.77	2.77	2.493e+41	0.274
11339	triHPacyl.ptmmpptmtpd	7.458e+43	3.40	3.40	2.488e+41	0.273
11340	triHPacyl.tmtmptmtpd	8.680e+43	3.51	3.51	2.413e+41	0.265
11341	triHPacyl.tmtmptmtpd	6.866e+43	3.38	3.38	2.359e+41	0.259
11342	triHPacyl.ptppmptmtpd	8.512e+42	2.14	2.14	2.357e+41	0.259
11343	triHPacyl.pptmptmtpd	8.179e+43	3.50	3.50	2.316e+41	0.254
11344	triHPacyl.mmtmptmtpd	2.652e+43	2.83	2.83	2.283e+41	0.251
11345	triHPacyl.mmpmptmtpd	5.734e+43	3.31	3.31	2.226e+41	0.245
11346	triHPacyl.pptmptmtpd	5.007e+43	3.23	3.23	2.205e+41	0.242
11347	triHPacyl.ptmmtmtpd	5.804e+43	3.34	3.34	2.142e+41	0.235
11348	triHPacyl.tmtmmtmtpd	3.452e+44	4.41	4.41	2.118e+41	0.233
11349	triHPacyl.pptmptmtpd	5.434e+43	3.31	3.31	2.101e+41	0.231
11350	triHPacyl.mpppptmtpd	2.519e+43	2.87	2.87	2.051e+41	0.225
11351	triHPacyl.pptmptmtpd	2.001e+43	2.73	2.73	2.044e+41	0.225

11352	triHPacyl.tpmmmtpmpd	2.422e+43	2.85	2.85	2.043e+41	0.224
11353	triHPacyl.pmtmmmmmd	2.170e+43	2.79	2.79	2.020e+41	0.222
11354	triHPacyl.pmtmptpmd	2.730e+44	4.31	4.31	1.980e+41	0.218
11355	triHPacyl.pptppmmmd	1.999e+43	2.75	2.75	1.970e+41	0.216
11356	triHPacyl.mmpmptmpd	6.437e+43	3.45	3.45	1.963e+41	0.216
11357	triHPacyl.ttmmmmpmmd	9.106e+43	3.67	3.67	1.920e+41	0.211
11358	triHPacyl.tmtmmtpmpd	7.062e+43	3.53	3.53	1.908e+41	0.21
11359	triHPacyl.mttppptmpd	5.049e+43	3.33	3.33	1.895e+41	0.208
11360	triHPacyl.tmmmmtpmd	6.740e+43	3.52	3.52	1.852e+41	0.204
11361	triHPacyl.pppppmpmd	1.488e+43	2.62	2.62	1.822e+41	0.2
11362	triHPacyl.tmtpmmpmd	3.510e+43	3.14	3.14	1.812e+41	0.199
11363	triHPacyl.pmmpppppd	2.352e+43	2.91	2.91	1.776e+41	0.195
11364	triHPacyl.ptmmpmpmd	7.221e+43	3.59	3.59	1.763e+41	0.194
11365	triHPacyl.tmmmmtpmd	4.576e+43	3.33	3.33	1.724e+41	0.189
11366	triHPacyl.tmtmmtpmd	1.401e+44	4.03	4.03	1.630e+41	0.179
11367	triHPacyl.mmpppmpmd	8.885e+42	2.39	2.39	1.618e+41	0.178
11368	triHPacyl.mmmmpmpmd	4.516e+43	3.36	3.36	1.607e+41	0.177
11369	triHPacyl.pptpptpmd	8.965e+43	3.77	3.77	1.603e+41	0.176
11370	triHPacyl.pmtmpmmmd	1.968e+43	2.87	2.87	1.597e+41	0.176
11371	triHPacyl.mmmmpmmmd	4.797e+43	3.40	3.40	1.590e+41	0.175
11372	triHPacyl.mttppmpmd	4.406e+43	3.38	3.38	1.524e+41	0.167
11373	triHPacyl.pppppmpmd	8.473e+43	3.77	3.77	1.519e+41	0.167
11374	triHPacyl.mmtmpmmmd	4.162e+43	3.36	3.36	1.491e+41	0.164
11375	triHPacyl.pptpptpmd	5.748e+43	3.57	3.57	1.451e+41	0.159
11376	triHPacyl.pptmmpmmmd	3.082e+43	3.20	3.20	1.427e+41	0.157
11377	triHPacyl.pmmmpmpmd	4.619e+43	3.46	3.46	1.399e+41	0.154
11378	triHPacyl.tmtpmmpmd	6.521e+43	3.67	3.67	1.381e+41	0.152
11379	triHPacyl.pppppmpmd	2.131e+43	3.01	3.01	1.358e+41	0.149
11380	triHPacyl.tpppmtmpd	5.206e+43	3.55	3.55	1.343e+41	0.148
11381	triHPacyl.mmtppmpmd	5.077e+43	3.54	3.54	1.337e+41	0.147
11382	triHPacyl.pmtmptmpd	3.948e+43	3.40	3.40	1.314e+41	0.144
11383	triHPacyl.pmmmmmpmd	6.345e+43	3.69	3.69	1.308e+41	0.144
11384	triHPacyl.ptmmtmpd	1.740e+43	2.93	2.93	1.282e+41	0.141
11385	triHPacyl.tpppmtmpd	3.589e+43	3.36	3.36	1.278e+41	0.14
11386	triHPacyl.pptppmpmd	6.449e+43	3.71	3.71	1.277e+41	0.14
11387	triHPacyl.ptppmpmpmd	1.404e+43	2.80	2.80	1.277e+41	0.14
11388	triHPacyl.pmtmmmmmd	2.112e+43	3.05	3.05	1.265e+41	0.139
11389	triHPacyl.tmpmmtmpd	3.560e+43	3.37	3.37	1.248e+41	0.137
11390	triHPacyl.mttmptmpd	1.860e+43	2.99	2.99	1.240e+41	0.136
11391	triHPacyl.pppppmpmd	1.401e+44	4.20	4.20	1.230e+41	0.135
11392	triHPacyl.pmtppmpmd	4.303e+43	3.50	3.50	1.223e+41	0.134
11393	triHPacyl.pttpmtmpd	7.734e+43	3.85	3.85	1.207e+41	0.133
11394	triHPacyl.tmtmmmmmd	6.263e+43	3.78	3.78	1.109e+41	0.122
11395	triHPacyl.ttmmtmpmd	5.602e+43	3.71	3.71	1.106e+41	0.121
11396	triHPacyl.pmpmptmpd	3.374e+43	3.41	3.41	1.105e+41	0.121
11397	triHPacyl.ptppmmpmd	1.875e+43	3.07	3.07	1.090e+41	0.12
11398	triHPacyl.ptppptmpd	8.991e+42	2.63	2.63	1.089e+41	0.12
11399	triHPacyl.tmtmmtmpd	5.960e+43	3.77	3.77	1.074e+41	0.118
11400	triHPacyl.ptmmtmpd	1.555e+43	2.97	2.97	1.073e+41	0.118
11401	triHPacyl.tmmmmtpmd	6.120e+43	3.78	3.78	1.072e+41	0.118
11402	triHPacyl.tptmtpmpd	1.454e+44	4.31	4.31	1.063e+41	0.117
11403	triHPacyl.mmpppptppd	7.237e+43	3.89	3.89	1.060e+41	0.116
11404	triHPacyl.ptmptmpd	2.144e+43	3.17	3.17	1.059e+41	0.116
11405	triHPacyl.tmmmmmmmd	5.240e+43	3.70	3.70	1.055e+41	0.116
11406	triHPacyl.tmtmmmmmd	4.389e+43	3.60	3.60	1.040e+41	0.114
11407	triHPacyl.tmtpmmmmd	4.153e+43	3.57	3.57	1.039e+41	0.114
11408	triHPacyl.tpppmtmpd	1.934e+43	3.12	3.12	1.038e+41	0.114
11409	triHPacyl.ptmmpmmpd	1.723e+43	3.05	3.05	1.033e+41	0.113
11410	triHPacyl.tmtmtpmpd	2.875e+44	4.73	4.73	1.022e+41	0.112
11411	triHPacyl.tmtmtpmpd	1.593e+44	4.38	4.38	1.021e+41	0.112
11412	triHPacyl.pmpmptppd	2.922e+43	3.38	3.38	1.003e+41	0.11
11413	triHPacyl.tptmmmpmd	6.128e+43	3.84	3.84	9.718e+40	0.107
11414	triHPacyl.mmpmptmpd	1.555e+43	3.03	3.03	9.712e+40	0.107
11415	triHPacyl.tmtmmtppd	8.759e+43	4.07	4.07	9.554e+40	0.105
11416	triHPacyl.tptmmtmpd	4.720e+43	3.71	3.71	9.418e+40	0.103
11417	triHPacyl.tpmmpmpd	1.433e+43	3.00	3.00	9.320e+40	0.102
11418	triHPacyl.tmtmmmmmd	3.707e+43	3.58	3.58	9.112e+40	0.1
11419	triHPacyl.tpmmpmmpmd	2.287e+43	3.30	3.30	9.034e+40	0.0993
11420	triHPacyl.pmtmtpmmd	1.471e+43	3.04	3.04	8.993e+40	0.0988
11421	triHPacyl.mtmmpmmpmd	3.324e+43	3.53	3.53	8.980e+40	0.0987
11422	triHPacyl.ptppptmpd	1.117e+43	2.88	2.88	8.904e+40	0.0978
11423	triHPacyl.ttmmtmpmd	9.383e+43	4.15	4.15	8.884e+40	0.0976

11424	triHPacyl.tttmmmpmpd	3.676e+43	3.60	3.60	8.727e+40	0.0959
11425	triHPacyl.tpmptmpmd	1.561e+43	3.09	3.09	8.697e+40	0.0956
11426	triHPacyl.pptpmtmpmd	9.257e+43	4.16	4.16	8.690e+40	0.0955
11427	triHPacyl.tptmmmmmpd	3.828e+43	3.64	3.64	8.607e+40	0.0946
11428	triHPacyl.pttppppmmd	3.026e+43	3.50	3.50	8.586e+40	0.0943
11429	triHPacyl.tmtpmtmpmd	6.839e+43	3.99	3.99	8.521e+40	0.0936
11430	triHPacyl.tttppmmmmmd	9.669e+42	2.83	2.83	8.323e+40	0.0915
11431	triHPacyl.tmmmpmtppd	2.730e+43	3.48	3.48	7.944e+40	0.0873
11432	triHPacyl.pmppmtmmd	3.449e+43	3.63	3.63	7.768e+40	0.0854
11433	triHPacyl.tmppmtmmd	1.129e+43	2.97	2.97	7.761e+40	0.0853
11434	triHPacyl.pmtmptmmd	3.667e+43	3.67	3.67	7.758e+40	0.0852
11435	triHPacyl.pptpppmmpd	3.673e+43	3.67	3.67	7.729e+40	0.0849
11436	triHPacyl.pmppmmmpmd	2.297e+43	3.40	3.40	7.633e+40	0.0839
11437	triHPacyl.pptpmtmmd	6.459e+43	4.02	4.02	7.605e+40	0.0836
11438	triHPacyl.tttmmmmmpd	1.837e+43	3.28	3.28	7.503e+40	0.0825
11439	triHPacyl.tpppmmtppd	7.839e+43	4.17	4.17	7.217e+40	0.0793
11440	triHPacyl.pppppmpmd	1.570e+43	3.21	3.21	7.210e+40	0.0792
11441	triHPacyl.pmtptmmd	2.480e+43	3.48	3.48	7.180e+40	0.0789
11442	triHPacyl.tpppmmpmd	4.411e+43	3.83	3.83	7.179e+40	0.0789
11443	triHPacyl.mmmmtmmpd	2.071e+43	3.38	3.38	7.157e+40	0.0786
11444	triHPacyl.mtmptmmd	1.090e+44	4.37	4.37	7.083e+40	0.0778
11445	triHPacyl.tttmmtmmd	1.789e+43	3.30	3.30	7.050e+40	0.0775
11446	triHPacyl.pmpppptpmd	8.588e+42	2.87	2.87	6.947e+40	0.0763
11447	triHPacyl.pmpmmtpmd	2.358e+43	3.48	3.48	6.833e+40	0.0751
11448	triHPacyl.mmpptmmpd	5.555e+43	4.00	4.00	6.803e+40	0.0748
11449	triHPacyl.pmtpptppd	9.832e+43	4.34	4.34	6.781e+40	0.0745
11450	triHPacyl.tttmmmmppd	2.537e+43	3.53	3.53	6.748e+40	0.0741
11451	triHPacyl.pppppppmpd	7.285e+43	4.17	4.17	6.704e+40	0.0737
11452	triHPacyl.pmmmpptppd	3.684e+43	3.77	3.77	6.643e+40	0.073
11453	triHPacyl.ptppmmmpmd	1.171e+43	3.09	3.09	6.552e+40	0.072
11454	triHPacyl.tmtpmmmmpd	3.705e+43	3.78	3.78	6.507e+40	0.0715
11455	triHPacyl.pmtmmpmmpd	2.314e+43	3.51	3.51	6.441e+40	0.0708
11456	triHPacyl.tmtpmmmppd	1.375e+44	4.58	4.58	6.317e+40	0.0694
11457	triHPacyl.tmppmmmmmd	2.446e+43	3.56	3.56	6.278e+40	0.069
11458	triHPacyl.ppmmtmpmd	8.134e+43	4.28	4.28	6.198e+40	0.0681
11459	triHPacyl.ptppppmpmd	2.170e+43	3.50	3.50	6.093e+40	0.067
11460	triHPacyl.pppmmmpmmd	1.985e+43	3.46	3.46	5.988e+40	0.0658
11461	triHPacyl.pmtpmtmmd	2.993e+43	3.71	3.71	5.946e+40	0.0653
11462	triHPacyl.pppmptppd	3.326e+43	3.77	3.77	5.939e+40	0.0653
11463	triHPacyl.tpppmtmmd	9.603e+43	4.41	4.41	5.927e+40	0.0651
11464	triHPacyl.tmtmptmmd	1.661e+44	4.73	4.73	5.909e+40	0.0649
11465	triHPacyl.tmtmptpmd	5.991e+44	5.51	5.51	5.821e+40	0.064
11466	triHPacyl.tmmmmmtppd	7.294e+43	4.25	4.25	5.800e+40	0.0637
11467	triHPacyl.pmmmpptppd	6.358e+43	4.18	4.18	5.724e+40	0.0629
11468	triHPacyl.pttppppmpd	2.673e+43	3.68	3.68	5.552e+40	0.061
11469	triHPacyl.pppmmmtmmpd	1.045e+43	3.13	3.13	5.516e+40	0.0606
11470	triHPacyl.pptppppmmd	1.483e+44	4.71	4.71	5.506e+40	0.0605
11471	triHPacyl.pppmpptmmd	6.367e+43	4.21	4.21	5.430e+40	0.0597
11472	triHPacyl.pttpptmmd	4.068e+43	3.95	3.95	5.422e+40	0.0596
11473	triHPacyl.pmtpmtmpmd	3.290e+43	3.83	3.83	5.361e+40	0.0589
11474	triHPacyl.tptmmtmmpd	2.677e+43	3.71	3.71	5.276e+40	0.058
11475	triHPacyl.tmmmmmmppd	4.573e+43	4.04	4.04	5.225e+40	0.0574
11476	triHPacyl.mmtmmpmmmd	5.559e+43	4.16	4.16	5.189e+40	0.057
11477	triHPacyl.pttmtmpmd	3.814e+43	3.95	3.95	5.037e+40	0.0553
11478	triHPacyl.tttpmmmppd	9.809e+43	4.52	4.52	4.999e+40	0.0549
11479	triHPacyl.mtmptmmd	1.666e+43	3.46	3.46	4.984e+40	0.0548
11480	triHPacyl.mmtppmmmd	4.013e+43	3.99	3.99	4.952e+40	0.0544
11481	triHPacyl.pmtptmmpd	8.410e+43	4.45	4.45	4.860e+40	0.0534
11482	triHPacyl.tpmptmmd	3.880e+43	3.98	3.98	4.860e+40	0.0534
11483	triHPacyl.pptmpptmmd	7.750e+43	4.40	4.40	4.805e+40	0.0528
11484	triHPacyl.tmtptmmd	1.294e+44	4.71	4.71	4.779e+40	0.0525
11485	triHPacyl.tpppmtppd	1.050e+44	4.59	4.59	4.770e+40	0.0524
11486	triHPacyl.tttptmmd	1.731e+43	3.51	3.51	4.762e+40	0.0523
11487	triHPacyl.pmtmptpmd	9.779e+43	4.56	4.56	4.657e+40	0.0512
11488	triHPacyl.tttmmtmmpd	4.106e+43	4.05	4.05	4.632e+40	0.0509
11489	triHPacyl.tmtpmtmmd	1.975e+44	4.98	4.98	4.617e+40	0.0507
11490	triHPacyl.mmpmpmtppd	5.577e+43	4.24	4.24	4.578e+40	0.0503
11491	triHPacyl.mtmptmpmd	9.787e+42	3.20	3.20	4.566e+40	0.0502
11492	triHPacyl.tttpmmmmd	1.659e+43	3.52	3.52	4.510e+40	0.0496
11493	triHPacyl.ppppptpmd	6.197e+43	4.31	4.31	4.503e+40	0.0495
11494	triHPacyl.mmpmpmmmpd	1.543e+43	3.48	3.48	4.475e+40	0.0492
11495	triHPacyl.pttpmtmmd	1.579e+43	3.51	3.51	4.410e+40	0.0485

11496	triHPacyl.pttppmmppd	6.616e+43	4.36	4.36	4.409e+40	0.0485
11497	triHPacyl.pmpmpmmmd	3.526e+43	3.99	3.99	4.398e+40	0.0483
11498	triHPacyl.ptppmtmpmd	3.548e+43	4.00	4.00	4.339e+40	0.0477
11499	triHPacyl.pptpmttmd	9.760e+43	4.61	4.61	4.303e+40	0.0473
11500	triHPacyl.ppmtmtmmd	1.083e+44	4.68	4.68	4.228e+40	0.0465
11501	triHPacyl.mmpppttmmd	3.581e+43	4.02	4.02	4.217e+40	0.0463
11502	triHPacyl.mmpppppmpd	2.099e+43	3.71	3.71	4.198e+40	0.0461
11503	triHPacyl.pppppmpmd	3.767e+43	4.05	4.05	4.195e+40	0.0461
11504	triHPacyl.pttppmtppd	8.958e+43	4.57	4.57	4.185e+40	0.046
11505	triHPacyl.mttppmmppd	6.218e+43	4.36	4.36	4.154e+40	0.0456
11506	triHPacyl.pttppmtppd	1.755e+43	3.61	3.61	4.134e+40	0.0454
11507	triHPacyl.pmmmtmmpd	1.151e+43	3.36	3.36	4.084e+40	0.0449
11508	triHPacyl.tmpmpmmmd	8.236e+42	3.18	3.18	3.968e+40	0.0436
11509	triHPacyl.ptppptmmd	2.475e+43	3.84	3.84	3.964e+40	0.0436
11510	triHPacyl.tmmmtmmd	1.587e+44	4.95	4.95	3.949e+40	0.0434
11511	triHPacyl.pmtmmmmmd	2.604e+43	3.87	3.87	3.939e+40	0.0433
11512	triHPacyl.ttpmmmmmd	1.020e+43	3.32	3.32	3.888e+40	0.0427
11513	triHPacyl.pmtppmtppd	6.216e+43	4.40	4.40	3.884e+40	0.0427
11514	triHPacyl.pptppmpd	2.258e+43	3.79	3.79	3.882e+40	0.0427
11515	triHPacyl.ptmtppmmpd	8.767e+43	4.61	4.61	3.823e+40	0.042
11516	triHPacyl.tptpmtppd	5.641e+43	4.36	4.36	3.777e+40	0.0415
11517	triHPacyl.tttmtpmpd	4.557e+43	4.24	4.24	3.741e+40	0.0411
11518	triHPacyl.tmtppmmmd	1.293e+44	4.86	4.86	3.720e+40	0.0409
11519	triHPacyl.tmmmtmmpd	1.163e+44	4.80	4.80	3.707e+40	0.0407
11520	triHPacyl.tptpmtppd	3.913e+43	4.15	4.15	3.688e+40	0.0405
11521	triHPacyl.pmmmtmmd	1.200e+44	4.83	4.83	3.641e+40	0.04
11522	triHPacyl.tmtppmpmpd	3.850e+44	5.53	5.53	3.615e+40	0.0397
11523	triHPacyl.tmmmtmmpd	5.955e+43	4.42	4.42	3.600e+40	0.0396
11524	triHPacyl.pttmtmmd	2.168e+43	3.82	3.82	3.559e+40	0.0391
11525	triHPacyl.mttppmmppd	6.444e+43	4.47	4.47	3.555e+40	0.0391
11526	triHPacyl.pmtppppmpd	5.190e+43	4.35	4.35	3.489e+40	0.0383
11527	triHPacyl.ttpmmmpmpd	2.226e+43	3.86	3.86	3.449e+40	0.0379
11528	triHPacyl.pppmpptppd	7.328e+43	4.57	4.57	3.442e+40	0.0378
11529	triHPacyl.tmmtpmpmd	1.975e+43	3.79	3.79	3.442e+40	0.0378
11530	triHPacyl.tmtppptppd	9.546e+43	4.73	4.73	3.393e+40	0.0373
11531	triHPacyl.pttppmmppd	2.207e+44	5.25	5.25	3.320e+40	0.0365
11532	triHPacyl.ttpmmmtmmd	4.037e+43	4.24	4.24	3.291e+40	0.0362
11533	triHPacyl.mtmmpmpmd	1.709e+44	5.11	5.11	3.229e+40	0.0355
11534	triHPacyl.pmtppmtppd	7.484e+43	4.62	4.62	3.227e+40	0.0355
11535	triHPacyl.ppttptppd	1.381e+44	4.99	4.99	3.182e+40	0.035
11536	triHPacyl.ppppmtmmd	4.900e+43	4.38	4.38	3.179e+40	0.0349
11537	triHPacyl.mmpppmmmd	8.724e+42	3.35	3.35	3.174e+40	0.0349
11538	triHPacyl.tptppmpmd	1.496e+44	5.05	5.05	3.149e+40	0.0346
11539	triHPacyl.pppppmmmd	5.021e+43	4.42	4.42	3.019e+40	0.0332
11540	triHPacyl.tmmmtmmpd	1.834e+44	5.19	5.19	3.019e+40	0.0332
11541	triHPacyl.tmpmtmmpd	7.897e+43	4.69	4.69	3.011e+40	0.0331
11542	triHPacyl.tmpmmtppd	5.391e+43	4.48	4.48	2.950e+40	0.0324
11543	triHPacyl.ppttptmmd	1.080e+44	4.89	4.89	2.948e+40	0.0324
11544	triHPacyl.pptppptmmd	4.550e+43	4.38	4.38	2.948e+40	0.0324
11545	triHPacyl.mtppmpmmd	2.806e+43	4.10	4.10	2.916e+40	0.032
11546	triHPacyl.mttppmmppd	2.238e+43	3.96	3.96	2.907e+40	0.0319
11547	triHPacyl.tmmppmmppd	9.579e+43	4.83	4.83	2.905e+40	0.0319
11548	triHPacyl.tmpmmmtmmd	4.885e+43	4.43	4.43	2.905e+40	0.0319
11549	triHPacyl.tmmmmmtmmd	7.280e+43	4.67	4.67	2.893e+40	0.0318
11550	triHPacyl.pppmpptmmd	1.014e+44	4.87	4.87	2.891e+40	0.0318
11551	triHPacyl.mtppppmmd	1.263e+43	3.63	3.63	2.859e+40	0.0314
11552	triHPacyl.ttpmmmpmd	1.595e+43	3.77	3.77	2.847e+40	0.0313
11553	triHPacyl.tptmmtppd	1.307e+44	5.03	5.03	2.845e+40	0.0313
11554	triHPacyl.ptmtmtpmd	6.128e+43	4.59	4.59	2.770e+40	0.0304
11555	triHPacyl.tppmmmpmd	1.623e+43	3.81	3.81	2.726e+40	0.03
11556	triHPacyl.tptpmtmmd	4.499e+43	4.42	4.42	2.723e+40	0.0299
11557	triHPacyl.tmtpptppd	2.687e+44	5.48	5.48	2.716e+40	0.0298
11558	triHPacyl.mmpppmtppd	2.300e+43	4.03	4.03	2.688e+40	0.0295
11559	triHPacyl.tmmptmmpd	6.317e+43	4.63	4.63	2.675e+40	0.0294
11560	triHPacyl.ppttptppd	8.823e+43	4.83	4.83	2.672e+40	0.0294
11561	triHPacyl.pppptppmmd	2.223e+44	5.38	5.38	2.671e+40	0.0294
11562	triHPacyl.tptmmtppd	8.717e+43	4.82	4.82	2.669e+40	0.0293
11563	triHPacyl.mmpmpmtppd	5.628e+43	4.56	4.56	2.664e+40	0.0293
11564	triHPacyl.tmpmptppd	3.009e+43	4.20	4.20	2.619e+40	0.0288
11565	triHPacyl.pptppmtppd	5.862e+43	4.60	4.60	2.592e+40	0.0285
11566	triHPacyl.mtppptmmd	1.370e+43	3.75	3.75	2.547e+40	0.028
11567	triHPacyl.pptppmtppd	3.991e+43	4.40	4.40	2.496e+40	0.0274

11568	triHPacyl.tptmmtttmpd	1.351e+44	5.13	5.13	2.463e+40	0.0271
11569	triHPacyl.pttpmmmpmd	1.646e+43	3.88	3.88	2.444e+40	0.0269
11570	triHPacyl.ttpmntmmmd	7.956e+42	3.45	3.45	2.432e+40	0.0267
11571	triHPacyl.ppptptmmd	2.183e+44	5.43	5.43	2.431e+40	0.0267
11572	triHPacyl.ttmptmpmd	7.286e+43	4.77	4.77	2.430e+40	0.0267
11573	triHPacyl.pmtppmmmpmd	3.729e+43	4.37	4.37	2.426e+40	0.0267
11574	triHPacyl.tptpmmmmmd	3.054e+43	4.26	4.26	2.416e+40	0.0265
11575	triHPacyl.ppppottmpd	3.229e+44	5.67	5.67	2.408e+40	0.0265
11576	triHPacyl.mttmptmpmd	3.504e+43	4.34	4.34	2.400e+40	0.0264
11577	triHPacyl.ttpmptmmd	4.635e+43	4.51	4.51	2.382e+40	0.0262
11578	triHPacyl.pppmptppd	8.920e+43	4.91	4.91	2.367e+40	0.026
11579	triHPacyl.tptmmmmmd	5.599e+43	4.64	4.64	2.342e+40	0.0257
11580	triHPacyl.tmtppmmmpd	4.850e+43	4.55	4.55	2.334e+40	0.0256
11581	triHPacyl.tttmnmmpmd	3.918e+43	4.43	4.43	2.329e+40	0.0256
11582	triHPacyl.pptppppppd	2.751e+44	5.59	5.59	2.324e+40	0.0255
11583	triHPacyl.tpmppmmmpmd	1.693e+43	3.94	3.94	2.301e+40	0.0253
11584	triHPacyl.pppmmntmmmd	8.605e+43	4.91	4.91	2.299e+40	0.0253
11585	triHPacyl.tptmmtmmmd	6.842e+43	4.77	4.77	2.298e+40	0.0252
11586	triHPacyl.ptppppppmd	1.884e+43	4.00	4.00	2.290e+40	0.0252
11587	triHPacyl.tttmptmmpd	1.091e+44	5.06	5.06	2.250e+40	0.0247
11588	triHPacyl.tptpmttmmmd	8.083e+43	4.88	4.88	2.243e+40	0.0246
11589	triHPacyl.pptmpppppd	9.474e+43	4.98	4.98	2.214e+40	0.0243
11590	triHPacyl.pmtppmtmmpd	6.430e+43	4.76	4.76	2.206e+40	0.0242
11591	triHPacyl.tptpmttppd	1.432e+44	5.24	5.24	2.198e+40	0.0242
11592	triHPacyl.pttmmmmppd	2.078e+43	4.09	4.09	2.189e+40	0.024
11593	triHPacyl.tmmmmmpmmd	2.568e+44	5.59	5.59	2.183e+40	0.024
11594	triHPacyl.tttptmtpmd	2.620e+43	4.23	4.23	2.168e+40	0.0238
11595	triHPacyl.pppmmtmmmd	7.328e+43	4.84	4.84	2.167e+40	0.0238
11596	triHPacyl.pppppptmmd	5.587e+43	4.69	4.69	2.156e+40	0.0237
11597	triHPacyl.pmtmmtmmpd	2.317e+43	4.17	4.17	2.127e+40	0.0234
11598	triHPacyl.pptpptmmpd	2.356e+44	5.55	5.55	2.123e+40	0.0233
11599	triHPacyl.ptppppptmmd	7.172e+43	4.85	4.85	2.108e+40	0.0232
11600	triHPacyl.pptppppmpd	1.280e+44	5.20	5.20	2.094e+40	0.023
11601	triHPacyl.pttpptmmpd	1.952e+43	4.08	4.08	2.082e+40	0.0229
11602	triHPacyl.pppmptmmpd	2.764e+43	4.29	4.29	2.072e+40	0.0228
11603	triHPacyl.tmpmmtmmpd	2.132e+43	4.14	4.14	2.041e+40	0.0224
11604	triHPacyl.pmmmpmmmpd	5.248e+43	4.68	4.68	2.031e+40	0.0223
11605	triHPacyl.mppmppppmd	1.665e+43	4.01	4.01	2.009e+40	0.0221
11606	triHPacyl.tptpmtmmpd	8.822e+43	5.00	5.00	2.003e+40	0.022
11607	triHPacyl.pppmmppppmd	3.513e+43	4.46	4.46	1.990e+40	0.0219
11608	triHPacyl.pttpmtmmpd	3.478e+43	4.45	4.45	1.978e+40	0.0217
11609	triHPacyl.ptmtppmmpd	1.168e+44	5.18	5.18	1.974e+40	0.0217
11610	triHPacyl.pmpmptmmpd	9.255e+42	3.67	3.67	1.948e+40	0.0214
11611	triHPacyl.ptppmtmmmd	7.238e+42	3.53	3.53	1.927e+40	0.0212
11612	triHPacyl.pmtppmmmmmd	2.677e+43	4.32	4.32	1.921e+40	0.0211
11613	triHPacyl.tmpmmtmmpd	4.156e+43	4.58	4.58	1.915e+40	0.021
11614	triHPacyl.pppppptmmd	7.918e+43	4.97	4.97	1.902e+40	0.0209
11615	triHPacyl.ptmtptmmpd	9.099e+43	5.06	5.06	1.884e+40	0.0207
11616	triHPacyl.mtppppmpmd	1.078e+43	3.79	3.79	1.879e+40	0.0206
11617	triHPacyl.ptppmmmmmd	8.479e+42	3.65	3.65	1.874e+40	0.0206
11618	triHPacyl.tpppmttmmmd	1.633e+44	5.41	5.41	1.872e+40	0.0206
11619	triHPacyl.tmpmmtmmmpd	2.814e+43	4.36	4.36	1.863e+40	0.0205
11620	triHPacyl.tmmntmmpmd	1.980e+44	5.53	5.53	1.840e+40	0.0202
11621	triHPacyl.pmmmpptmmpd	5.315e+43	4.76	4.76	1.810e+40	0.0199
11622	triHPacyl.tttmmtmmpd	2.167e+43	4.23	4.23	1.809e+40	0.0199
11623	triHPacyl.tppmmmmpppd	2.277e+43	4.26	4.26	1.791e+40	0.0197
11624	triHPacyl.pppppptppmd	6.711e+43	4.91	4.91	1.785e+40	0.0196
11625	triHPacyl.pmtppptpppd	2.547e+44	5.71	5.71	1.770e+40	0.0195
11626	triHPacyl.ptppmmmpmd	1.700e+43	4.09	4.09	1.769e+40	0.0194
11627	triHPacyl.tmtptmtpmd	2.735e+44	5.76	5.76	1.749e+40	0.0192
11628	triHPacyl.tmpmptmmpd	5.898e+43	4.85	4.85	1.734e+40	0.0191
11629	triHPacyl.tppmptmmpd	3.328e+43	4.51	4.51	1.724e+40	0.0189
11630	triHPacyl.mmpptppppd	5.343e+43	4.79	4.79	1.723e+40	0.0189
11631	triHPacyl.pmtppmmmmmd	2.128e+43	4.24	4.24	1.722e+40	0.0189
11632	triHPacyl.pppmmmpmpmd	3.353e+43	4.53	4.53	1.687e+40	0.0185
11633	triHPacyl.pmtppmmmmmd	1.983e+43	4.21	4.21	1.687e+40	0.0185
11634	triHPacyl.pppppppppmd	4.759e+43	4.74	4.74	1.679e+40	0.0185
11635	triHPacyl.tttppmmmpmd	4.820e+43	4.75	4.75	1.677e+40	0.0184
11636	triHPacyl.pmpmptmmpd	8.115e+43	5.07	5.07	1.655e+40	0.0182
11637	triHPacyl.pppmmmpmpd	4.885e+42	3.39	3.39	1.654e+40	0.0182
11638	triHPacyl.mmtppmmmpd	5.818e+43	4.87	4.87	1.648e+40	0.0181
11639	triHPacyl.mppppptmmpd	1.013e+43	3.83	3.83	1.642e+40	0.018

11640	triHPacyl.tppppptpmd	9.259e+43	5.15	5.15	1.639e+40	0.018
11641	triHPacyl.mmttpmtmmd	8.005e+43	5.07	5.07	1.632e+40	0.0179
11642	triHPacyl.tmtppmpppd	1.580e+44	5.48	5.48	1.597e+40	0.0175
11643	triHPacyl.tmtppmtmmpd	3.217e+44	5.92	5.92	1.571e+40	0.0173
11644	triHPacyl.pmpmpmtppmd	5.450e+43	4.86	4.86	1.560e+40	0.0171
11645	triHPacyl.mttppmmmpd	2.164e+43	4.32	4.32	1.554e+40	0.0171
11646	triHPacyl.ttpmmmtppd	3.078e+43	4.53	4.53	1.547e+40	0.017
11647	triHPacyl.pppmpmtppmd	9.256e+42	3.81	3.81	1.541e+40	0.0169
11648	triHPacyl.pppmpmtmmd	5.076e+43	4.84	4.84	1.515e+40	0.0167
11649	triHPacyl.ppptptppmd	2.180e+44	5.71	5.71	1.507e+40	0.0166
11650	triHPacyl.tmpppptpmd	3.831e+43	4.68	4.68	1.501e+40	0.0165
11651	triHPacyl.ptmpmtppd	4.102e+43	4.72	4.72	1.488e+40	0.0164
11652	triHPacyl.tttptmtpmd	7.279e+43	5.07	5.07	1.487e+40	0.0163
11653	triHPacyl.tmtmtmtpd	3.320e+44	5.98	5.98	1.450e+40	0.0159
11654	triHPacyl.mtppptmmpd	7.079e+43	5.07	5.07	1.446e+40	0.0159
11655	triHPacyl.tppppmtppd	2.030e+43	4.32	4.32	1.442e+40	0.0158
11656	triHPacyl.ppptptppd	4.413e+43	4.79	4.79	1.432e+40	0.0157
11657	triHPacyl.ppttppmmmd	5.731e+43	4.95	4.95	1.432e+40	0.0157
11658	triHPacyl.ptmpmmppd	3.069e+43	4.57	4.57	1.428e+40	0.0157
11659	triHPacyl.mtppptppd	1.397e+44	5.48	5.48	1.421e+40	0.0156
11660	triHPacyl.pttpmtppd	1.100e+44	5.35	5.35	1.398e+40	0.0154
11661	triHPacyl.tpppmtmmd	1.047e+44	5.32	5.32	1.392e+40	0.0153
11662	triHPacyl.mppppmtmmd	9.397e+43	5.26	5.26	1.386e+40	0.0152
11663	triHPacyl.tttptmtpd	2.521e+44	5.85	5.85	1.385e+40	0.0152
11664	triHPacyl.ppptptppd	2.441e+44	5.83	5.83	1.383e+40	0.0152
11665	triHPacyl.mttppppmd	5.739e+43	4.97	4.97	1.366e+40	0.015
11666	triHPacyl.tppmmppmd	4.623e+43	4.85	4.85	1.362e+40	0.015
11667	triHPacyl.mmtppttppd	9.819e+43	5.30	5.30	1.362e+40	0.015
11668	triHPacyl.pttmmmmmpd	1.960e+43	4.36	4.36	1.310e+40	0.0144
11669	triHPacyl.pptpmtppd	3.878e+43	4.78	4.78	1.287e+40	0.0141
11670	triHPacyl.pptpmpmpd	7.879e+43	5.21	5.21	1.260e+40	0.0139
11671	triHPacyl.ppptppppd	2.267e+44	5.84	5.84	1.260e+40	0.0138
11672	triHPacyl.ttmtmtmmpd	5.543e+44	6.38	6.38	1.249e+40	0.0137
11673	triHPacyl.tttptmtpmd	5.069e+43	4.95	4.95	1.248e+40	0.0137
11674	triHPacyl.mtppppppmd	2.304e+43	4.49	4.49	1.244e+40	0.0137
11675	triHPacyl.pptpmpmpmd	5.951e+43	5.05	5.05	1.243e+40	0.0137
11676	triHPacyl.tmmmmmtppd	1.787e+44	5.71	5.71	1.240e+40	0.0136
11677	triHPacyl.pptmmtppd	3.410e+43	4.72	4.72	1.239e+40	0.0136
11678	triHPacyl.pmmmpmtppd	7.543e+43	5.20	5.20	1.236e+40	0.0136
11679	triHPacyl.pppmpmpmpmd	6.589e+43	5.12	5.12	1.227e+40	0.0135
11680	triHPacyl.mmtppptppd	4.738e+43	4.93	4.93	1.224e+40	0.0134
11681	triHPacyl.ttmmmtmmd	1.553e+44	5.64	5.64	1.216e+40	0.0134
11682	triHPacyl.ppptptppd	1.455e+44	5.60	5.60	1.204e+40	0.0132
11683	triHPacyl.tmtpmtppd	6.735e+44	6.52	6.52	1.190e+40	0.0131
11684	triHPacyl.pppppptppd	8.451e+43	5.29	5.29	1.187e+40	0.013
11685	triHPacyl.tptpmtppd	9.519e+43	5.37	5.37	1.174e+40	0.0129
11686	triHPacyl.ptmtptppd	1.351e+43	4.21	4.21	1.150e+40	0.0126
11687	triHPacyl.mtmmmtppd	4.262e+43	4.90	4.90	1.144e+40	0.0126
11688	triHPacyl.pmmmtmmpd	1.464e+43	4.28	4.28	1.113e+40	0.0122
11689	triHPacyl.tptmmmtppd	1.435e+44	5.64	5.64	1.110e+40	0.0122
11690	triHPacyl.pttmttppd	1.167e+44	5.53	5.53	1.097e+40	0.012
11691	triHPacyl.ptmtmtppd	1.275e+43	4.21	4.21	1.093e+40	0.012
11692	triHPacyl.tmtmtmtpd	1.251e+44	5.57	5.57	1.092e+40	0.012
11693	triHPacyl.mppmpptppd	8.210e+42	3.96	3.96	1.077e+40	0.0118
11694	triHPacyl.ppppmtppd	2.099e+43	4.52	4.52	1.074e+40	0.0118
11695	triHPacyl.ppttptppd	1.655e+44	5.76	5.76	1.060e+40	0.0117
11696	triHPacyl.pppppppppd	2.690e+44	6.05	6.05	1.057e+40	0.0116
11697	triHPacyl.mtttptppd	4.072e+43	4.92	4.92	1.057e+40	0.0116
11698	triHPacyl.ppppmtppd	9.426e+43	5.42	5.42	1.053e+40	0.0116
11699	triHPacyl.pptpmpppd	1.858e+44	5.83	5.83	1.052e+40	0.0116
11700	triHPacyl.mttmptmmd	2.376e+43	4.61	4.61	1.048e+40	0.0115
11701	triHPacyl.ptmmmtmmd	1.598e+44	5.74	5.74	1.044e+40	0.0115
11702	triHPacyl.tmpppmtmmd	7.306e+43	5.28	5.28	1.044e+40	0.0115
11703	triHPacyl.tptmmmmppd	2.287e+43	4.59	4.59	1.040e+40	0.0114
11704	triHPacyl.ptmtppmpmd	6.047e+43	5.17	5.17	1.039e+40	0.0114
11705	triHPacyl.tttmmtmmd	2.751e+43	4.71	4.71	1.027e+40	0.0113
11706	triHPacyl.pppppppppd	3.048e+43	4.77	4.77	1.022e+40	0.0112
11707	triHPacyl.tmtmttppd	2.007e+44	5.90	5.90	1.019e+40	0.0112
11708	triHPacyl.tmmmpptppd	5.087e+43	5.08	5.08	1.014e+40	0.0111
11709	triHPacyl.mmmmpptppd	3.616e+43	4.88	4.88	1.014e+40	0.0111
11710	triHPacyl.tttmptppd	4.697e+43	5.04	5.04	1.002e+40	0.011
11711	triHPacyl.pmmtpppmd	1.992e+43	4.53	4.53	9.945e+39	0.0109

11712	triHPacyl.pmppptmpmd	7.707e+42	3.97	3.97	9.832e+39	0.0108
11713	triHPacyl.mmtmpttpmd	9.120e+43	5.46	5.46	9.681e+39	0.0106
11714	triHPacyl.pmmmpmpppd	4.089e+43	4.98	4.98	9.659e+39	0.0106
11715	triHPacyl.tmpnmtmpmd	1.990e+43	4.55	4.55	9.658e+39	0.0106
11716	triHPacyl.ppptptmpd	5.260e+44	6.51	6.51	9.572e+39	0.0105
11717	triHPacyl.pmttpttpmd	1.507e+44	5.76	5.76	9.534e+39	0.0105
11718	triHPacyl.tptpmmpmd	1.139e+44	5.60	5.60	9.503e+39	0.0104
11719	triHPacyl.tmpmnmppd	1.045e+43	4.18	4.18	9.486e+39	0.0104
11720	triHPacyl.mpmmpptmpd	5.131e+43	5.13	5.13	9.462e+39	0.0104
11721	triHPacyl.tmttmnmppd	1.656e+44	5.83	5.83	9.385e+39	0.0103
11722	triHPacyl.pttpmtmpmd	4.045e+43	5.00	5.00	9.194e+39	0.0101
11723	triHPacyl.ttmtmmpmd	1.072e+44	5.58	5.58	9.159e+39	0.0101
11724	triHPacyl.tmmpmtmpd	2.609e+43	4.74	4.74	9.121e+39	0.01
11725	triHPacyl.tptmptmpd	1.168e+44	5.64	5.64	9.083e+39	0.00998
11726	triHPacyl.ttmmpptmpd	1.372e+44	5.74	5.74	8.981e+39	0.00987
11727	triHPacyl.pmtpmnmppd	3.690e+43	4.97	4.97	8.852e+39	0.00973
11728	triHPacyl.tmmmmmtmmd	1.533e+44	5.82	5.82	8.835e+39	0.00971
11729	triHPacyl.pppppptmpd	1.801e+44	5.92	5.92	8.822e+39	0.00969
11730	triHPacyl.mttmptmpd	3.145e+43	4.88	4.88	8.752e+39	0.00962
11731	triHPacyl.ppttpptppd	1.058e+44	5.60	5.60	8.733e+39	0.0096
11732	triHPacyl.mttppmtmmd	2.242e+43	4.68	4.68	8.731e+39	0.00959
11733	triHPacyl.ptmtptmpd	1.175e+44	5.67	5.67	8.721e+39	0.00958
11734	triHPacyl.pmmppptmpd	2.293e+43	4.70	4.70	8.659e+39	0.00951
11735	triHPacyl.tmmpptmmd	1.867e+44	5.95	5.95	8.646e+39	0.0095
11736	triHPacyl.tppmmmpmmd	1.574e+45	7.23	7.23	8.456e+39	0.00929
11737	triHPacyl.ppmmmmpmmd	2.298e+43	4.72	4.72	8.407e+39	0.00924
11738	triHPacyl.mmpppptppd	2.387e+43	4.74	4.74	8.381e+39	0.00921
11739	triHPacyl.ppptptmpd	3.344e+44	6.32	6.32	8.323e+39	0.00915
11740	triHPacyl.pmttptmpd	1.382e+44	5.80	5.80	8.291e+39	0.00911
11741	triHPacyl.pmpppmmpmd	8.430e+42	4.13	4.13	8.259e+39	0.00907
11742	triHPacyl.tpmmmmtmpd	5.413e+43	5.24	5.24	8.242e+39	0.00906
11743	triHPacyl.tpmnmtmmd	5.979e+43	5.30	5.30	8.200e+39	0.00901
11744	triHPacyl.tmmmpptppd	6.914e+43	5.39	5.39	8.168e+39	0.00897
11745	triHPacyl.mttppmpmd	2.959e+44	6.26	6.26	8.102e+39	0.0089
11746	triHPacyl.tppppptmpd	1.964e+43	4.65	4.65	8.101e+39	0.0089
11747	triHPacyl.mmpmpppmmd	5.111e+43	5.22	5.22	8.055e+39	0.00885
11748	triHPacyl.ptttmtmpd	5.924e+43	5.31	5.31	8.049e+39	0.00884
11749	triHPacyl.tmppptmmd	5.336e+43	5.25	5.25	7.997e+39	0.00879
11750	triHPacyl.tpmnmtmmd	9.490e+43	5.59	5.59	7.993e+39	0.00878
11751	triHPacyl.ttmnmtmmd	1.544e+44	5.89	5.89	7.875e+39	0.00865
11752	triHPacyl.pppmptmpd	1.717e+44	5.96	5.96	7.854e+39	0.00863
11753	triHPacyl.ppmppmpmd	3.171e+43	4.95	4.95	7.849e+39	0.00863
11754	triHPacyl.tpmnmtpppd	3.900e+43	5.08	5.08	7.828e+39	0.0086
11755	triHPacyl.tmmnmtmmd	1.591e+44	5.92	5.92	7.780e+39	0.00855
11756	triHPacyl.pmpmtmnmmd	3.336e+43	4.99	4.99	7.729e+39	0.00849
11757	triHPacyl.pttpmtpppd	4.476e+44	6.54	6.54	7.642e+39	0.0084
11758	triHPacyl.ppmptmmpd	8.606e+43	5.56	5.56	7.617e+39	0.00837
11759	triHPacyl.pmmnmtmmd	1.136e+44	5.73	5.73	7.616e+39	0.00837
11760	triHPacyl.ptppptmmd	4.907e+43	5.23	5.23	7.542e+39	0.00829
11761	triHPacyl.pmtmmtmpd	2.185e+43	4.75	4.75	7.510e+39	0.00825
11762	triHPacyl.tptpmnmppd	5.343e+43	5.29	5.29	7.442e+39	0.00818
11763	triHPacyl.mtppptmpd	4.064e+43	5.13	5.13	7.416e+39	0.00815
11764	triHPacyl.mmpmptpppd	3.525e+43	5.05	5.05	7.401e+39	0.00813
11765	triHPacyl.tmtmmtmmd	1.108e+44	5.74	5.74	7.292e+39	0.00801
11766	triHPacyl.tmmmpptppd	3.241e+43	5.01	5.01	7.271e+39	0.00799
11767	triHPacyl.tmtmnmppd	3.235e+44	6.38	6.38	7.271e+39	0.00799
11768	triHPacyl.pppmptmpd	7.989e+43	5.56	5.56	7.056e+39	0.00775
11769	triHPacyl.tmtmmtmpd	9.407e+44	7.04	7.04	7.014e+39	0.00771
11770	triHPacyl.ppttptmpd	3.640e+44	6.48	6.48	6.973e+39	0.00766
11771	triHPacyl.ttppppppmd	2.580e+43	4.90	4.90	6.960e+39	0.00765
11772	triHPacyl.ptmtpppmmd	1.596e+44	5.99	5.99	6.926e+39	0.00761
11773	triHPacyl.pmttppmmpd	8.956e+43	5.64	5.64	6.922e+39	0.00761
11774	triHPacyl.ppmnmtmpd	2.451e+44	6.25	6.25	6.848e+39	0.00752
11775	triHPacyl.tpmnmtmpd	8.880e+43	5.65	5.65	6.842e+39	0.00752
11776	triHPacyl.tptmptmpd	1.879e+44	6.09	6.09	6.833e+39	0.00751
11777	triHPacyl.tmtmmtmmd	6.800e+43	5.49	5.49	6.774e+39	0.00744
11778	triHPacyl.tptmptmpd	2.115e+44	6.17	6.17	6.734e+39	0.0074
11779	triHPacyl.mtmtptmpd	5.501e+43	5.37	5.37	6.691e+39	0.00735
11780	triHPacyl.ppttptmpd	7.849e+43	5.59	5.59	6.661e+39	0.00732
11781	triHPacyl.ppmnmppmd	7.599e+43	5.57	5.57	6.646e+39	0.0073
11782	triHPacyl.tmtmmtmpd	1.774e+44	6.08	6.08	6.641e+39	0.0073
11783	triHPacyl.tptmnmppd	8.690e+42	4.28	4.28	6.614e+39	0.00727

11784	triHPacyl.pppmpttmd	1.465e+44	5.97	5.97	6.600e+39	0.00725
11785	triHPacyl.ppptppmmpd	7.502e+43	5.57	5.57	6.594e+39	0.00725
11786	triHPacyl.tmmmpmtmpd	7.737e+43	5.59	5.59	6.572e+39	0.00722
11787	triHPacyl.tptpmtmpmd	4.513e+43	5.27	5.27	6.556e+39	0.0072
11788	triHPacyl.pmpmptmmd	4.373e+43	5.25	5.25	6.543e+39	0.00719
11789	triHPacyl.ttppttmd	1.606e+43	4.66	4.66	6.481e+39	0.00712
11790	triHPacyl.pppmppmmd	1.486e+44	5.99	5.99	6.466e+39	0.00711
11791	triHPacyl.ttmtmmpmd	5.421e+43	5.39	5.39	6.405e+39	0.00704
11792	triHPacyl.pppmptmmd	1.677e+44	6.07	6.07	6.330e+39	0.00696
11793	triHPacyl.mtpppttmd	1.369e+43	4.59	4.59	6.236e+39	0.00685
11794	triHPacyl.ttpppmmpmd	6.072e+43	5.48	5.48	6.221e+39	0.00684
11795	triHPacyl.pmtppmpppd	1.473e+44	6.01	6.01	6.185e+39	0.0068
11796	triHPacyl.tpmpttmd	1.179e+44	5.88	5.88	6.182e+39	0.00679
11797	triHPacyl.pmpmmtppd	4.103e+43	5.25	5.25	6.169e+39	0.00678
11798	triHPacyl.tmtmtmpmd	4.988e+44	6.74	6.74	6.159e+39	0.00677
11799	triHPacyl.pttpmtppmd	6.634e+44	6.91	6.91	6.147e+39	0.00675
11800	triHPacyl.ptmpmtppd	3.243e+43	5.11	5.11	6.116e+39	0.00672
11801	triHPacyl.pptppmppd	6.901e+43	5.56	5.56	6.101e+39	0.0067
11802	triHPacyl.pmpmttmd	1.255e+44	5.92	5.92	6.089e+39	0.00669
11803	triHPacyl.pttpmmmmmd	1.869e+43	4.79	4.79	6.085e+39	0.00669
11804	triHPacyl.ttpmptppmd	1.552e+43	4.68	4.68	6.078e+39	0.00668
11805	triHPacyl.tpppmtppmd	1.301e+44	5.95	5.95	6.067e+39	0.00667
11806	triHPacyl.tmmmtppmd	1.261e+44	5.93	5.93	6.023e+39	0.00662
11807	triHPacyl.tmtmtmpmd	3.905e+44	6.61	6.61	5.963e+39	0.00655
11808	triHPacyl.tttmmmmmd	2.363e+43	4.94	4.94	5.961e+39	0.00655
11809	triHPacyl.tpmmttppd	1.271e+44	5.94	5.94	5.942e+39	0.00653
11810	triHPacyl.ttpmmmpd	2.907e+43	5.07	5.07	5.909e+39	0.00649
11811	triHPacyl.tmpmmmtppd	7.606e+43	5.64	5.64	5.891e+39	0.00647
11812	triHPacyl.mmmmmmpd	4.948e+43	5.39	5.39	5.855e+39	0.00643
11813	triHPacyl.ppttppmmd	2.068e+44	6.25	6.25	5.817e+39	0.00639
11814	triHPacyl.tmtmmpmd	1.121e+44	5.88	5.88	5.791e+39	0.00636
11815	triHPacyl.pppttmd	1.083e+44	5.87	5.87	5.724e+39	0.00629
11816	triHPacyl.pmpmtmpmd	1.116e+44	5.89	5.89	5.717e+39	0.00628
11817	triHPacyl.tmmptmmd	1.532e+44	6.08	6.08	5.711e+39	0.00628
11818	triHPacyl.pptppppd	8.053e+43	5.70	5.70	5.698e+39	0.00626
11819	triHPacyl.ttmtmtmpmd	1.673e+43	4.76	4.76	5.697e+39	0.00626
11820	triHPacyl.mtppmmmd	1.625e+43	4.74	4.74	5.681e+39	0.00624
11821	triHPacyl.mmtpmtmd	4.353e+43	5.33	5.33	5.669e+39	0.00623
11822	triHPacyl.ttmtmmpd	8.240e+43	5.71	5.71	5.665e+39	0.00623
11823	triHPacyl.ptmpmmpd	1.216e+43	4.58	4.58	5.637e+39	0.00619
11824	triHPacyl.pttpmmmpd	1.872e+43	4.84	4.84	5.620e+39	0.00618
11825	triHPacyl.ptpmmtppd	1.187e+43	4.56	4.56	5.617e+39	0.00617
11826	triHPacyl.ptmtmmpd	7.090e+43	5.63	5.63	5.576e+39	0.00613
11827	triHPacyl.pmmmpmtmd	8.985e+43	5.78	5.78	5.564e+39	0.00611
11828	triHPacyl.tppmmpmd	6.713e+43	5.60	5.60	5.559e+39	0.00611
11829	triHPacyl.tttpmtmd	5.068e+43	5.44	5.44	5.545e+39	0.00609
11830	triHPacyl.pmpptmmd	1.377e+43	4.66	4.66	5.515e+39	0.00606
11831	triHPacyl.mmppttppd	5.452e+43	5.49	5.49	5.479e+39	0.00602
11832	triHPacyl.ttpmmtppd	5.566e+43	5.50	5.50	5.457e+39	0.006
11833	triHPacyl.ptppmtppd	2.423e+43	5.01	5.01	5.413e+39	0.00595
11834	triHPacyl.tpmmmtpd	6.807e+43	5.63	5.63	5.390e+39	0.00592
11835	triHPacyl.pttppmmd	6.482e+43	5.61	5.61	5.315e+39	0.00584
11836	triHPacyl.tttpmmtmd	3.527e+43	5.25	5.25	5.304e+39	0.00583
11837	triHPacyl.ttpmmtmmd	9.788e+42	4.48	4.48	5.292e+39	0.00582
11838	triHPacyl.pptppppd	1.483e+44	6.11	6.11	5.245e+39	0.00576
11839	triHPacyl.ttpmttmd	3.731e+43	5.29	5.29	5.236e+39	0.00575
11840	triHPacyl.pmmmmmpd	1.510e+43	4.75	4.75	5.235e+39	0.00575
11841	triHPacyl.ppttppmmd	4.083e+44	6.72	6.72	5.225e+39	0.00574
11842	triHPacyl.tmtmmtmpd	9.312e+43	5.85	5.85	5.123e+39	0.00563
11843	triHPacyl.tptpmmtmd	6.181e+43	5.60	5.60	5.106e+39	0.00561
11844	triHPacyl.mtmmmmmpd	6.990e+43	5.68	5.68	5.064e+39	0.00556
11845	triHPacyl.tttppmtppd	1.392e+44	6.09	6.09	5.062e+39	0.00556
11846	triHPacyl.mmmppmtmd	1.107e+43	4.59	4.59	5.059e+39	0.00556
11847	triHPacyl.ptmtpttmd	1.859e+44	6.27	6.27	5.057e+39	0.00556
11848	triHPacyl.mmpmmtppd	2.727e+43	5.12	5.12	5.054e+39	0.00555
11849	triHPacyl.mmmmpmmpd	5.617e+43	5.56	5.56	5.007e+39	0.0055
11850	triHPacyl.tptpmtppd	5.732e+43	5.58	5.58	4.962e+39	0.00545
11851	triHPacyl.pppmppppd	2.047e+43	4.97	4.97	4.943e+39	0.00543
11852	triHPacyl.tmtppppd	4.898e+44	6.86	6.86	4.886e+39	0.00537
11853	triHPacyl.ttmtmpmd	1.753e+44	6.25	6.25	4.866e+39	0.00535
11854	triHPacyl.tmtppmmd	8.217e+43	5.81	5.81	4.838e+39	0.00532
11855	triHPacyl.pmttmmmd	3.934e+43	5.37	5.37	4.837e+39	0.00532

11856	triHPacyl.pmmmpmmnd	9.980e+43	5.93	5.93	4.802e+39	0.00528
11857	triHPacyl.ttpmmmtmpd	4.411e+43	5.44	5.44	4.765e+39	0.00524
11858	triHPacyl.mppmmmtmpd	2.837e+43	5.18	5.18	4.764e+39	0.00523
11859	triHPacyl.pptppmpmd	4.166e+43	5.41	5.41	4.753e+39	0.00522
11860	triHPacyl.tppmmmtmpd	3.486e+43	5.31	5.31	4.707e+39	0.00517
11861	triHPacyl.ttpmmtmpd	3.043e+43	5.24	5.24	4.670e+39	0.00513
11862	triHPacyl.tttmmmtmpd	9.185e+43	5.90	5.90	4.660e+39	0.00512
11863	triHPacyl.pmtmptmpd	2.894e+43	5.21	5.21	4.645e+39	0.0051
11864	triHPacyl.pptmmpmpd	4.928e+43	5.53	5.53	4.632e+39	0.00509
11865	triHPacyl.tmpmptmpd	2.173e+43	5.04	5.04	4.598e+39	0.00505
11866	triHPacyl.ptppppmpd	2.793e+43	5.20	5.20	4.578e+39	0.00503
11867	triHPacyl.tppppmmnd	8.383e+42	4.48	4.48	4.561e+39	0.00501
11868	triHPacyl.tmtmmtppd	1.316e+44	6.12	6.12	4.554e+39	0.005
11869	triHPacyl.tmtppmmnd	1.086e+44	6.01	6.01	4.546e+39	0.005
11870	triHPacyl.tmttmtmmnd	3.097e+44	6.64	6.64	4.543e+39	0.00499
11871	triHPacyl.tmttmmmpmd	2.767e+44	6.57	6.57	4.530e+39	0.00498
11872	triHPacyl.pmpmmmtmnd	5.394e+43	5.62	5.62	4.363e+39	0.00479
11873	triHPacyl.mtmmtmpmnd	1.082e+44	6.03	6.03	4.360e+39	0.00479
11874	triHPacyl.ptmtmmmpmd	1.069e+44	6.03	6.03	4.342e+39	0.00477
11875	triHPacyl.pmpppptmpd	2.615e+43	5.19	5.19	4.340e+39	0.00477
11876	triHPacyl.mmmtpmtpmd	1.074e+44	6.03	6.03	4.330e+39	0.00476
11877	triHPacyl.ttmmtmpmnd	1.442e+44	6.22	6.22	4.243e+39	0.00466
11878	triHPacyl.tppmptmpd	2.852e+43	5.25	5.25	4.242e+39	0.00466
11879	triHPacyl.pmtmppmpd	2.267e+43	5.12	5.12	4.230e+39	0.00465
11880	triHPacyl.pppmptppmd	5.428e+43	5.64	5.64	4.221e+39	0.00464
11881	triHPacyl.tmttmmmmnd	2.265e+44	6.49	6.49	4.211e+39	0.00463
11882	triHPacyl.pppmmpmpmd	2.718e+43	5.23	5.23	4.195e+39	0.00461
11883	triHPacyl.tmttmmmmnd	5.980e+43	5.70	5.70	4.188e+39	0.0046
11884	triHPacyl.pmmmpmpmnd	2.079e+44	6.45	6.45	4.182e+39	0.0046
11885	triHPacyl.ptppmtpmd	2.069e+43	5.07	5.07	4.171e+39	0.00458
11886	triHPacyl.tppmmpmnd	6.449e+43	5.75	5.75	4.158e+39	0.00457
11887	triHPacyl.tppmmpmpd	3.658e+43	5.42	5.42	4.151e+39	0.00456
11888	triHPacyl.mtmtpmmpmd	5.179e+43	5.62	5.62	4.149e+39	0.00456
11889	triHPacyl.tttmptmpd	6.430e+43	5.76	5.76	4.128e+39	0.00454
11890	triHPacyl.mtppmmpmd	4.596e+43	5.55	5.55	4.128e+39	0.00454
11891	triHPacyl.tmpmmtmpd	6.509e+43	5.77	5.77	4.088e+39	0.00449
11892	triHPacyl.tppmmmmpd	4.183e+43	5.51	5.51	4.066e+39	0.00447
11893	triHPacyl.mmmmpptppd	5.426e+43	5.67	5.67	4.032e+39	0.00443
11894	triHPacyl.mttmmtmpd	3.077e+43	5.33	5.33	4.014e+39	0.00441
11895	triHPacyl.pttmptmmpd	1.844e+43	5.03	5.03	4.011e+39	0.00441
11896	triHPacyl.tmtmtpmd	2.092e+44	6.48	6.48	4.008e+39	0.0044
11897	triHPacyl.mmpmtpmd	3.383e+43	5.39	5.39	4.003e+39	0.0044
11898	triHPacyl.pttpmmtmnd	1.939e+43	5.06	5.06	3.989e+39	0.00438
11899	triHPacyl.ptttmmpmd	2.672e+44	6.63	6.63	3.935e+39	0.00432
11900	triHPacyl.ppttptmpmd	9.561e+43	6.02	6.02	3.912e+39	0.0043
11901	triHPacyl.mttptmpmd	3.051e+43	5.34	5.34	3.902e+39	0.00429
11902	triHPacyl.pmtptmpmd	1.048e+44	6.08	6.08	3.896e+39	0.00428
11903	triHPacyl.mtttptmpmd	4.845e+43	5.62	5.62	3.879e+39	0.00426
11904	triHPacyl.mttptmmpd	1.010e+44	6.06	6.06	3.871e+39	0.00425
11905	triHPacyl.mppmptmpd	1.386e+43	4.88	4.88	3.867e+39	0.00425
11906	triHPacyl.tmtmtpmd	1.275e+44	6.20	6.20	3.850e+39	0.00423
11907	triHPacyl.ptttptmpd	6.735e+43	5.82	5.82	3.846e+39	0.00423
11908	triHPacyl.pmmmpmpmd	1.474e+43	4.92	4.92	3.845e+39	0.00422
11909	triHPacyl.mtpmptmpd	1.972e+43	5.10	5.10	3.803e+39	0.00418
11910	triHPacyl.pmtmtpmd	1.285e+43	4.85	4.85	3.794e+39	0.00417
11911	triHPacyl.ttmppmmmpd	2.742e+43	5.30	5.30	3.792e+39	0.00417
11912	triHPacyl.mttmptppmd	7.490e+43	5.90	5.90	3.757e+39	0.00413
11913	triHPacyl.pmtmmtppmd	6.561e+43	5.82	5.82	3.753e+39	0.00412
11914	triHPacyl.tmtmptppmd	2.721e+44	6.68	6.68	3.729e+39	0.0041
11915	triHPacyl.ttptmmpmnd	1.167e+44	6.17	6.17	3.726e+39	0.00409
11916	triHPacyl.tppmptmnd	4.213e+43	5.57	5.57	3.694e+39	0.00406
11917	triHPacyl.tttmtpmd	6.374e+43	5.82	5.82	3.673e+39	0.00404
11918	triHPacyl.tmtppmtpmd	7.783e+43	5.95	5.95	3.609e+39	0.00397
11919	triHPacyl.tmpmmtmpd	7.986e+43	5.97	5.97	3.591e+39	0.00395
11920	triHPacyl.tptpmtmpd	1.322e+44	6.27	6.27	3.575e+39	0.00393
11921	triHPacyl.ppmmtmtpmd	1.651e+44	6.40	6.40	3.574e+39	0.00393
11922	triHPacyl.tttptmpmd	1.547e+44	6.37	6.37	3.569e+39	0.00392
11923	triHPacyl.pmpppppmd	1.355e+43	4.91	4.91	3.563e+39	0.00392
11924	triHPacyl.pmtppmmmpd	5.578e+43	5.76	5.76	3.561e+39	0.00391
11925	triHPacyl.pttpmmmnd	1.584e+43	5.02	5.02	3.500e+39	0.00385
11926	triHPacyl.ppptptmpd	3.210e+44	6.81	6.81	3.489e+39	0.00383
11927	triHPacyl.tppmptmpd	9.616e+43	6.10	6.10	3.482e+39	0.00383

11928	triHPacyl.pmtmptmpmd	9.639e+43	6.11	6.11	3.431e+39	0.00377
11929	triHPacyl.tttmmttppmd	3.002e+44	6.79	6.79	3.398e+39	0.00373
11930	triHPacyl.tttptmmmpd	3.959e+43	5.58	5.58	3.382e+39	0.00372
11931	triHPacyl.ptttmmmmmpd	2.833e+43	5.39	5.39	3.361e+39	0.00369
11932	triHPacyl.ptptmmmpmd	2.212e+44	6.61	6.61	3.361e+39	0.00369
11933	triHPacyl.tmtttmmmpd	3.526e+44	6.89	6.89	3.349e+39	0.00368
11934	triHPacyl.ppttptmmpd	1.169e+44	6.24	6.24	3.345e+39	0.00368
11935	triHPacyl.tttmmptppmd	3.466e+44	6.88	6.88	3.345e+39	0.00368
11936	triHPacyl.pmtptmmpmd	2.628e+43	5.35	5.35	3.343e+39	0.00367
11937	triHPacyl.tptmptmmpd	3.111e+43	5.45	5.45	3.330e+39	0.00366
11938	triHPacyl.tpppttppd	1.459e+44	6.37	6.37	3.324e+39	0.00365
11939	triHPacyl.mmtmmttppmd	1.306e+44	6.31	6.31	3.318e+39	0.00365
11940	triHPacyl.tptmptppmd	1.354e+45	7.70	7.70	3.308e+39	0.00364
11941	triHPacyl.mmtptmtpd	1.114e+44	6.22	6.22	3.306e+39	0.00363
11942	triHPacyl.pptmppppd	7.037e+43	5.95	5.95	3.253e+39	0.00357
11943	triHPacyl.pmpmmmmmpd	5.845e+43	5.84	5.84	3.236e+39	0.00356
11944	triHPacyl.ppmtmmpmd	1.074e+44	6.21	6.21	3.226e+39	0.00354
11945	triHPacyl.ptmmmtppmd	3.010e+44	6.82	6.82	3.225e+39	0.00354
11946	triHPacyl.pptmppppmd	1.641e+44	6.46	6.46	3.222e+39	0.00354
11947	triHPacyl.mttppppmmd	6.327e+43	5.90	5.90	3.197e+39	0.00351
11948	triHPacyl.pptmptmmd	2.292e+44	6.67	6.67	3.189e+39	0.0035
11949	triHPacyl.ptppmmpmd	2.311e+43	5.30	5.30	3.177e+39	0.00349
11950	triHPacyl.pmtmmpmpd	6.273e+43	5.90	5.90	3.169e+39	0.00348
11951	triHPacyl.tttmmpmmmpd	6.841e+43	5.95	5.95	3.163e+39	0.00348
11952	triHPacyl.pmtmmpmpmd	2.170e+43	5.27	5.27	3.163e+39	0.00348
11953	triHPacyl.pmtmmmmppd	2.476e+43	5.35	5.35	3.142e+39	0.00345
11954	triHPacyl.ptttmmpmd	5.268e+43	5.80	5.80	3.112e+39	0.00342
11955	triHPacyl.mmpppppmmpd	3.229e+43	5.52	5.52	3.096e+39	0.0034
11956	triHPacyl.ptmptppd	1.082e+43	4.87	4.87	3.064e+39	0.00337
11957	triHPacyl.ptttppppmd	5.056e+44	7.16	7.16	3.059e+39	0.00336
11958	triHPacyl.ppptptmmd	2.385e+44	6.72	6.72	3.049e+39	0.00335
11959	triHPacyl.mtppptmmd	1.700e+43	5.15	5.15	3.026e+39	0.00332
11960	triHPacyl.tpttmmtpmd	1.346e+44	6.38	6.38	3.012e+39	0.00331
11961	triHPacyl.mmtppmtpd	1.160e+44	6.30	6.30	3.006e+39	0.0033
11962	triHPacyl.mppmptmmpd	1.446e+43	5.06	5.06	2.994e+39	0.00329
11963	triHPacyl.ptppptmmpd	1.444e+43	5.06	5.06	2.987e+39	0.00328
11964	triHPacyl.tttpmmtppd	5.660e+43	5.87	5.87	2.986e+39	0.00328
11965	triHPacyl.ppptppppd	3.052e+44	6.88	6.88	2.983e+39	0.00328
11966	triHPacyl.ptttmmpmpd	1.434e+43	5.06	5.06	2.980e+39	0.00327
11967	triHPacyl.ttttmmmpd	5.854e+43	5.89	5.89	2.978e+39	0.00327
11968	triHPacyl.tpppmtmmpd	7.995e+43	6.08	6.08	2.963e+39	0.00326
11969	triHPacyl.pmtmptmmpd	1.611e+44	6.51	6.51	2.936e+39	0.00323
11970	triHPacyl.ptppmpmpd	9.639e+42	4.83	4.83	2.921e+39	0.00321
11971	triHPacyl.mmmmmttppd	6.817e+43	6.00	6.00	2.894e+39	0.00318
11972	triHPacyl.tpmmpmmpmd	3.560e+43	5.62	5.62	2.886e+39	0.00317
11973	triHPacyl.tttpmmmmpd	3.964e+43	5.68	5.68	2.872e+39	0.00316
11974	triHPacyl.pptppppppd	1.393e+44	6.43	6.43	2.870e+39	0.00315
11975	triHPacyl.pmtmmpmpmd	5.646e+43	5.90	5.90	2.846e+39	0.00313
11976	triHPacyl.tpptmmpmmd	1.666e+44	6.55	6.55	2.843e+39	0.00312
11977	triHPacyl.pmmmpmtpmd	1.498e+44	6.49	6.49	2.825e+39	0.0031
11978	triHPacyl.tmtppptppd	1.949e+44	6.65	6.65	2.809e+39	0.00309
11979	triHPacyl.tmttptmmpd	3.350e+44	6.97	6.97	2.787e+39	0.00306
11980	triHPacyl.ptppptmmpd	1.071e+43	4.92	4.92	2.772e+39	0.00305
11981	triHPacyl.mtpmmpmmpd	2.307e+43	5.38	5.38	2.770e+39	0.00304
11982	triHPacyl.mtttppmmpd	5.099e+43	5.86	5.86	2.765e+39	0.00304
11983	triHPacyl.mppmmpmmpd	4.017e+43	5.72	5.72	2.752e+39	0.00302
11984	triHPacyl.mmttppmmpd	1.140e+44	6.34	6.34	2.742e+39	0.00301
11985	triHPacyl.ptpmmmtmmpd	8.693e+42	4.81	4.81	2.727e+39	0.003
11986	triHPacyl.tpttmmmpmd	1.677e+44	6.57	6.57	2.726e+39	0.003
11987	triHPacyl.tttppmpmmd	3.811e+43	5.69	5.69	2.723e+39	0.00299
11988	triHPacyl.ptpmmmmppd	1.385e+43	5.09	5.09	2.699e+39	0.00297
11989	triHPacyl.pmttptppd	1.245e+44	6.40	6.40	2.697e+39	0.00296
11990	triHPacyl.tppmmpmmpd	2.046e+43	5.33	5.33	2.691e+39	0.00296
11991	triHPacyl.tppppptmmd	2.784e+44	6.89	6.89	2.681e+39	0.00295
11992	triHPacyl.ppmtppmmpd	8.074e+43	6.15	6.15	2.671e+39	0.00294
11993	triHPacyl.pppmmpmmmpd	4.940e+43	5.86	5.86	2.651e+39	0.00291
11994	triHPacyl.ttttmmmpmd	1.815e+44	6.64	6.64	2.635e+39	0.0029
11995	triHPacyl.ptttmtpmmd	7.825e+43	6.14	6.14	2.619e+39	0.00288
11996	triHPacyl.mtmppptmmpd	2.290e+44	6.78	6.78	2.613e+39	0.00287
11997	triHPacyl.ptpmpmmpd	1.022e+43	4.93	4.93	2.612e+39	0.00287
11998	triHPacyl.tmtmptmmpd	1.290e+44	6.45	6.45	2.589e+39	0.00284
11999	triHPacyl.tmpmptppd	8.022e+43	6.17	6.17	2.570e+39	0.00282

12000	triHPacyl.mttmpmtmpd	1.197e+44	6.42	6.42	2.522e+39	0.00277
12001	triHPacyl.pmttptmpd	1.511e+44	6.56	6.56	2.520e+39	0.00277
12002	triHPacyl.pptmpppmd	5.525e+43	5.96	5.96	2.517e+39	0.00277
12003	triHPacyl.mmmppmtmmd	4.428e+43	5.83	5.83	2.506e+39	0.00275
12004	triHPacyl.mtmtppmmpd	7.206e+43	6.12	6.12	2.501e+39	0.00275
12005	triHPacyl.ppmtmmpmmd	1.683e+44	6.63	6.63	2.500e+39	0.00275
12006	triHPacyl.pmpmtmmpd	3.573e+43	5.71	5.71	2.490e+39	0.00274
12007	triHPacyl.tpttmtmpd	1.869e+44	6.69	6.69	2.484e+39	0.00273
12008	triHPacyl.tmmppmmpd	9.924e+43	6.32	6.32	2.475e+39	0.00272
12009	triHPacyl.mtmtptmpd	1.055e+44	6.36	6.36	2.471e+39	0.00272
12010	triHPacyl.ptppmtmpd	4.661e+43	5.87	5.87	2.462e+39	0.00271
12011	triHPacyl.pppmptppd	4.681e+43	5.88	5.88	2.442e+39	0.00268
12012	triHPacyl.mtppmmmd	2.641e+43	5.54	5.54	2.438e+39	0.00268
12013	triHPacyl.mmtmmtmmd	2.928e+43	5.60	5.60	2.438e+39	0.00268
12014	triHPacyl.mmpmppppd	5.269e+43	5.95	5.95	2.431e+39	0.00267
12015	triHPacyl.mttmpmmmd	2.834e+43	5.59	5.59	2.416e+39	0.00265
12016	triHPacyl.pptppppmd	2.829e+44	6.96	6.96	2.405e+39	0.00264
12017	triHPacyl.ppptppmmd	6.467e+43	6.08	6.08	2.404e+39	0.00264
12018	triHPacyl.tppmtmpd	1.305e+43	5.13	5.13	2.399e+39	0.00264
12019	triHPacyl.ttpmmpmd	3.589e+43	5.73	5.73	2.392e+39	0.00263
12020	triHPacyl.mtppptppd	1.145e+44	6.43	6.43	2.387e+39	0.00262
12021	triHPacyl.ttmpmmmd	2.550e+43	5.53	5.53	2.385e+39	0.00262
12022	triHPacyl.ptppppmmd	1.266e+43	5.12	5.12	2.366e+39	0.0026
12023	triHPacyl.tppmptppd	9.847e+43	6.34	6.34	2.356e+39	0.00259
12024	triHPacyl.tmmmtmpd	5.768e+44	7.40	7.40	2.355e+39	0.00259
12025	triHPacyl.tppmmpmd	8.448e+43	6.25	6.25	2.348e+39	0.00258
12026	triHPacyl.tptmppppd	1.818e+44	6.71	6.71	2.339e+39	0.00257
12027	triHPacyl.pmmptmpd	1.361e+44	6.54	6.54	2.335e+39	0.00257
12028	triHPacyl.ppptptmpd	5.722e+43	6.03	6.03	2.329e+39	0.00256
12029	triHPacyl.tttmptmpd	5.604e+43	6.01	6.01	2.328e+39	0.00256
12030	triHPacyl.mmtmpmtmpd	1.141e+44	6.44	6.44	2.327e+39	0.00256
12031	triHPacyl.tpmmmmpmd	3.613e+43	5.75	5.75	2.324e+39	0.00255
12032	triHPacyl.ptmppmmpd	2.637e+43	5.57	5.57	2.322e+39	0.00255
12033	triHPacyl.pmtptmpd	2.394e+43	5.51	5.51	2.310e+39	0.00254
12034	triHPacyl.ttmmmtppd	3.924e+44	7.18	7.18	2.303e+39	0.00253
12035	triHPacyl.mttmpmtmpd	2.252e+44	6.86	6.86	2.285e+39	0.00251
12036	triHPacyl.pptpmpppd	1.016e+44	6.38	6.38	2.272e+39	0.0025
12037	triHPacyl.mmpptppd	1.132e+44	6.45	6.45	2.271e+39	0.0025
12038	triHPacyl.ttptppmmd	1.054e+44	6.41	6.41	2.265e+39	0.00249
12039	triHPacyl.tmmtmtmmd	4.565e+43	5.91	5.91	2.262e+39	0.00249
12040	triHPacyl.mmtptmpd	1.703e+44	6.70	6.70	2.256e+39	0.00248
12041	triHPacyl.pppmmpmd	5.675e+43	6.04	6.04	2.255e+39	0.00248
12042	triHPacyl.pmtptmmd	3.376e+43	5.73	5.73	2.251e+39	0.00247
12043	triHPacyl.pmtmtmpd	1.048e+44	6.41	6.41	2.248e+39	0.00247
12044	triHPacyl.mtppptmpd	7.663e+42	4.85	4.85	2.242e+39	0.00246
12045	triHPacyl.mmpmmpmd	1.065e+43	5.05	5.05	2.236e+39	0.00246
12046	triHPacyl.ptmmpmmpd	3.808e+43	5.81	5.81	2.229e+39	0.00245
12047	triHPacyl.pptppppd	3.204e+44	7.09	7.09	2.208e+39	0.00243
12048	triHPacyl.mmtppmtmpd	4.748e+43	5.95	5.95	2.195e+39	0.00241
12049	triHPacyl.mtppmmpmd	2.646e+43	5.61	5.61	2.182e+39	0.0024
12050	triHPacyl.ttmtmtmpd	1.228e+44	6.52	6.52	2.180e+39	0.00239
12051	triHPacyl.pppmmpmmpd	2.033e+43	5.46	5.46	2.153e+39	0.00237
12052	triHPacyl.pmttmmpd	9.354e+44	7.74	7.74	2.142e+39	0.00235
12053	triHPacyl.ppptptmpd	2.056e+44	6.84	6.84	2.138e+39	0.00235
12054	triHPacyl.ptmmtppmd	1.743e+44	6.74	6.74	2.131e+39	0.00234
12055	triHPacyl.pptppmmpd	6.799e+43	6.19	6.19	2.120e+39	0.00233
12056	triHPacyl.mtmtptmpd	1.443e+44	6.64	6.64	2.112e+39	0.00232
12057	triHPacyl.tptmtpppd	4.152e+44	7.27	7.27	2.095e+39	0.0023
12058	triHPacyl.pttpmtpmd	3.777e+43	5.84	5.84	2.094e+39	0.0023
12059	triHPacyl.tttmmtmpd	5.497e+43	6.07	6.07	2.080e+39	0.00229
12060	triHPacyl.ptppptmpd	2.231e+43	5.55	5.55	2.037e+39	0.00224
12061	triHPacyl.mmpmmpmd	1.125e+43	5.14	5.14	2.036e+39	0.00224
12062	triHPacyl.ttmtptmpd	2.002e+43	5.48	5.48	2.036e+39	0.00224
12063	triHPacyl.tttmmpmd	5.303e+43	6.06	6.06	2.033e+39	0.00223
12064	triHPacyl.tttmtmpd	8.727e+43	6.36	6.36	2.017e+39	0.00222
12065	triHPacyl.mtppmmpd	2.891e+43	5.71	5.71	2.016e+39	0.00221
12066	triHPacyl.pttpptmpd	2.808e+43	5.69	5.69	2.011e+39	0.00221
12067	triHPacyl.mtppptmpd	4.004e+43	5.90	5.90	2.008e+39	0.00221
12068	triHPacyl.tmpmtmpd	5.907e+43	6.13	6.13	2.008e+39	0.00221
12069	triHPacyl.mmmmtppd	4.992e+43	6.03	6.03	2.006e+39	0.0022
12070	triHPacyl.ppmmtppd	4.774e+43	6.01	6.01	2.006e+39	0.0022
12071	triHPacyl.tmtmtmpd	2.070e+45	8.26	8.26	1.999e+39	0.0022

12072	triHPacyl.pmmmtmpmd	1.027e+43	5.10	5.10	1.993e+39	0.00219
12073	triHPacyl.pptpnmppmd	9.525e+43	6.42	6.42	1.988e+39	0.00218
12074	triHPacyl.mttmpmmpmd	4.045e+43	5.91	5.91	1.987e+39	0.00218
12075	triHPacyl.mppmptpmd	8.705e+43	6.37	6.37	1.986e+39	0.00218
12076	triHPacyl.ttttmmmpmd	1.349e+44	6.63	6.63	1.980e+39	0.00218
12077	triHPacyl.ppptppppmd	3.878e+44	7.27	7.27	1.967e+39	0.00216
12078	triHPacyl.mpppmtppmd	4.019e+43	5.92	5.92	1.960e+39	0.00215
12079	triHPacyl.pmmmpmtmpmd	1.095e+44	6.52	6.52	1.952e+39	0.00214
12080	triHPacyl.ppmtmmtmmd	1.895e+44	6.85	6.85	1.951e+39	0.00214
12081	triHPacyl.ttmmpmpmmd	2.328e+44	6.97	6.97	1.941e+39	0.00213
12082	triHPacyl.ptmtptpmd	3.856e+43	5.90	5.90	1.926e+39	0.00212
12083	triHPacyl.ptttmmppd	9.349e+43	6.43	6.43	1.922e+39	0.00211
12084	triHPacyl.tpptmtppd	3.116e+44	7.15	7.15	1.922e+39	0.00211
12085	triHPacyl.mmmmmmpmd	1.073e+44	6.52	6.52	1.912e+39	0.0021
12086	triHPacyl.tptmtmmd	1.389e+44	6.67	6.67	1.911e+39	0.0021
12087	triHPacyl.pmpmtmmd	1.709e+44	6.81	6.81	1.870e+39	0.00205
12088	triHPacyl.tptmptmmd	1.821e+44	6.85	6.85	1.868e+39	0.00205
12089	triHPacyl.tptmtmmpd	1.113e+44	6.56	6.56	1.863e+39	0.00205
12090	triHPacyl.ppppmmmpd	2.633e+43	5.70	5.70	1.850e+39	0.00203
12091	triHPacyl.ppppmtppd	1.510e+44	6.74	6.74	1.843e+39	0.00203
12092	triHPacyl.ttptmtmmd	6.294e+44	7.60	7.60	1.842e+39	0.00202
12093	triHPacyl.pmtmmtmmd	6.606e+43	6.26	6.26	1.833e+39	0.00201
12094	triHPacyl.pmttptppd	3.625e+44	7.27	7.27	1.832e+39	0.00201
12095	triHPacyl.pptmptmmd	6.774e+43	6.27	6.27	1.826e+39	0.00201
12096	triHPacyl.tmmpmtmmd	1.707e+44	6.83	6.83	1.819e+39	0.002
12097	triHPacyl.pmmmpmtmmd	1.338e+43	5.31	5.31	1.813e+39	0.00199
12098	triHPacyl.mttppptppd	8.766e+43	6.43	6.43	1.804e+39	0.00198
12099	triHPacyl.ttmppmmpmd	6.063e+43	6.22	6.22	1.797e+39	0.00197
12100	triHPacyl.ptmppmmpmd	6.844e+43	6.29	6.29	1.787e+39	0.00196
12101	triHPacyl.ppptptmmd	8.574e+43	6.43	6.43	1.777e+39	0.00195
12102	triHPacyl.ttmmttppd	3.745e+44	7.31	7.31	1.773e+39	0.00195
12103	triHPacyl.pttmmtmmd	2.513e+44	7.07	7.07	1.765e+39	0.00194
12104	triHPacyl.ptttmtmmd	2.526e+44	7.08	7.08	1.755e+39	0.00193
12105	triHPacyl.mmtpmmtmmd	7.316e+43	6.34	6.34	1.750e+39	0.00192
12106	triHPacyl.ttppptmmd	3.274e+43	5.86	5.86	1.749e+39	0.00192
12107	triHPacyl.pptmptmmd	1.417e+44	6.74	6.74	1.742e+39	0.00191
12108	triHPacyl.mtmmpmmpmd	1.632e+44	6.83	6.83	1.732e+39	0.0019
12109	triHPacyl.tpptmtmmd	2.904e+44	7.17	7.17	1.726e+39	0.0019
12110	triHPacyl.mtmtpppmd	1.764e+44	6.88	6.88	1.719e+39	0.00189
12111	triHPacyl.tptmtmmd	3.299e+44	7.25	7.25	1.717e+39	0.00189
12112	triHPacyl.pmpmtmmd	6.788e+43	6.31	6.31	1.713e+39	0.00188
12113	triHPacyl.pmtmmtmmd	9.027e+43	6.48	6.48	1.707e+39	0.00188
12114	triHPacyl.mtptptmmd	1.435e+43	5.39	5.39	1.697e+39	0.00186
12115	triHPacyl.tptmmtppd	1.609e+44	6.83	6.83	1.691e+39	0.00186
12116	triHPacyl.tmpmmpmmd	4.333e+43	6.05	6.05	1.685e+39	0.00185
12117	triHPacyl.tptmmpmmd	6.408e+43	6.29	6.29	1.684e+39	0.00185
12118	triHPacyl.pmtmmpmmd	2.800e+43	5.80	5.80	1.680e+39	0.00185
12119	triHPacyl.tmppmtmmd	6.311e+43	6.28	6.28	1.671e+39	0.00184
12120	triHPacyl.tmmpptppmd	1.463e+44	6.79	6.79	1.663e+39	0.00183
12121	triHPacyl.pmttptmmd	1.140e+44	6.64	6.64	1.656e+39	0.00182
12122	triHPacyl.tmtmmtppd	1.150e+44	6.65	6.65	1.654e+39	0.00182
12123	triHPacyl.pmtmptmmd	1.239e+44	6.70	6.70	1.642e+39	0.0018
12124	triHPacyl.pmpmtmmd	1.039e+43	5.22	5.22	1.637e+39	0.0018
12125	triHPacyl.ppttptppmd	7.096e+44	7.74	7.74	1.630e+39	0.00179
12126	triHPacyl.mttmmtmmd	5.319e+43	6.20	6.20	1.623e+39	0.00178
12127	triHPacyl.tttmmtmmd	7.255e+43	6.39	6.39	1.607e+39	0.00177
12128	triHPacyl.pmtmptmmd	2.055e+43	5.64	5.64	1.603e+39	0.00176
12129	triHPacyl.tptmmpmmd	2.919e+44	7.23	7.23	1.591e+39	0.00175
12130	triHPacyl.pmttptppd	1.043e+44	6.61	6.61	1.589e+39	0.00175
12131	triHPacyl.tttmmtmmd	7.836e+43	6.44	6.44	1.582e+39	0.00174
12132	triHPacyl.tpptmmtppd	1.412e+44	6.80	6.80	1.562e+39	0.00172
12133	triHPacyl.tptmmpmmd	1.719e+44	6.92	6.92	1.561e+39	0.00172
12134	triHPacyl.mmpmmtmmd	1.852e+43	5.60	5.60	1.542e+39	0.00169
12135	triHPacyl.tmtmtpppd	3.307e+44	7.32	7.32	1.533e+39	0.00169
12136	triHPacyl.ttppmmtppd	3.138e+43	5.92	5.92	1.529e+39	0.00168
12137	triHPacyl.pmtppmtmmd	7.454e+43	6.44	6.44	1.523e+39	0.00167
12138	triHPacyl.tmttptmmd	4.857e+44	7.56	7.56	1.513e+39	0.00166
12139	triHPacyl.tmtmmpppd	7.385e+43	6.44	6.44	1.509e+39	0.00166
12140	triHPacyl.mppmptmmd	7.611e+42	5.09	5.09	1.500e+39	0.00165
12141	triHPacyl.mttmmtmmd	3.486e+43	6.00	6.00	1.481e+39	0.00163
12142	triHPacyl.tpmtmmpmd	2.015e+44	7.05	7.05	1.470e+39	0.00161
12143	triHPacyl.ptttptmmd	1.070e+44	6.68	6.68	1.462e+39	0.00161

12144	triHPacyl.tmtpptmpmd	3.662e+44	7.41	7.41	1.455e+39	0.0016
12145	triHPacyl.mtmmpmtmmmd	7.480e+43	6.47	6.47	1.447e+39	0.00159
12146	triHPacyl.tppppmtpmmd	2.103e+43	5.72	5.72	1.440e+39	0.00158
12147	triHPacyl.pmmmpmtmmmd	1.176e+44	6.75	6.75	1.433e+39	0.00157
12148	triHPacyl.mmmmpmtpmmd	1.532e+43	5.53	5.53	1.425e+39	0.00157
12149	triHPacyl.tttmmmtpmmd	4.457e+43	6.18	6.18	1.408e+39	0.00155
12150	triHPacyl.pppmpmpmmmd	4.308e+43	6.16	6.16	1.399e+39	0.00154
12151	triHPacyl.mmtppptpppd	2.646e+44	7.25	7.25	1.392e+39	0.00153
12152	triHPacyl.mptmptmmpmd	1.167e+44	6.76	6.76	1.386e+39	0.00152
12153	triHPacyl.tmtpptmpmd	9.505e+43	6.64	6.64	1.385e+39	0.00152
12154	triHPacyl.tptpptmmmd	6.715e+43	6.43	6.43	1.385e+39	0.00152
12155	triHPacyl.mmttptmmpmd	9.016e+43	6.61	6.61	1.384e+39	0.00152
12156	triHPacyl.tmpmtmmmpmd	4.737e+43	6.23	6.23	1.375e+39	0.00151
12157	triHPacyl.tptpptmmmd	9.977e+43	6.67	6.67	1.370e+39	0.00151
12158	triHPacyl.ppmmtmmmpmd	7.951e+43	6.55	6.55	1.356e+39	0.00149
12159	triHPacyl.tmpppmtpmmd	3.743e+43	6.11	6.11	1.329e+39	0.00146
12160	triHPacyl.tmpmmtpmmd	1.858e+43	5.69	5.69	1.325e+39	0.00146
12161	triHPacyl.pttpmmtppd	1.181e+44	6.80	6.80	1.324e+39	0.00145
12162	triHPacyl.tmmmpmtmmmd	1.751e+44	7.03	7.03	1.318e+39	0.00145
12163	triHPacyl.mmmmmmtmpmd	7.729e+43	6.55	6.55	1.312e+39	0.00144
12164	triHPacyl.ppttppmpmd	7.492e+43	6.53	6.53	1.301e+39	0.00143
12165	triHPacyl.pmttmmmmmd	6.885e+43	6.49	6.49	1.298e+39	0.00143
12166	triHPacyl.tppppptpmmd	1.357e+44	6.89	6.89	1.292e+39	0.00142
12167	triHPacyl.tptmmmpppd	8.128e+43	6.59	6.59	1.283e+39	0.00141
12168	triHPacyl.tpttmmmmmd	7.559e+43	6.55	6.55	1.278e+39	0.0014
12169	triHPacyl.pppptpppd	3.915e+44	7.53	7.53	1.278e+39	0.0014
12170	triHPacyl.tttmptmmpmd	3.676e+43	6.12	6.12	1.269e+39	0.00139
12171	triHPacyl.ttttmtmpmd	1.625e+44	7.01	7.01	1.267e+39	0.00139
12172	triHPacyl.pmmmmmmmpmd	1.922e+43	5.74	5.74	1.267e+39	0.00139
12173	triHPacyl.ptttptpmmd	2.935e+44	7.37	7.37	1.263e+39	0.00139
12174	triHPacyl.tmmmtmmmpmd	2.122e+44	7.18	7.18	1.258e+39	0.00138
12175	triHPacyl.ttttmmpppd	1.921e+44	7.12	7.12	1.256e+39	0.00138
12176	triHPacyl.tptpmmpmd	3.667e+43	6.13	6.13	1.256e+39	0.00138
12177	triHPacyl.ppmmtmmmpmd	9.583e+43	6.70	6.70	1.256e+39	0.00138
12178	triHPacyl.tttmmmpmmmd	1.407e+44	6.93	6.93	1.251e+39	0.00137
12179	triHPacyl.ttttppmmpmd	7.856e+43	6.59	6.59	1.239e+39	0.00136
12180	triHPacyl.mmpmptmmmd	1.173e+45	8.21	8.21	1.235e+39	0.00136
12181	triHPacyl.pmpppmtpmmd	2.361e+43	5.88	5.88	1.232e+39	0.00135
12182	triHPacyl.tmpmmtpmmd	2.578e+43	5.93	5.93	1.232e+39	0.00135
12183	triHPacyl.tmmmpmtpmmd	1.602e+44	7.02	7.02	1.225e+39	0.00135
12184	triHPacyl.pmttmttppmd	2.637e+44	7.32	7.32	1.220e+39	0.00134
12185	triHPacyl.pmtpmmtppd	8.755e+43	6.67	6.67	1.207e+39	0.00133
12186	triHPacyl.tmttmtppmd	3.762e+44	7.54	7.54	1.204e+39	0.00132
12187	triHPacyl.mmpmptmmmd	2.726e+43	5.98	5.98	1.196e+39	0.00131
12188	triHPacyl.tmpmmmpmd	1.483e+43	5.62	5.62	1.196e+39	0.00131
12189	triHPacyl.tmpmmmpmd	1.628e+43	5.68	5.68	1.193e+39	0.00131
12190	triHPacyl.pmpmtmmpmd	7.511e+43	6.59	6.59	1.189e+39	0.00131
12191	triHPacyl.pmmmmtpmmd	7.975e+43	6.63	6.63	1.187e+39	0.0013
12192	triHPacyl.tmtpppmmpmd	2.358e+44	7.27	7.27	1.187e+39	0.0013
12193	triHPacyl.tptmmmpmd	1.469e+44	6.99	6.99	1.185e+39	0.0013
12194	triHPacyl.tmpmmmpmd	3.754e+43	6.18	6.18	1.174e+39	0.00129
12195	triHPacyl.mtmmpmtppd	3.012e+45	8.80	8.80	1.172e+39	0.00129
12196	triHPacyl.mmpmpmpppd	6.250e+43	6.49	6.49	1.172e+39	0.00129
12197	triHPacyl.tptmptpmmd	2.384e+44	7.29	7.29	1.166e+39	0.00128
12198	triHPacyl.mtttptpmmd	1.091e+44	6.82	6.82	1.165e+39	0.00128
12199	triHPacyl.mtppmtmmmd	8.142e+43	6.65	6.65	1.163e+39	0.00128
12200	triHPacyl.ttttmtpmmd	1.801e+44	7.12	7.12	1.162e+39	0.00128
12201	triHPacyl.tmmmpmmmpmd	9.951e+43	6.77	6.77	1.158e+39	0.00127
12202	triHPacyl.mtppmtpmmd	5.705e+43	6.44	6.44	1.153e+39	0.00127
12203	triHPacyl.pmttppmpmd	7.297e+43	6.59	6.59	1.152e+39	0.00127
12204	triHPacyl.pmtmptpppd	7.930e+43	6.64	6.64	1.152e+39	0.00127
12205	triHPacyl.pmttmtmpmd	7.521e+43	6.61	6.61	1.144e+39	0.00126
12206	triHPacyl.tppppptppmd	8.095e+43	6.66	6.66	1.138e+39	0.00125
12207	triHPacyl.mttmmmmppd	3.925e+43	6.23	6.23	1.135e+39	0.00125
12208	triHPacyl.tmpmptppmd	6.027e+43	6.49	6.49	1.134e+39	0.00125
12209	triHPacyl.mmpmtppmd	6.715e+43	6.55	6.55	1.133e+39	0.00125
12210	triHPacyl.pmtppmtpmmd	9.689e+43	6.77	6.77	1.133e+39	0.00124
12211	triHPacyl.pmmtppmmmd	2.978e+43	6.07	6.07	1.131e+39	0.00124
12212	triHPacyl.pttpmmmmmd	4.829e+43	6.36	6.36	1.120e+39	0.00123
12213	triHPacyl.pmpppmtmmmd	1.086e+43	5.48	5.48	1.115e+39	0.00122
12214	triHPacyl.mtpmptmpmd	1.865e+43	5.80	5.80	1.113e+39	0.00122
12215	triHPacyl.ttmptmpmd	5.157e+43	6.41	6.41	1.102e+39	0.00121

12216	triHPacyl.tpmmpmtmpmd	3.828e+43	6.24	6.24	1.091e+39	0.0012
12217	triHPacyl.tpmmpptmpd	1.008e+44	6.82	6.82	1.089e+39	0.0012
12218	triHPacyl.ttmtnmtmpd	2.098e+44	7.26	7.26	1.086e+39	0.00119
12219	triHPacyl.mmpmpmtmpmd	5.039e+43	6.41	6.41	1.073e+39	0.00118
12220	triHPacyl.ttmtnmpmd	3.727e+43	6.23	6.23	1.071e+39	0.00118
12221	triHPacyl.mmpmpmpmd	2.792e+43	6.07	6.07	1.056e+39	0.00116
12222	triHPacyl.tpptmtmpmd	3.215e+44	7.53	7.53	1.056e+39	0.00116
12223	triHPacyl.pmtptmpd	2.493e+44	7.38	7.38	1.055e+39	0.00116
12224	triHPacyl.tmpmpmmmd	1.002e+44	6.84	6.84	1.047e+39	0.00115
12225	triHPacyl.tmpmtmpmd	6.839e+43	6.61	6.61	1.047e+39	0.00115
12226	triHPacyl.tptmtmpd	1.488e+44	7.07	7.07	1.046e+39	0.00115
12227	triHPacyl.tmpmtmpd	1.163e+44	6.93	6.93	1.040e+39	0.00114
12228	triHPacyl.pttmtnmmd	8.584e+43	6.75	6.75	1.033e+39	0.00114
12229	triHPacyl.tmpmpmtmpd	1.181e+44	6.94	6.94	1.030e+39	0.00113
12230	triHPacyl.pmpmtmpmd	6.879e+43	6.62	6.62	1.027e+39	0.00113
12231	triHPacyl.tmpmtmpd	8.535e+43	6.76	6.76	1.023e+39	0.00112
12232	triHPacyl.pmpmtmpmd	1.428e+44	7.07	7.07	1.015e+39	0.00112
12233	triHPacyl.tmpmtmpd	6.484e+43	6.60	6.60	1.015e+39	0.00111
12234	triHPacyl.pptmpmpmd	1.056e+44	6.89	6.89	1.007e+39	0.00111
12235	triHPacyl.tmtmpmpmd	3.294e+44	7.58	7.58	9.946e+38	0.00109
12236	triHPacyl.pmpmtmpmd	6.344e+43	6.60	6.60	9.935e+38	0.00109
12237	triHPacyl.tmpmtmpmd	1.158e+44	6.96	6.96	9.906e+38	0.00109
12238	triHPacyl.pmpmtmpmd	1.549e+44	7.13	7.13	9.876e+38	0.00109
12239	triHPacyl.tptmtmpmd	3.675e+44	7.65	7.65	9.872e+38	0.00108
12240	triHPacyl.pmpmtmpmd	8.527e+43	6.78	6.78	9.865e+38	0.00108
12241	triHPacyl.ttmmpmpd	5.680e+44	7.91	7.91	9.848e+38	0.00108
12242	triHPacyl.ttmmpmpd	4.395e+44	7.76	7.76	9.837e+38	0.00108
12243	triHPacyl.tmpmpmpmd	1.023e+44	6.89	6.89	9.811e+38	0.00108
12244	triHPacyl.pmpmpmpmd	2.984e+44	7.53	7.53	9.807e+38	0.00108
12245	triHPacyl.mtptmpmd	9.012e+44	8.19	8.19	9.695e+38	0.00107
12246	triHPacyl.ttmppmpmd	8.002e+43	6.75	6.75	9.681e+38	0.00106
12247	triHPacyl.ttpptmpmd	6.336e+43	6.62	6.62	9.612e+38	0.00106
12248	triHPacyl.pmpptmpmd	1.151e+44	6.97	6.97	9.604e+38	0.00106
12249	triHPacyl.pmpmtmpmd	7.425e+43	6.71	6.71	9.581e+38	0.00105
12250	triHPacyl.tmtmpmpmd	2.059e+44	7.32	7.32	9.559e+38	0.00105
12251	triHPacyl.pmtmtmpmd	4.867e+43	6.47	6.47	9.498e+38	0.00104
12252	triHPacyl.ttmmpmpd	4.100e+43	6.36	6.36	9.485e+38	0.00104
12253	triHPacyl.mtppmtmpmd	4.946e+43	6.48	6.48	9.483e+38	0.00104
12254	triHPacyl.ttmmpmpd	8.272e+43	6.79	6.79	9.421e+38	0.00104
12255	triHPacyl.mtppmtmpd	2.524e+44	7.46	7.46	9.343e+38	0.00103
12256	triHPacyl.ttpptmpd	4.989e+43	6.49	6.49	9.267e+38	0.00102
12257	triHPacyl.pmtmpmpd	3.939e+43	6.35	6.35	9.257e+38	0.00102
12258	triHPacyl.ttpppmpmd	3.298e+43	6.25	6.25	9.254e+38	0.00102
12259	triHPacyl.pmtmtmpmd	6.159e+43	6.62	6.62	9.246e+38	0.00102
12260	triHPacyl.tptpmtppd	2.579e+44	7.48	7.48	9.226e+38	0.00101
12261	triHPacyl.ttpmtppd	1.895e+43	5.92	5.92	9.194e+38	0.00101
12262	triHPacyl.tptpmtppd	1.299e+44	7.07	7.07	9.188e+38	0.00101
12263	triHPacyl.tmpptmpmd	1.673e+43	5.85	5.85	9.173e+38	0.00101
12264	triHPacyl.tmpmtppd	3.010e+43	6.20	6.20	9.147e+38	0.00101
12265	triHPacyl.ptmmmmmmmd	1.634e+44	7.21	7.21	9.074e+38	0.000997
12266	triHPacyl.ppttmppd	5.748e+44	7.97	7.97	9.003e+38	0.000989
12267	triHPacyl.tmmmpmpd	3.260e+43	6.26	6.26	8.902e+38	0.000978
12268	triHPacyl.mtmtmpmd	1.371e+43	5.75	5.75	8.878e+38	0.000976
12269	triHPacyl.tmtptmpmd	1.640e+44	7.23	7.23	8.856e+38	0.000973
12270	triHPacyl.ptmmmtmpd	2.906e+44	7.58	7.58	8.764e+38	0.000963
12271	triHPacyl.tmtmtppd	3.520e+44	7.69	7.69	8.755e+38	0.000962
12272	triHPacyl.pmttppmd	3.120e+44	7.62	7.62	8.726e+38	0.000959
12273	triHPacyl.mtmtppmd	1.900e+44	7.33	7.33	8.720e+38	0.000958
12274	triHPacyl.tpmtmpd	8.208e+43	6.83	6.83	8.704e+38	0.000956
12275	triHPacyl.mmtmpmpmd	5.477e+43	6.59	6.59	8.623e+38	0.000947
12276	triHPacyl.pmtmtppd	1.361e+44	7.14	7.14	8.609e+38	0.000946
12277	triHPacyl.tmpmtmpd	1.222e+44	7.07	7.07	8.580e+38	0.000943
12278	triHPacyl.pmpmtmpd	1.183e+44	7.06	7.06	8.580e+38	0.000943
12279	triHPacyl.pmpmpmpd	6.297e+43	6.68	6.68	8.571e+38	0.000942
12280	triHPacyl.mmtmpmpd	1.855e+44	7.32	7.32	8.565e+38	0.000941
12281	triHPacyl.tppmpmpmd	9.939e+43	6.95	6.95	8.540e+38	0.000938
12282	triHPacyl.pmtmtmpd	7.135e+43	6.76	6.76	8.455e+38	0.000929
12283	triHPacyl.tmtmpmpmd	3.469e+44	7.71	7.71	8.408e+38	0.000924
12284	triHPacyl.tpmmpptppd	1.819e+44	7.33	7.33	8.382e+38	0.000921
12285	triHPacyl.mppmtppd	5.619e+43	6.63	6.63	8.364e+38	0.000919
12286	triHPacyl.tptmtppmd	2.410e+44	7.50	7.50	8.355e+38	0.000918
12287	triHPacyl.mtptmpmd	6.415e+43	6.71	6.71	8.329e+38	0.000915

12288	triHPacyl.mmtpmmtppd	1.656e+44	7.27	7.27	8.320e+38	0.000914
12289	triHPacyl.tmtmtmmmpd	1.877e+44	7.35	7.35	8.306e+38	0.000913
12290	triHPacyl.mptmtmmmpd	5.869e+43	6.66	6.66	8.268e+38	0.000908
12291	triHPacyl.tpttmtmpmd	1.224e+44	7.10	7.10	8.213e+38	0.000902
12292	triHPacyl.ttpmmmmmpd	1.697e+43	5.94	5.94	7.960e+38	0.000875
12293	triHPacyl.tmmmpmtmmd	1.323e+44	7.17	7.17	7.933e+38	0.000872
12294	triHPacyl.ptppmmppmd	9.359e+43	6.97	6.97	7.883e+38	0.000866
12295	triHPacyl.mttptmtmmd	2.802e+43	6.25	6.25	7.845e+38	0.000862
12296	triHPacyl.pppmptppd	4.180e+43	6.49	6.49	7.792e+38	0.000856
12297	triHPacyl.mtppmpmpd	1.797e+43	5.99	5.99	7.769e+38	0.000854
12298	triHPacyl.tmtmtmmmpd	7.902e+43	6.88	6.88	7.695e+38	0.000846
12299	triHPacyl.pmmppmpmpd	7.120e+42	5.45	5.45	7.636e+38	0.000839
12300	triHPacyl.pmpppmmmpd	9.655e+42	5.64	5.64	7.564e+38	0.000831
12301	triHPacyl.tmtpttppd	3.330e+44	7.75	7.75	7.530e+38	0.000827
12302	triHPacyl.mmpppptppd	1.362e+43	5.85	5.85	7.475e+38	0.000821
12303	triHPacyl.tmpmmpmpd	2.409e+43	6.20	6.20	7.284e+38	0.0008
12304	triHPacyl.mmppttmmmd	1.563e+44	7.32	7.32	7.269e+38	0.000799
12305	triHPacyl.tpttmtppd	1.855e+44	7.42	7.42	7.254e+38	0.000797
12306	triHPacyl.tmtmmmpmpd	2.764e+44	7.67	7.67	7.197e+38	0.000791
12307	triHPacyl.tmtpmmtmpd	1.274e+45	8.58	8.58	7.196e+38	0.000791
12308	triHPacyl.pttmttppmd	8.488e+43	6.96	6.96	7.189e+38	0.00079
12309	triHPacyl.mmtmtmmpd	8.424e+43	6.96	6.96	7.184e+38	0.000789
12310	triHPacyl.tmtmptmpd	2.742e+44	7.67	7.67	7.137e+38	0.000784
12311	triHPacyl.tptmpmpmpd	1.242e+44	7.20	7.20	7.121e+38	0.000783
12312	triHPacyl.mtptppmmd	4.488e+43	6.59	6.59	7.106e+38	0.000781
12313	triHPacyl.ttmppmmmpd	7.991e+43	6.93	6.93	7.102e+38	0.00078
12314	triHPacyl.ttpmptppd	3.981e+43	6.52	6.52	7.095e+38	0.00078
12315	triHPacyl.tppmmmpppd	5.933e+43	6.76	6.76	7.059e+38	0.000776
12316	triHPacyl.pppmpppppd	2.499e+44	7.62	7.62	7.035e+38	0.000773
12317	triHPacyl.tmtmttppd	4.031e+44	7.91	7.91	6.995e+38	0.000769
12318	triHPacyl.ppptppmpmd	5.942e+43	6.77	6.77	6.988e+38	0.000768
12319	triHPacyl.tptmtmmmpd	1.922e+44	7.47	7.47	6.981e+38	0.000767
12320	triHPacyl.mtppmpmpmd	2.193e+43	6.17	6.17	6.979e+38	0.000767
12321	triHPacyl.ppttptppd	4.492e+44	7.98	7.98	6.940e+38	0.000763
12322	triHPacyl.mmpmptmpmd	2.067e+43	6.14	6.14	6.939e+38	0.000763
12323	triHPacyl.ttttmmmmmpd	7.833e+43	6.95	6.95	6.817e+38	0.000749
12324	triHPacyl.mptmmpmpmd	3.381e+44	7.82	7.82	6.800e+38	0.000747
12325	triHPacyl.tmtptppmd	2.451e+44	7.63	7.63	6.789e+38	0.000746
12326	triHPacyl.tmtptmmmpd	1.117e+45	8.53	8.53	6.781e+38	0.000745
12327	triHPacyl.mtppmtmpmd	2.600e+43	6.29	6.29	6.779e+38	0.000745
12328	triHPacyl.mtppmpppd	1.758e+44	7.43	7.43	6.771e+38	0.000744
12329	triHPacyl.ptmmpmmmpd	2.419e+44	7.62	7.62	6.752e+38	0.000742
12330	triHPacyl.tttppmmppd	1.661e+44	7.40	7.40	6.738e+38	0.00074
12331	triHPacyl.tttpttmmmd	2.485e+43	6.28	6.28	6.643e+38	0.00073
12332	triHPacyl.ppttmtppmd	4.247e+44	7.97	7.97	6.624e+38	0.000728
12333	triHPacyl.ppmmtmmpd	9.123e+43	7.06	7.06	6.590e+38	0.000724
12334	triHPacyl.tmtmtmmmpd	3.293e+44	7.83	7.83	6.550e+38	0.00072
12335	triHPacyl.tmpptppmd	8.724e+43	7.04	7.04	6.528e+38	0.000717
12336	triHPacyl.tttptppmd	3.077e+44	7.79	7.79	6.509e+38	0.000715
12337	triHPacyl.tppmmtmpd	3.303e+44	7.83	7.83	6.494e+38	0.000714
12338	triHPacyl.tpptmtmmmd	7.976e+44	8.36	8.36	6.476e+38	0.000712
12339	triHPacyl.pmpmtppmd	1.459e+44	7.35	7.35	6.402e+38	0.000703
12340	triHPacyl.pptpmmpd	2.017e+44	7.55	7.55	6.401e+38	0.000703
12341	triHPacyl.tpptmmmpd	8.176e+43	7.01	7.01	6.369e+38	0.0007
12342	triHPacyl.ptpmmmtppd	3.257e+43	6.47	6.47	6.325e+38	0.000695
12343	triHPacyl.mmtpmmtmpd	6.680e+43	6.90	6.90	6.323e+38	0.000695
12344	triHPacyl.tmmpptppd	1.343e+44	7.31	7.31	6.309e+38	0.000693
12345	triHPacyl.pmtpmmpmd	3.374e+43	6.49	6.49	6.303e+38	0.000693
12346	triHPacyl.tppmptppd	6.223e+43	6.86	6.86	6.286e+38	0.000691
12347	triHPacyl.pppmmpmpd	5.333e+43	6.77	6.77	6.266e+38	0.000689
12348	triHPacyl.tmtmptppd	3.196e+44	7.84	7.84	6.260e+38	0.000688
12349	triHPacyl.pmppttppd	2.516e+43	6.33	6.33	6.204e+38	0.000682
12350	triHPacyl.mmtmptmpd	1.161e+44	7.25	7.25	6.065e+38	0.000666
12351	triHPacyl.mtmmpptppd	8.893e+44	8.47	8.47	6.000e+38	0.000659
12352	triHPacyl.pmmtptppmd	3.617e+43	6.56	6.56	5.994e+38	0.000659
12353	triHPacyl.mttptppmd	1.639e+44	7.47	7.47	5.956e+38	0.000654
12354	triHPacyl.tmtmtmpd	2.365e+44	7.69	7.69	5.948e+38	0.000654
12355	triHPacyl.mppmmtppd	2.329e+43	6.30	6.30	5.945e+38	0.000653
12356	triHPacyl.pppppppppd	8.612e+43	7.09	7.09	5.877e+38	0.000646
12357	triHPacyl.pmmmttppd	8.312e+43	7.07	7.07	5.870e+38	0.000645
12358	triHPacyl.mtttppmpd	1.892e+44	7.56	7.56	5.868e+38	0.000645
12359	triHPacyl.mmtppptmmd	6.291e+43	6.91	6.91	5.865e+38	0.000644

12360	triHPacyl.ptppppptppd	3.191e+43	6.50	6.50	5.863e+38	0.000644
12361	triHPacyl.pmtppppmmd	2.340e+43	6.33	6.33	5.744e+38	0.000631
12362	triHPacyl.mmpmmpmmd	9.896e+43	7.19	7.19	5.735e+38	0.00063
12363	triHPacyl.mmpptptmpmd	4.793e+43	6.76	6.76	5.727e+38	0.000629
12364	triHPacyl.tppppptmpd	1.138e+44	7.28	7.28	5.701e+38	0.000626
12365	triHPacyl.pmpmtmpmmd	1.218e+44	7.32	7.32	5.692e+38	0.000625
12366	triHPacyl.ptttmtppd	1.583e+44	7.48	7.48	5.666e+38	0.000623
12367	triHPacyl.pmtppptmmd	2.967e+43	6.48	6.48	5.647e+38	0.000621
12368	triHPacyl.ttpmmtmmd	3.787e+43	6.63	6.63	5.633e+38	0.000619
12369	triHPacyl.mmtppmtpd	3.435e+44	7.94	7.94	5.621e+38	0.000618
12370	triHPacyl.tptppmtpd	5.993e+43	6.90	6.90	5.616e+38	0.000617
12371	triHPacyl.mpmtpmtpd	1.371e+44	7.40	7.40	5.614e+38	0.000617
12372	triHPacyl.tttmtmmd	3.026e+44	7.87	7.87	5.612e+38	0.000617
12373	triHPacyl.mtmmpmmd	2.210e+44	7.69	7.69	5.541e+38	0.000609
12374	triHPacyl.tttmtmmd	2.140e+44	7.67	7.67	5.536e+38	0.000608
12375	triHPacyl.pptppmtpd	2.524e+44	7.77	7.77	5.525e+38	0.000607
12376	triHPacyl.tpmmmmpmmd	4.804e+43	6.78	6.78	5.495e+38	0.000604
12377	triHPacyl.mtmmpmmd	6.324e+43	6.95	6.95	5.486e+38	0.000603
12378	triHPacyl.ttmmpmtpd	1.888e+44	7.60	7.60	5.475e+38	0.000602
12379	triHPacyl.ttpmmpmmd	6.619e+43	6.98	6.98	5.448e+38	0.000599
12380	triHPacyl.pmttptmmd	1.686e+44	7.54	7.54	5.448e+38	0.000599
12381	triHPacyl.ttpmmpmmd	3.833e+43	6.66	6.66	5.414e+38	0.000595
12382	triHPacyl.mpmmpmtpd	2.373e+44	7.75	7.75	5.408e+38	0.000594
12383	triHPacyl.mtmmpmmd	1.584e+44	7.51	7.51	5.333e+38	0.000586
12384	triHPacyl.tpppmtpmd	2.302e+44	7.74	7.74	5.314e+38	0.000584
12385	triHPacyl.pmttptmmd	1.082e+44	7.29	7.29	5.295e+38	0.000582
12386	triHPacyl.pptmmpmmd	7.433e+43	7.07	7.07	5.238e+38	0.000576
12387	triHPacyl.tptptmmd	9.419e+43	7.22	7.22	5.170e+38	0.000568
12388	triHPacyl.pptmtpmmd	4.363e+44	8.14	8.14	5.159e+38	0.000567
12389	triHPacyl.pptmmpmmd	8.375e+43	7.15	7.15	5.157e+38	0.000567
12390	triHPacyl.ttmmpmmpd	3.271e+44	7.97	7.97	5.127e+38	0.000563
12391	triHPacyl.tmpmtpmmd	9.147e+43	7.21	7.21	5.109e+38	0.000561
12392	triHPacyl.mmtmmtmmd	5.089e+43	6.86	6.86	5.102e+38	0.000561
12393	triHPacyl.tmtmtpmmd	3.068e+44	7.93	7.93	5.090e+38	0.000559
12394	triHPacyl.tptmtpmmd	7.859e+43	7.12	7.12	5.071e+38	0.000557
12395	triHPacyl.mttppmtpd	1.164e+44	7.36	7.36	5.070e+38	0.000557
12396	triHPacyl.tptmmpmmd	9.993e+43	7.28	7.28	4.983e+38	0.000547
12397	triHPacyl.pptptmmd	2.781e+44	7.89	7.89	4.956e+38	0.000545
12398	triHPacyl.tpmmpmmd	7.440e+43	7.11	7.11	4.947e+38	0.000544
12399	triHPacyl.tptptmmd	1.427e+44	7.50	7.50	4.939e+38	0.000543
12400	triHPacyl.tttmtpmmd	4.925e+44	8.24	8.24	4.921e+38	0.000541
12401	triHPacyl.tmpmtpmmd	1.231e+44	7.41	7.41	4.906e+38	0.000539
12402	triHPacyl.pptmmpmmd	1.535e+44	7.54	7.54	4.894e+38	0.000538
12403	triHPacyl.mmttptmmd	1.800e+44	7.64	7.64	4.883e+38	0.000537
12404	triHPacyl.tmpmmpmmd	4.225e+43	6.78	6.78	4.860e+38	0.000534
12405	triHPacyl.ptmmpmmd	2.911e+43	6.56	6.56	4.816e+38	0.000529
12406	triHPacyl.tttptmmd	4.345e+43	6.81	6.81	4.766e+38	0.000524
12407	triHPacyl.tmpmmpmmd	5.641e+43	6.96	6.96	4.761e+38	0.000523
12408	triHPacyl.pptptmmd	7.350e+43	7.12	7.12	4.761e+38	0.000523
12409	triHPacyl.mtppmtpmmd	1.343e+43	6.11	6.11	4.758e+38	0.000523
12410	triHPacyl.ttptmmpmmd	6.860e+43	7.08	7.08	4.737e+38	0.000521
12411	triHPacyl.tmmpmtpmmd	1.510e+44	7.56	7.56	4.734e+38	0.00052
12412	triHPacyl.mmtmtpmmd	7.528e+43	7.14	7.14	4.727e+38	0.000519
12413	triHPacyl.tmmpmmpmmd	8.956e+43	7.25	7.25	4.710e+38	0.000518
12414	triHPacyl.tmpmmpmmd	1.070e+44	7.36	7.36	4.682e+38	0.000514
12415	triHPacyl.tmmtmtpmmd	4.775e+43	6.88	6.88	4.648e+38	0.000511
12416	triHPacyl.tmmtmtpmmd	3.782e+44	8.12	8.12	4.621e+38	0.000508
12417	triHPacyl.ppmmpmmd	1.306e+44	7.48	7.48	4.609e+38	0.000506
12418	triHPacyl.pttptmmd	7.348e+43	7.14	7.14	4.607e+38	0.000506
12419	triHPacyl.tppppmtpd	2.532e+44	7.88	7.88	4.594e+38	0.000505
12420	triHPacyl.pmpmmpmmd	5.437e+43	6.97	6.97	4.577e+38	0.000503
12421	triHPacyl.ptttmmpmmd	1.061e+44	7.38	7.38	4.498e+38	0.000494
12422	triHPacyl.tmpmtpmmd	9.453e+43	7.31	7.31	4.482e+38	0.000492
12423	triHPacyl.ppmmpmmd	1.100e+44	7.40	7.40	4.468e+38	0.000491
12424	triHPacyl.pmpmtpmmd	1.661e+44	7.65	7.65	4.457e+38	0.00049
12425	triHPacyl.ttpmmpmmd	2.008e+43	6.39	6.39	4.426e+38	0.000486
12426	triHPacyl.tmmpmmpmmd	8.259e+43	7.24	7.24	4.396e+38	0.000483
12427	triHPacyl.mmtmtpmmd	3.367e+43	6.71	6.71	4.392e+38	0.000483
12428	triHPacyl.tptptmmd	3.647e+44	8.13	8.13	4.375e+38	0.000481
12429	triHPacyl.mtppmmpmmd	2.173e+43	6.45	6.45	4.348e+38	0.000478
12430	triHPacyl.tttmtmmd	6.412e+43	7.10	7.10	4.328e+38	0.000476
12431	triHPacyl.pmpmmpmmd	5.660e+43	7.03	7.03	4.308e+38	0.000473

12432	triHPacyl.mmppmmpmnd	1.110e+43	6.06	6.06	4.268e+38	0.000469
12433	triHPacyl.tppmmmtpmnd	7.026e+43	7.16	7.16	4.259e+38	0.000468
12434	triHPacyl.mmmppptmnd	1.051e+44	7.40	7.40	4.249e+38	0.000467
12435	triHPacyl.tmtptmmpd	1.656e+44	7.68	7.68	4.226e+38	0.000464
12436	triHPacyl.mttptmmpd	5.950e+43	7.07	7.07	4.224e+38	0.000464
12437	triHPacyl.ptppmmtppd	1.529e+44	7.63	7.63	4.222e+38	0.000464
12438	triHPacyl.mmtptmmpd	2.757e+44	7.98	7.98	4.203e+38	0.000462
12439	triHPacyl.tmmmpmtpmd	1.483e+45	8.99	8.99	4.192e+38	0.000461
12440	triHPacyl.ttttptmmpd	1.081e+44	7.43	7.43	4.185e+38	0.00046
12441	triHPacyl.tpmtmmpmd	1.829e+44	7.74	7.74	4.182e+38	0.00046
12442	triHPacyl.mppmmpmmpd	1.940e+43	6.41	6.41	4.168e+38	0.000458
12443	triHPacyl.tmtppppppd	3.482e+44	8.13	8.13	4.148e+38	0.000456
12444	triHPacyl.pmttmmpmd	9.326e+43	7.35	7.35	4.134e+38	0.000454
12445	triHPacyl.pttptmmpd	2.877e+43	6.65	6.65	4.109e+38	0.000452
12446	triHPacyl.ptmptmmpd	1.505e+44	7.64	7.64	4.108e+38	0.000451
12447	triHPacyl.ptmmmpmmpd	3.043e+44	8.06	8.06	4.062e+38	0.000446
12448	triHPacyl.tttptmmpd	1.543e+44	7.66	7.66	4.043e+38	0.000444
12449	triHPacyl.tmtmmtmmpd	2.943e+44	8.05	8.05	4.038e+38	0.000444
12450	triHPacyl.tmmptmmpd	1.303e+44	7.56	7.56	4.029e+38	0.000443
12451	triHPacyl.pmpmptmmpd	2.167e+43	6.49	6.49	4.026e+38	0.000442
12452	triHPacyl.tmtmmtmmpd	3.343e+44	8.13	8.13	4.012e+38	0.000441
12453	triHPacyl.mtppppppmd	2.231e+43	6.52	6.52	3.990e+38	0.000438
12454	triHPacyl.tppmmtmmpd	1.529e+44	7.66	7.66	3.989e+38	0.000438
12455	triHPacyl.tmtptmmpd	1.319e+44	7.58	7.58	3.972e+38	0.000436
12456	triHPacyl.pmtmmmpmd	6.743e+43	7.18	7.18	3.972e+38	0.000436
12457	triHPacyl.pmtptmmpd	5.551e+43	7.07	7.07	3.950e+38	0.000434
12458	triHPacyl.pmtmmpmmpd	8.673e+44	8.71	8.71	3.950e+38	0.000434
12459	triHPacyl.tppppppmd	1.008e+44	7.42	7.42	3.935e+38	0.000432
12460	triHPacyl.tptptmmpd	1.004e+44	7.42	7.42	3.918e+38	0.00043
12461	triHPacyl.pptptmmpd	3.918e+44	8.24	8.24	3.902e+38	0.000429
12462	triHPacyl.tmtmmpmmpd	3.002e+43	6.71	6.71	3.901e+38	0.000429
12463	triHPacyl.tmtmmtmmpd	3.147e+44	8.11	8.11	3.883e+38	0.000427
12464	triHPacyl.tmmmpmmpmd	1.362e+44	7.61	7.61	3.866e+38	0.000425
12465	triHPacyl.mtppptppmd	3.811e+43	6.86	6.86	3.853e+38	0.000423
12466	triHPacyl.mptmmtmmpd	2.900e+43	6.70	6.70	3.836e+38	0.000421
12467	triHPacyl.tmtmmtmmpd	4.645e+44	8.35	8.35	3.831e+38	0.000421
12468	triHPacyl.ptmmmtmmpd	3.304e+44	8.15	8.15	3.829e+38	0.000421
12469	triHPacyl.pmttppmmpd	2.001e+44	7.85	7.85	3.828e+38	0.000421
12470	triHPacyl.tttptmmpd	3.151e+44	8.12	8.12	3.819e+38	0.00042
12471	triHPacyl.tmtmmtmmpd	2.234e+44	7.92	7.92	3.784e+38	0.000416
12472	triHPacyl.tttptmmpd	9.412e+43	7.41	7.41	3.778e+38	0.000415
12473	triHPacyl.pptptmmpd	7.932e+44	8.68	8.68	3.754e+38	0.000413
12474	triHPacyl.mptmmtmmpd	3.395e+43	6.80	6.80	3.753e+38	0.000412
12475	triHPacyl.mtptptmmpd	2.178e+43	6.54	6.54	3.723e+38	0.000409
12476	triHPacyl.mmmppmmpmd	2.423e+43	6.61	6.61	3.720e+38	0.000409
12477	triHPacyl.tmtmmtmmpd	2.163e+44	7.91	7.91	3.718e+38	0.000409
12478	triHPacyl.ptpmtmmpd	4.265e+43	6.95	6.95	3.718e+38	0.000409
12479	triHPacyl.pmttppmmpd	1.489e+44	7.69	7.69	3.708e+38	0.000407
12480	triHPacyl.mmmmpmmpmd	5.148e+43	7.06	7.06	3.705e+38	0.000407
12481	triHPacyl.pmtmmtmmpd	2.177e+44	7.92	7.92	3.693e+38	0.000406
12482	triHPacyl.tmmmpmtpmd	1.220e+44	7.58	7.58	3.672e+38	0.000404
12483	triHPacyl.tmpmtpmtpd	1.066e+44	7.50	7.50	3.672e+38	0.000404
12484	triHPacyl.mppmmmpmmpd	2.743e+43	6.69	6.69	3.668e+38	0.000403
12485	triHPacyl.ptppptppmd	4.392e+43	6.97	6.97	3.665e+38	0.000403
12486	triHPacyl.tttmtpmmpd	9.702e+43	7.45	7.45	3.650e+38	0.000401
12487	triHPacyl.mtmmpmtpmd	8.026e+43	7.33	7.33	3.642e+38	0.0004
12488	triHPacyl.tmpmptmmpd	2.716e+44	8.06	8.06	3.633e+38	0.000399
12489	triHPacyl.tmtmmtmmpd	1.741e+44	7.80	7.80	3.631e+38	0.000399
12490	triHPacyl.mppmptmmpd	5.403e+43	7.10	7.10	3.626e+38	0.000398
12491	triHPacyl.pptmmtmmpd	9.545e+43	7.44	7.44	3.623e+38	0.000398
12492	triHPacyl.mtttptmmpd	1.129e+44	7.54	7.54	3.615e+38	0.000397
12493	triHPacyl.mttppmmpmd	7.085e+43	7.27	7.27	3.578e+38	0.000393
12494	triHPacyl.tmtmmpmmpd	2.428e+44	8.01	8.01	3.558e+38	0.000391
12495	triHPacyl.tmmptmmpd	8.254e+43	7.37	7.37	3.527e+38	0.000388
12496	triHPacyl.pmtppmmpd	8.672e+43	7.40	7.40	3.515e+38	0.000386
12497	triHPacyl.mmmmpmtpmd	5.477e+43	7.13	7.13	3.503e+38	0.000385
12498	triHPacyl.pptptmmpd	1.102e+45	8.92	8.92	3.493e+38	0.000384
12499	triHPacyl.mtttppmmpd	3.175e+44	8.19	8.19	3.446e+38	0.000379
12500	triHPacyl.ttptmtpmmpd	2.550e+44	8.06	8.06	3.426e+38	0.000376
12501	triHPacyl.tppmtmmpd	5.200e+44	8.49	8.49	3.415e+38	0.000375
12502	triHPacyl.mtpmmpmmpd	3.969e+43	6.96	6.96	3.377e+38	0.000371
12503	triHPacyl.tmtmmtmmpd	3.450e+44	8.25	8.25	3.373e+38	0.000371

12504	triHPacyl.mmttptmpmd	1.829e+44	7.87	7.87	3.364e+38	0.00037
12505	triHPacyl.mtppmtmmmd	1.179e+43	6.24	6.24	3.363e+38	0.00037
12506	triHPacyl.ttptpmmpmd	7.338e+44	8.71	8.71	3.336e+38	0.000367
12507	triHPacyl.tpptmmtpmd	1.561e+44	7.78	7.78	3.328e+38	0.000366
12508	triHPacyl.ttmtmtppd	3.797e+44	8.32	8.32	3.323e+38	0.000365
12509	triHPacyl.tmppmmppd	1.834e+43	6.51	6.51	3.322e+38	0.000365
12510	triHPacyl.pmtpmmpmd	2.553e+43	6.71	6.71	3.320e+38	0.000365
12511	triHPacyl.ttptmpmpmd	1.084e+44	7.57	7.57	3.317e+38	0.000364
12512	triHPacyl.mppmpmtmpd	1.084e+44	7.57	7.57	3.313e+38	0.000364
12513	triHPacyl.pppmpmmmd	2.848e+43	6.78	6.78	3.283e+38	0.000361
12514	triHPacyl.tmtptppd	1.922e+44	7.92	7.92	3.281e+38	0.000361
12515	triHPacyl.ttptmpppd	4.837e+43	7.10	7.10	3.275e+38	0.00036
12516	triHPacyl.mmtppmtmpmd	1.118e+44	7.60	7.60	3.268e+38	0.000359
12517	triHPacyl.ptmmtpmmmd	2.332e+44	8.04	8.04	3.264e+38	0.000359
12518	triHPacyl.ttmmmpmmmd	6.385e+44	8.64	8.64	3.221e+38	0.000354
12519	triHPacyl.mtmmptmmmd	8.413e+44	8.81	8.81	3.215e+38	0.000353
12520	triHPacyl.mmmmtmtpd	1.539e+44	7.80	7.80	3.212e+38	0.000353
12521	triHPacyl.pppmtmpd	2.634e+43	6.75	6.75	3.198e+38	0.000351
12522	triHPacyl.tttppmpmd	1.038e+45	8.94	8.94	3.191e+38	0.000351
12523	triHPacyl.ttptptmpmd	3.909e+44	8.37	8.37	3.147e+38	0.000346
12524	triHPacyl.pttmtmpmd	1.580e+44	7.83	7.83	3.143e+38	0.000345
12525	triHPacyl.tppmtmpmd	1.518e+44	7.80	7.80	3.137e+38	0.000345
12526	triHPacyl.ptmppmpmd	4.551e+43	7.09	7.09	3.121e+38	0.000343
12527	triHPacyl.ppmtptmmmd	7.552e+44	8.77	8.77	3.097e+38	0.00034
12528	triHPacyl.ttmptmpd	2.165e+44	8.02	8.02	3.096e+38	0.00034
12529	triHPacyl.mmmmtmpmd	1.953e+43	6.59	6.59	3.082e+38	0.000339
12530	triHPacyl.tttmtmpmd	7.610e+43	7.40	7.40	3.069e+38	0.000337
12531	triHPacyl.mmtmtmpmd	1.392e+44	7.78	7.78	3.015e+38	0.000331
12532	triHPacyl.mtmmmpmmmd	8.222e+43	7.46	7.46	3.006e+38	0.00033
12533	triHPacyl.ppttpmpd	4.952e+44	8.53	8.53	3.001e+38	0.00033
12534	triHPacyl.pmpmtmpd	1.481e+43	6.44	6.44	2.998e+38	0.000329
12535	triHPacyl.mttmtmpd	9.137e+43	7.53	7.53	2.990e+38	0.000329
12536	triHPacyl.tptmtmpmd	1.512e+44	7.84	7.84	2.943e+38	0.000323
12537	triHPacyl.ttppmtmmmd	1.135e+43	6.30	6.30	2.935e+38	0.000323
12538	triHPacyl.mmmmtmpmd	9.172e+43	7.55	7.55	2.921e+38	0.000321
12539	triHPacyl.tmppptmpmd	1.991e+43	6.64	6.64	2.919e+38	0.000321
12540	triHPacyl.mtppmmmmmd	2.236e+43	6.71	6.71	2.914e+38	0.00032
12541	triHPacyl.ttmptmpd	8.818e+43	7.52	7.52	2.909e+38	0.00032
12542	triHPacyl.tpmtppppd	2.881e+44	8.23	8.23	2.901e+38	0.000319
12543	triHPacyl.mttmmmmmd	5.207e+43	7.21	7.21	2.891e+38	0.000318
12544	triHPacyl.tmtptppmd	6.058e+44	8.68	8.68	2.890e+38	0.000318
12545	triHPacyl.ptmpmtmpmd	3.566e+44	8.36	8.36	2.879e+38	0.000316
12546	triHPacyl.pppmpmpmd	5.955e+43	7.30	7.30	2.874e+38	0.000316
12547	triHPacyl.pttppptppd	5.519e+43	7.25	7.25	2.872e+38	0.000316
12548	triHPacyl.tmmptmpd	1.011e+44	7.61	7.61	2.871e+38	0.000315
12549	triHPacyl.pmpmtmmmd	2.163e+44	8.07	8.07	2.860e+38	0.000314
12550	triHPacyl.mptpmtmmmd	5.028e+43	7.20	7.20	2.850e+38	0.000313
12551	triHPacyl.mtppppmpmd	2.105e+43	6.69	6.69	2.808e+38	0.000309
12552	triHPacyl.mtmtmpmmmd	5.109e+44	8.59	8.59	2.804e+38	0.000308
12553	triHPacyl.pppppmpd	5.072e+43	7.22	7.22	2.796e+38	0.000307
12554	triHPacyl.ptmtmpmpd	1.548e+44	7.88	7.88	2.795e+38	0.000307
12555	triHPacyl.ptmmpptmpd	3.428e+44	8.36	8.36	2.788e+38	0.000306
12556	triHPacyl.mmtpmmpmd	1.163e+44	7.72	7.72	2.783e+38	0.000306
12557	triHPacyl.pmmtptmpmd	1.657e+44	7.93	7.93	2.772e+38	0.000305
12558	triHPacyl.tpttmppmd	2.548e+44	8.19	8.19	2.752e+38	0.000302
12559	triHPacyl.mttptmpmd	4.014e+43	7.09	7.09	2.749e+38	0.000302
12560	triHPacyl.pmmmmmpmd	1.541e+43	6.52	6.52	2.744e+38	0.000302
12561	triHPacyl.ppmtpmpd	1.568e+44	7.90	7.90	2.744e+38	0.000301
12562	triHPacyl.tmmmtppd	2.230e+44	8.11	8.11	2.734e+38	0.0003
12563	triHPacyl.pppmpmpd	2.408e+44	8.16	8.16	2.732e+38	0.0003
12564	triHPacyl.mttptmpmd	1.229e+44	7.76	7.76	2.721e+38	0.000299
12565	triHPacyl.mtmtmpd	9.604e+43	7.62	7.62	2.711e+38	0.000298
12566	triHPacyl.pmtmpppd	5.366e+43	7.27	7.27	2.710e+38	0.000298
12567	triHPacyl.pttpmppd	2.484e+44	8.19	8.19	2.664e+38	0.000293
12568	triHPacyl.ptttmtmpmd	3.338e+44	8.38	8.38	2.639e+38	0.00029
12569	triHPacyl.mppptmpd	7.566e+43	7.49	7.49	2.633e+38	0.000289
12570	triHPacyl.ptptmpmpmd	4.835e+43	7.23	7.23	2.616e+38	0.000287
12571	triHPacyl.mmpmmmpmd	2.575e+43	6.86	6.86	2.590e+38	0.000285
12572	triHPacyl.ttmtmtmpmd	3.946e+44	8.49	8.49	2.569e+38	0.000282
12573	triHPacyl.tppppmpmd	2.571e+43	6.86	6.86	2.568e+38	0.000282
12574	triHPacyl.ppmmtmmmpd	1.128e+44	7.75	7.75	2.548e+38	0.00028
12575	triHPacyl.mmtmmmpmd	1.348e+44	7.86	7.86	2.545e+38	0.00028

12576	triHPacyl.mmptpmtppmd	1.188e+44	7.78	7.78	2.544e+38	0.000279
12577	triHPacyl.tpppmtpppd	3.332e+44	8.40	8.40	2.529e+38	0.000278
12578	triHPacyl.pmppttppd	4.199e+43	7.17	7.17	2.529e+38	0.000278
12579	triHPacyl.tpptmmtmmd	3.371e+44	8.41	8.41	2.526e+38	0.000278
12580	triHPacyl.tmpmpmmpd	1.958e+43	6.71	6.71	2.518e+38	0.000277
12581	triHPacyl.ttptmtpppd	1.615e+44	7.97	7.97	2.509e+38	0.000276
12582	triHPacyl.tpmmtppmd	8.899e+43	7.63	7.63	2.470e+38	0.000271
12583	triHPacyl.tmmtmmpd	1.940e+44	8.10	8.10	2.457e+38	0.00027
12584	triHPacyl.tmmpmmpd	1.214e+44	7.82	7.82	2.455e+38	0.00027
12585	triHPacyl.tmttptppd	5.458e+44	8.71	8.71	2.452e+38	0.000269
12586	triHPacyl.tttppmmpd	2.750e+44	8.31	8.31	2.441e+38	0.000268
12587	triHPacyl.pmpmtmmd	1.760e+43	6.67	6.67	2.431e+38	0.000267
12588	triHPacyl.tpptmtppd	2.678e+44	8.30	8.30	2.426e+38	0.000267
12589	triHPacyl.mpttptppd	7.002e+43	7.50	7.50	2.414e+38	0.000265
12590	triHPacyl.pmttmmpd	8.535e+43	7.62	7.62	2.403e+38	0.000264
12591	triHPacyl.tmmpmmtppd	8.357e+43	7.61	7.61	2.398e+38	0.000263
12592	triHPacyl.tpttmmpd	9.702e+43	7.70	7.70	2.391e+38	0.000263
12593	triHPacyl.pttppmmpd	2.244e+43	6.84	6.84	2.334e+38	0.000256
12594	triHPacyl.mptmtpmd	1.237e+44	7.86	7.86	2.324e+38	0.000255
12595	triHPacyl.tmttptppd	5.602e+44	8.76	8.76	2.319e+38	0.000255
12596	triHPacyl.mppmmpd	3.249e+43	7.07	7.07	2.313e+38	0.000254
12597	triHPacyl.tpptmtppd	8.481e+43	7.64	7.64	2.311e+38	0.000254
12598	triHPacyl.tmpmtppd	1.167e+44	7.84	7.84	2.282e+38	0.000251
12599	triHPacyl.mmpmmpd	2.195e+43	6.84	6.84	2.270e+38	0.000249
12600	triHPacyl.mtpmtpmd	1.341e+44	7.92	7.92	2.262e+38	0.000249
12601	triHPacyl.tppmtpmd	3.860e+43	7.18	7.18	2.255e+38	0.000248
12602	triHPacyl.tptmtppd	6.280e+44	8.85	8.85	2.254e+38	0.000248
12603	triHPacyl.ttmtptppd	2.150e+44	8.21	8.21	2.254e+38	0.000248
12604	triHPacyl.tttppmmpd	8.639e+43	7.67	7.67	2.244e+38	0.000247
12605	triHPacyl.ttttmmpd	1.217e+44	7.87	7.87	2.240e+38	0.000246
12606	triHPacyl.mppmtpmd	9.822e+43	7.75	7.75	2.239e+38	0.000246
12607	triHPacyl.ptmttppd	3.314e+44	8.47	8.47	2.235e+38	0.000246
12608	triHPacyl.pppmmpd	3.710e+44	8.54	8.54	2.235e+38	0.000246
12609	triHPacyl.pmttptppd	3.139e+44	8.44	8.44	2.225e+38	0.000244
12610	triHPacyl.pttmtpmd	6.910e+43	7.54	7.54	2.217e+38	0.000244
12611	triHPacyl.mmttppmd	1.099e+44	7.82	7.82	2.210e+38	0.000243
12612	triHPacyl.tttmtppd	9.010e+43	7.70	7.70	2.209e+38	0.000243
12613	triHPacyl.mttppmmpd	8.933e+43	7.70	7.70	2.204e+38	0.000242
12614	triHPacyl.pptmmpd	1.364e+44	7.95	7.95	2.194e+38	0.000241
12615	triHPacyl.pmtmtpd	1.118e+44	7.84	7.84	2.188e+38	0.00024
12616	triHPacyl.tmmptmmpd	1.307e+44	7.93	7.93	2.186e+38	0.00024
12617	triHPacyl.tptmtpmd	1.002e+45	9.14	9.14	2.185e+38	0.00024
12618	triHPacyl.ptppmtpd	3.999e+43	7.22	7.22	2.184e+38	0.00024
12619	triHPacyl.tttmtpppd	1.038e+44	7.79	7.79	2.181e+38	0.00024
12620	triHPacyl.mttppmmpd	5.068e+43	7.37	7.37	2.156e+38	0.000237
12621	triHPacyl.mmtppmmpd	3.185e+44	8.47	8.47	2.151e+38	0.000236
12622	triHPacyl.mptpmpd	2.059e+44	8.21	8.21	2.147e+38	0.000236
12623	triHPacyl.pmpmtmmpd	8.711e+43	7.70	7.70	2.145e+38	0.000236
12624	triHPacyl.mppppmmpd	1.956e+44	8.18	8.18	2.143e+38	0.000235
12625	triHPacyl.ptttmmpd	8.469e+43	7.68	7.68	2.141e+38	0.000235
12626	triHPacyl.ttptmtpmd	1.233e+44	7.91	7.91	2.136e+38	0.000235
12627	triHPacyl.mppmmpd	6.761e+43	7.55	7.55	2.135e+38	0.000235
12628	triHPacyl.mppmmpmmpd	1.016e+44	7.79	7.79	2.132e+38	0.000234
12629	triHPacyl.ptmptppd	5.125e+44	8.76	8.76	2.128e+38	0.000234
12630	triHPacyl.mmtmtpmd	4.191e+43	7.27	7.27	2.127e+38	0.000234
12631	triHPacyl.tptmtppd	6.066e+44	8.87	8.87	2.098e+38	0.000231
12632	triHPacyl.tpmtmtpd	9.034e+43	7.74	7.74	2.079e+38	0.000228
12633	triHPacyl.tpptmmpd	7.641e+43	7.64	7.64	2.077e+38	0.000228
12634	triHPacyl.pptmtpmd	1.448e+44	8.02	8.02	2.077e+38	0.000228
12635	triHPacyl.mmmmtmmpd	2.602e+44	8.37	8.37	2.068e+38	0.000227
12636	triHPacyl.pptmpppd	2.500e+44	8.35	8.35	2.065e+38	0.000227
12637	triHPacyl.pmttppmpd	1.057e+44	7.84	7.84	2.060e+38	0.000226
12638	triHPacyl.pppmmpd	9.457e+43	7.77	7.77	2.058e+38	0.000226
12639	triHPacyl.mtppmtpmd	1.135e+44	7.88	7.88	2.047e+38	0.000225
12640	triHPacyl.mmmtpmmpd	3.422e+43	7.17	7.17	2.044e+38	0.000225
12641	triHPacyl.mmpmmpd	5.175e+43	7.42	7.42	2.030e+38	0.000223
12642	triHPacyl.tmtmtpmd	2.723e+45	9.78	9.78	2.029e+38	0.000223
12643	triHPacyl.pmtmmpd	9.205e+43	7.77	7.77	2.027e+38	0.000223
12644	triHPacyl.tmtmtpmd	7.631e+44	9.03	9.03	2.020e+38	0.000222
12645	triHPacyl.pmmmtmmpd	3.226e+43	7.14	7.14	2.020e+38	0.000222
12646	triHPacyl.pttppmmpd	3.080e+44	8.49	8.49	2.018e+38	0.000222
12647	triHPacyl.pmmmmmpd	1.056e+44	7.85	7.85	2.016e+38	0.000222

12648	triHPacyl.mtmppptmmd	2.122e+43	6.90	6.90	2.007e+38	0.000221
12649	triHPacyl.tptmptpppd	1.125e+44	7.89	7.89	2.002e+38	0.00022
12650	triHPacyl.ppptpmtmmd	4.875e+44	8.77	8.77	1.994e+38	0.000219
12651	triHPacyl.tpttpptmmd	4.355e+44	8.70	8.70	1.990e+38	0.000219
12652	triHPacyl.tmmpmtpppd	6.680e+43	7.59	7.59	1.983e+38	0.000218
12653	triHPacyl.tpmtmppmd	1.067e+44	7.87	7.87	1.968e+38	0.000216
12654	triHPacyl.pmpptmtpd	1.517e+43	6.71	6.71	1.964e+38	0.000216
12655	triHPacyl.ppmtmmmmmd	1.128e+44	7.91	7.91	1.960e+38	0.000215
12656	triHPacyl.mttmptpppd	5.367e+43	7.47	7.47	1.943e+38	0.000213
12657	triHPacyl.mtmmttmmd	2.593e+44	8.41	8.41	1.939e+38	0.000213
12658	triHPacyl.ttptmtpmd	2.821e+44	8.46	8.46	1.933e+38	0.000212
12659	triHPacyl.mtttptpppd	1.401e+44	8.05	8.05	1.924e+38	0.000211
12660	triHPacyl.tpmptmtpd	5.888e+43	7.53	7.53	1.913e+38	0.00021
12661	triHPacyl.pmtmmpmmd	3.570e+43	7.24	7.24	1.910e+38	0.00021
12662	triHPacyl.mmpptpmd	1.109e+43	6.54	6.54	1.910e+38	0.00021
12663	triHPacyl.tmtmmpmmd	1.133e+44	7.93	7.93	1.884e+38	0.000207
12664	triHPacyl.mmmmtmtpmd	5.524e+43	7.51	7.51	1.881e+38	0.000207
12665	triHPacyl.pmtpttmmd	4.749e+43	7.42	7.42	1.868e+38	0.000205
12666	triHPacyl.pttpmtmmd	6.751e+43	7.63	7.63	1.859e+38	0.000204
12667	triHPacyl.mmmtpmmpmd	3.895e+43	7.31	7.31	1.852e+38	0.000203
12668	triHPacyl.mmtmppmmd	2.047e+44	8.30	8.30	1.851e+38	0.000203
12669	triHPacyl.tpmtmtpmd	2.940e+44	8.51	8.51	1.847e+38	0.000203
12670	triHPacyl.tttmtpmd	7.462e+43	7.70	7.70	1.844e+38	0.000203
12671	triHPacyl.pmtmmpmmd	2.319e+44	8.37	8.37	1.844e+38	0.000203
12672	triHPacyl.tmtppmmpd	4.890e+44	8.82	8.82	1.837e+38	0.000202
12673	triHPacyl.tmpmptppd	1.271e+44	8.02	8.02	1.826e+38	0.000201
12674	triHPacyl.tttmmpppd	8.457e+43	7.78	7.78	1.826e+38	0.000201
12675	triHPacyl.mttptmtpmd	2.133e+44	8.33	8.33	1.823e+38	0.0002
12676	triHPacyl.mtpmmpmmd	3.467e+43	7.25	7.25	1.817e+38	0.0002
12677	triHPacyl.mppmtpmmd	7.890e+43	7.74	7.74	1.814e+38	0.000199
12678	triHPacyl.mtttptppd	1.777e+44	8.23	8.23	1.808e+38	0.000199
12679	triHPacyl.pmtmtpmmd	2.639e+44	8.46	8.46	1.801e+38	0.000198
12680	triHPacyl.ttmpttmmd	2.013e+44	8.30	8.30	1.796e+38	0.000197
12681	triHPacyl.tptmmpmmd	9.404e+43	7.85	7.85	1.787e+38	0.000196
12682	triHPacyl.ptmtmtpmd	4.374e+44	8.77	8.77	1.787e+38	0.000196
12683	triHPacyl.ptpmpmmpd	1.369e+43	6.71	6.71	1.780e+38	0.000196
12684	triHPacyl.ppptmppmd	1.095e+44	7.95	7.95	1.779e+38	0.000195
12685	triHPacyl.ptppmmpmd	7.210e+43	7.70	7.70	1.779e+38	0.000195
12686	triHPacyl.mmpmmpmmd	2.478e+43	7.06	7.06	1.776e+38	0.000195
12687	triHPacyl.ptppptmmd	2.879e+43	7.15	7.15	1.769e+38	0.000194
12688	triHPacyl.pmtptpmd	1.153e+44	7.98	7.98	1.769e+38	0.000194
12689	triHPacyl.ttmtpmmpmd	1.486e+44	8.13	8.13	1.764e+38	0.000194
12690	triHPacyl.mtmptmtpd	4.730e+43	7.45	7.45	1.763e+38	0.000194
12691	triHPacyl.ptmmpmtpd	5.211e+44	8.88	8.88	1.757e+38	0.000193
12692	triHPacyl.tmmpmmpmmd	1.053e+44	7.94	7.94	1.732e+38	0.00019
12693	triHPacyl.ptmptpmd	5.226e+43	7.52	7.52	1.729e+38	0.00019
12694	triHPacyl.tmptmtpmd	1.001e+44	7.91	7.91	1.728e+38	0.00019
12695	triHPacyl.pmtmmpmmd	1.995e+43	6.95	6.95	1.722e+38	0.000189
12696	triHPacyl.pmtmtpmmd	1.131e+44	7.99	7.99	1.709e+38	0.000188
12697	triHPacyl.pttmtpmmd	7.210e+43	7.72	7.72	1.707e+38	0.000188
12698	triHPacyl.mttmmpmmd	6.801e+43	7.69	7.69	1.705e+38	0.000187
12699	triHPacyl.ptpmtmtpd	3.559e+43	7.30	7.30	1.701e+38	0.000187
12700	triHPacyl.ppmptmmd	1.610e+44	8.21	8.21	1.692e+38	0.000186
12701	triHPacyl.pptmmpmmd	3.563e+44	8.68	8.68	1.682e+38	0.000185
12702	triHPacyl.pmtmmpmmd	1.452e+44	8.15	8.15	1.681e+38	0.000185
12703	triHPacyl.ptppmtmmd	3.128e+43	7.24	7.24	1.663e+38	0.000183
12704	triHPacyl.pmtmtpmmd	1.475e+44	8.18	8.18	1.632e+38	0.000179
12705	triHPacyl.mmpmtpmmd	4.236e+43	7.43	7.43	1.629e+38	0.000179
12706	triHPacyl.ptttmtpppd	2.077e+44	8.38	8.38	1.629e+38	0.000179
12707	triHPacyl.mttptmtpd	1.587e+43	6.85	6.85	1.621e+38	0.000178
12708	triHPacyl.tmtppmmpd	4.714e+44	8.88	8.88	1.611e+38	0.000177
12709	triHPacyl.mmmmpmtpd	7.415e+43	7.78	7.78	1.604e+38	0.000176
12710	triHPacyl.mmmppptppd	4.838e+43	7.52	7.52	1.599e+38	0.000176
12711	triHPacyl.mptpmtmmd	2.313e+43	7.09	7.09	1.592e+38	0.000175
12712	triHPacyl.pptmppmmd	3.245e+44	8.67	8.67	1.579e+38	0.000173
12713	triHPacyl.tptmmpmmd	8.893e+43	7.89	7.89	1.578e+38	0.000173
12714	triHPacyl.pmtmtpmmd	3.207e+43	7.29	7.29	1.566e+38	0.000172
12715	triHPacyl.mptmmpmmd	7.581e+43	7.81	7.81	1.562e+38	0.000172
12716	triHPacyl.tttppmmpd	8.009e+43	7.84	7.84	1.559e+38	0.000171
12717	triHPacyl.pmtptpmd	2.550e+44	8.53	8.53	1.557e+38	0.000171
12718	triHPacyl.tpmtmtpd	2.223e+44	8.45	8.45	1.556e+38	0.000171
12719	triHPacyl.ttppmtpmd	1.544e+44	8.23	8.23	1.553e+38	0.000171

12720	triHPacyl.mmmmmmtppd	1.266e+44	8.12	8.12	1.548e+38	0.00017
12721	triHPacyl.mtmmppmmmpd	8.947e+43	7.91	7.91	1.540e+38	0.000169
12722	triHPacyl.tptppptpmd	1.102e+44	8.04	8.04	1.538e+38	0.000169
12723	triHPacyl.tpptmtpppd	5.941e+44	9.04	9.04	1.534e+38	0.000169
12724	triHPacyl.tpmmmtmmd	4.220e+44	8.84	8.84	1.530e+38	0.000168
12725	triHPacyl.mptpmttppd	5.314e+43	7.61	7.61	1.527e+38	0.000168
12726	triHPacyl.tppmmmtmmd	3.067e+44	8.65	8.65	1.523e+38	0.000167
12727	triHPacyl.tptmpptpmd	1.387e+44	8.18	8.18	1.516e+38	0.000167
12728	triHPacyl.tptpmtppmd	6.604e+44	9.12	9.12	1.504e+38	0.000165
12729	triHPacyl.tttmptmmd	5.178e+43	7.60	7.60	1.501e+38	0.000165
12730	triHPacyl.pptmpptmmd	1.164e+44	8.09	8.09	1.498e+38	0.000165
12731	triHPacyl.mtmtmmpmpd	2.498e+44	8.54	8.54	1.491e+38	0.000164
12732	triHPacyl.pmttmmmmpd	7.168e+43	7.80	7.80	1.487e+38	0.000163
12733	triHPacyl.tmmtpmtppd	2.188e+44	8.47	8.47	1.484e+38	0.000163
12734	triHPacyl.ptppmtppd	4.106e+43	7.47	7.47	1.480e+38	0.000163
12735	triHPacyl.pmtmtppmd	5.710e+44	9.04	9.04	1.478e+38	0.000162
12736	triHPacyl.mmmmpmtmmd	2.059e+44	8.44	8.44	1.474e+38	0.000162
12737	triHPacyl.ptmmmtmmd	3.257e+44	8.71	8.71	1.461e+38	0.00016
12738	triHPacyl.pppmpptpmd	1.199e+44	8.12	8.12	1.460e+38	0.00016
12739	triHPacyl.ppppmtppd	3.940e+43	7.46	7.46	1.458e+38	0.00016
12740	triHPacyl.ttpppmmmd	2.016e+43	7.06	7.06	1.451e+38	0.000159
12741	triHPacyl.tmpmttppd	1.662e+44	8.32	8.32	1.447e+38	0.000159
12742	triHPacyl.pmtmmtpppd	5.117e+43	7.62	7.62	1.441e+38	0.000158
12743	triHPacyl.mppmptmmd	2.092e+44	8.46	8.46	1.440e+38	0.000158
12744	triHPacyl.tpptmtmmd	1.420e+44	8.23	8.23	1.435e+38	0.000158
12745	triHPacyl.mtppmmmpd	7.020e+43	7.81	7.81	1.429e+38	0.000157
12746	triHPacyl.mmmmpmtppd	8.843e+43	7.95	7.95	1.422e+38	0.000156
12747	triHPacyl.ttttptpmd	3.955e+44	8.85	8.85	1.421e+38	0.000156
12748	triHPacyl.mtttptpmd	9.792e+43	8.01	8.01	1.421e+38	0.000156
12749	triHPacyl.tttmtmmpd	8.133e+43	7.90	7.90	1.421e+38	0.000156
12750	triHPacyl.mmtppmtmmd	8.320e+43	7.92	7.92	1.416e+38	0.000156
12751	triHPacyl.tmpppptpmd	1.235e+44	8.16	8.16	1.415e+38	0.000156
12752	triHPacyl.tmpppptmmd	9.223e+43	7.98	7.98	1.406e+38	0.000155
12753	triHPacyl.pttpmtppmd	2.102e+44	8.48	8.48	1.395e+38	0.000153
12754	triHPacyl.pppmtppmpd	2.531e+44	8.59	8.59	1.395e+38	0.000153
12755	triHPacyl.tppppmtmmd	9.527e+43	8.01	8.01	1.394e+38	0.000153
12756	triHPacyl.mtmtmmmpmd	8.924e+43	7.97	7.97	1.386e+38	0.000152
12757	triHPacyl.ttttptpmd	1.448e+44	8.26	8.26	1.384e+38	0.000152
12758	triHPacyl.mtmtptmmd	1.411e+43	6.88	6.88	1.375e+38	0.000151
12759	triHPacyl.pmmtpptppd	1.912e+44	8.44	8.44	1.357e+38	0.000149
12760	triHPacyl.mmpptmmpd	2.859e+44	8.68	8.68	1.353e+38	0.000149
12761	triHPacyl.pmpmtmmmpd	6.878e+43	7.84	7.84	1.338e+38	0.000147
12762	triHPacyl.pmmtpppmpd	1.291e+43	6.84	6.84	1.338e+38	0.000147
12763	triHPacyl.tpttmmpppd	3.521e+44	8.82	8.82	1.331e+38	0.000146
12764	triHPacyl.mmtmmtmmd	1.450e+44	8.29	8.29	1.321e+38	0.000145
12765	triHPacyl.mtttppmmmpd	2.375e+44	8.59	8.59	1.319e+38	0.000145
12766	triHPacyl.tmpppmtppd	3.718e+43	7.48	7.48	1.317e+38	0.000145
12767	triHPacyl.mppmptmmd	2.097e+44	8.52	8.52	1.308e+38	0.000144
12768	triHPacyl.mmmmpmtppd	6.606e+43	7.83	7.83	1.307e+38	0.000144
12769	triHPacyl.pmmppptpmd	7.392e+43	7.90	7.90	1.291e+38	0.000142
12770	triHPacyl.ttpppmmmpd	4.052e+43	7.55	7.55	1.282e+38	0.000141
12771	triHPacyl.tmmtpppmpd	3.375e+43	7.44	7.44	1.273e+38	0.00014
12772	triHPacyl.tmpmtmmmmmd	6.469e+43	7.84	7.84	1.268e+38	0.000139
12773	triHPacyl.ptptmpmpmd	5.307e+43	7.72	7.72	1.256e+38	0.000138
12774	triHPacyl.mtptpmmmpd	5.739e+43	7.77	7.77	1.255e+38	0.000138
12775	triHPacyl.mttmmtmmpd	6.121e+43	7.81	7.81	1.254e+38	0.000138
12776	triHPacyl.tptpmmppmd	9.776e+43	8.09	8.09	1.245e+38	0.000137
12777	triHPacyl.mmtppppppd	5.181e+44	9.09	9.09	1.242e+38	0.000136
12778	triHPacyl.mmtmptpppd	1.141e+44	8.19	8.19	1.240e+38	0.000136
12779	triHPacyl.mppmtppmpd	1.985e+44	8.52	8.52	1.227e+38	0.000135
12780	triHPacyl.pmttmmtppd	1.505e+44	8.36	8.36	1.220e+38	0.000134
12781	triHPacyl.mmtmttppd	1.421e+44	8.33	8.33	1.217e+38	0.000134
12782	triHPacyl.ttpppmtppd	9.061e+43	8.06	8.06	1.215e+38	0.000134
12783	triHPacyl.mttmmtmmd	5.347e+43	7.75	7.75	1.211e+38	0.000133
12784	triHPacyl.pppmmtpppd	6.025e+43	7.82	7.82	1.207e+38	0.000133
12785	triHPacyl.mtpppmtppd	2.196e+43	7.22	7.22	1.206e+38	0.000133
12786	triHPacyl.mmtmptmmd	1.705e+44	8.44	8.44	1.203e+38	0.000132
12787	triHPacyl.tptpmtpppd	4.030e+44	8.96	8.96	1.203e+38	0.000132
12788	triHPacyl.mmtppmmppd	4.033e+44	8.96	8.96	1.200e+38	0.000132
12789	triHPacyl.ttpmmmtppd	8.994e+43	8.06	8.06	1.200e+38	0.000132
12790	triHPacyl.ttmtppmpd	2.477e+44	8.67	8.67	1.196e+38	0.000131
12791	triHPacyl.ttptpmpmd	2.171e+44	8.59	8.59	1.192e+38	0.000131

12792	triHPacyl.mttptmtmmd	7.442e+43	7.96	7.96	1.191e+38	0.000131
12793	triHPacyl.tmptmtpmmd	5.205e+43	7.74	7.74	1.189e+38	0.000131
12794	triHPacyl.tptppmpmmd	2.469e+44	8.67	8.67	1.188e+38	0.000131
12795	triHPacyl.tppnmmtmmd	1.996e+44	8.55	8.55	1.179e+38	0.00013
12796	triHPacyl.tpmpptmmd	7.321e+43	7.95	7.95	1.177e+38	0.000129
12797	triHPacyl.pmpmtmmd	2.707e+44	8.74	8.74	1.166e+38	0.000128
12798	triHPacyl.ptmtmtmmd	2.675e+43	7.36	7.36	1.165e+38	0.000128
12799	triHPacyl.mmmmmpppd	1.018e+44	8.16	8.16	1.152e+38	0.000127
12800	triHPacyl.ttmtmtpppd	8.691e+44	9.44	9.44	1.152e+38	0.000127
12801	triHPacyl.mmppptmmpd	3.436e+43	7.52	7.52	1.150e+38	0.000126
12802	triHPacyl.pmttmtpmmd	1.354e+44	8.34	8.34	1.145e+38	0.000126
12803	triHPacyl.mmmmmmtmmd	2.248e+44	8.64	8.64	1.143e+38	0.000126
12804	triHPacyl.mmtmmpmmd	6.141e+43	7.87	7.87	1.140e+38	0.000125
12805	triHPacyl.pmmppmtmmd	1.281e+44	8.31	8.31	1.139e+38	0.000125
12806	triHPacyl.tptmpmmpd	4.695e+43	7.71	7.71	1.137e+38	0.000125
12807	triHPacyl.pmttmtpppd	6.456e+44	9.27	9.27	1.136e+38	0.000125
12808	triHPacyl.tpttptmmpd	1.274e+44	8.31	8.31	1.134e+38	0.000125
12809	triHPacyl.mmtppmtmmd	7.921e+43	8.02	8.02	1.132e+38	0.000124
12810	triHPacyl.pmpmmtmmpd	3.724e+43	7.58	7.58	1.127e+38	0.000124
12811	triHPacyl.mptpmmtmmd	4.972e+43	7.75	7.75	1.122e+38	0.000123
12812	triHPacyl.tttppmtmmd	6.599e+43	7.92	7.92	1.121e+38	0.000123
12813	triHPacyl.ttmppmmpmd	4.611e+43	7.71	7.71	1.110e+38	0.000122
12814	triHPacyl.mtppmmmpd	2.184e+43	7.27	7.27	1.103e+38	0.000121
12815	triHPacyl.mtmmpmtppd	8.151e+44	9.43	9.43	1.102e+38	0.000121
12816	triHPacyl.mppmmpmmpd	2.229e+43	7.28	7.28	1.100e+38	0.000121
12817	triHPacyl.ptttmmmmmd	8.003e+43	8.05	8.05	1.092e+38	0.00012
12818	triHPacyl.pmttptmmpd	1.636e+44	8.48	8.48	1.088e+38	0.00012
12819	triHPacyl.mmptpmmpmd	1.070e+44	8.23	8.23	1.083e+38	0.000119
12820	triHPacyl.ttptmmmmmd	7.627e+43	8.04	8.04	1.067e+38	0.000117
12821	triHPacyl.pmmtptmmpd	2.752e+44	8.80	8.80	1.063e+38	0.000117
12822	triHPacyl.tmtmpmtmmd	2.853e+44	8.83	8.83	1.059e+38	0.000116
12823	triHPacyl.tmmpmmpmd	4.303e+43	7.70	7.70	1.058e+38	0.000116
12824	triHPacyl.mmtptmmpd	8.256e+43	8.09	8.09	1.056e+38	0.000116
12825	triHPacyl.mmmmpmmpd	3.016e+43	7.49	7.49	1.051e+38	0.000116
12826	triHPacyl.tmtmptmmpd	5.392e+44	9.21	9.21	1.049e+38	0.000115
12827	triHPacyl.mptmmtmmd	7.041e+43	8.00	8.00	1.046e+38	0.000115
12828	triHPacyl.mmttptppmd	3.395e+44	8.94	8.94	1.045e+38	0.000115
12829	triHPacyl.mmtpmmmmd	6.785e+43	7.98	7.98	1.036e+38	0.000114
12830	triHPacyl.pmpmptmmpd	3.233e+43	7.55	7.55	1.024e+38	0.000113
12831	triHPacyl.tmptmmpmd	4.245e+43	7.71	7.71	1.021e+38	0.000112
12832	triHPacyl.mmptptppmd	1.388e+44	8.42	8.42	1.021e+38	0.000112
12833	triHPacyl.mmmmtmmpd	2.620e+44	8.81	8.81	1.008e+38	0.000111
12834	triHPacyl.ttppptmmd	4.808e+43	7.80	7.80	1.004e+38	0.00011
12835	triHPacyl.mtttpppppd	2.608e+44	8.81	8.81	1.004e+38	0.00011
12836	triHPacyl.tmtppmmpmd	7.722e+43	8.08	8.08	9.965e+37	0.00011
12837	triHPacyl.mmppmtmmpd	2.593e+43	7.44	7.44	9.893e+37	0.000109
12838	triHPacyl.pmtppptmmpd	1.815e+44	8.60	8.60	9.787e+37	0.000108
12839	triHPacyl.mtpppmtppd	3.325e+43	7.60	7.60	9.718e+37	0.000107
12840	triHPacyl.mppppmmpmd	1.639e+44	8.55	8.55	9.645e+37	0.000106
12841	triHPacyl.mmttmmtmmd	2.495e+44	8.81	8.81	9.581e+37	0.000105
12842	triHPacyl.ppmtptppd	1.362e+45	9.83	9.83	9.468e+37	0.000104
12843	triHPacyl.tpttmtppmd	5.328e+44	9.27	9.27	9.451e+37	0.000104
12844	triHPacyl.mppmmpmmd	1.958e+43	7.30	7.30	9.451e+37	0.000104
12845	triHPacyl.tppmptmmd	7.374e+43	8.09	8.09	9.450e+37	0.000104
12846	triHPacyl.tppmmpmmpd	6.460e+43	8.01	8.01	9.411e+37	0.000103
12847	triHPacyl.mppppmtmmd	2.300e+44	8.77	8.77	9.393e+37	0.000103
12848	triHPacyl.mmttptpppd	3.684e+44	9.05	9.05	9.386e+37	0.000103
12849	triHPacyl.tmttptmmpd	6.653e+44	9.40	9.40	9.369e+37	0.000103
12850	triHPacyl.tptppmmmd	7.641e+43	8.12	8.12	9.322e+37	0.000102
12851	triHPacyl.pmmppmmmpd	1.940e+43	7.30	7.30	9.305e+37	0.000102
12852	triHPacyl.mptmmmpmd	1.424e+44	8.49	8.49	9.289e+37	0.000102
12853	triHPacyl.mmttmtmmpd	2.869e+44	8.91	8.91	9.284e+37	0.000102
12854	triHPacyl.tmttppmmpd	7.794e+44	9.51	9.51	9.269e+37	0.000102
12855	triHPacyl.ttppmtmmpd	3.849e+43	7.72	7.72	9.179e+37	0.000101
12856	triHPacyl.tppppmtmmd	4.090e+44	9.13	9.13	9.146e+37	0.0001
12857	triHPacyl.ptmtmtpppd	2.305e+44	8.79	8.79	9.098e+37	0.0001
12858	triHPacyl.ttptmmtppd	1.468e+44	8.52	8.52	9.089e+37	9.99e-05
12859	triHPacyl.tmtppmtmmd	1.461e+44	8.52	8.52	9.028e+37	9.92e-05
12860	triHPacyl.pmttppmmpd	9.476e+43	8.27	8.27	8.886e+37	9.76e-05
12861	triHPacyl.tppptmmpd	4.721e+44	9.24	9.24	8.824e+37	9.7e-05
12862	triHPacyl.pttmtppmd	1.911e+44	8.70	8.70	8.806e+37	9.68e-05
12863	triHPacyl.ptmttpppd	5.654e+44	9.35	9.35	8.732e+37	9.59e-05

12864	triHPacyl.tpttptmmnd	1.899e+44	8.70	8.70	8.716e+37	9.58e-05
12865	triHPacyl.mmtptpmmnd	3.541e+43	7.70	7.70	8.702e+37	9.56e-05
12866	triHPacyl.ppmpmpmpd	4.848e+43	7.89	7.89	8.671e+37	9.53e-05
12867	triHPacyl.tmttptmpd	2.680e+44	8.91	8.91	8.642e+37	9.5e-05
12868	triHPacyl.pmpptmpmd	2.958e+43	7.60	7.60	8.542e+37	9.39e-05
12869	triHPacyl.mttptmtpmd	6.770e+43	8.10	8.10	8.483e+37	9.32e-05
12870	triHPacyl.pmpmtttmpd	2.544e+44	8.89	8.89	8.458e+37	9.29e-05
12871	triHPacyl.tmtmpmpmpd	3.540e+44	9.09	9.09	8.442e+37	9.28e-05
12872	triHPacyl.tmttptmpd	9.331e+44	9.67	9.67	8.438e+37	9.27e-05
12873	triHPacyl.pmpmmpmpmd	7.420e+43	8.16	8.16	8.436e+37	9.27e-05
12874	triHPacyl.mtppmtmnd	4.344e+43	7.84	7.84	8.419e+37	9.25e-05
12875	triHPacyl.pmppttmmnd	9.035e+43	8.28	8.28	8.399e+37	9.23e-05
12876	triHPacyl.tmpmtmpmnd	4.325e+43	7.84	7.84	8.360e+37	9.19e-05
12877	triHPacyl.tttmpmmmpd	4.190e+43	7.83	7.83	8.325e+37	9.15e-05
12878	triHPacyl.ptppmmmpd	1.511e+43	7.22	7.22	8.305e+37	9.13e-05
12879	triHPacyl.tpmtmtpmpd	2.196e+44	8.82	8.82	8.305e+37	9.13e-05
12880	triHPacyl.mpppmmtppd	1.293e+44	8.50	8.50	8.268e+37	9.08e-05
12881	triHPacyl.mpppmmpmnd	1.290e+44	8.50	8.50	8.267e+37	9.08e-05
12882	triHPacyl.pmpmtmpmd	9.611e+43	8.33	8.33	8.250e+37	9.07e-05
12883	triHPacyl.mmpmmtmpd	1.412e+43	7.18	7.18	8.239e+37	9.05e-05
12884	triHPacyl.tmttmtmpd	3.293e+44	9.06	9.06	8.212e+37	9.02e-05
12885	triHPacyl.mtptppmpmd	1.201e+44	8.47	8.47	8.143e+37	8.95e-05
12886	triHPacyl.mmpptmpmpd	3.428e+43	7.72	7.72	8.142e+37	8.95e-05
12887	triHPacyl.pmpptmpmpd	6.178e+43	8.07	8.07	8.131e+37	8.93e-05
12888	triHPacyl.mmttptmpd	1.797e+44	8.72	8.72	8.038e+37	8.83e-05
12889	triHPacyl.ttpmmpmnd	2.112e+43	7.44	7.44	8.035e+37	8.83e-05
12890	triHPacyl.tpmmmmtmnd	2.244e+44	8.85	8.85	8.018e+37	8.81e-05
12891	triHPacyl.pmpmtpppd	1.329e+44	8.54	8.54	8.010e+37	8.8e-05
12892	triHPacyl.pmpmpptmpd	2.774e+44	8.98	8.98	7.987e+37	8.78e-05
12893	triHPacyl.pmpptmpmnd	3.041e+43	7.66	7.66	7.931e+37	8.71e-05
12894	triHPacyl.tpttptmpd	3.350e+44	9.10	9.10	7.901e+37	8.68e-05
12895	triHPacyl.mptpmtpmd	1.027e+44	8.39	8.39	7.889e+37	8.67e-05
12896	triHPacyl.tmppttppd	4.420e+44	9.27	9.27	7.865e+37	8.64e-05
12897	triHPacyl.mtpmpmtppd	6.527e+43	8.13	8.13	7.846e+37	8.62e-05
12898	triHPacyl.tmpmmtmpd	5.307e+43	8.01	8.01	7.812e+37	8.58e-05
12899	triHPacyl.tmpppmpmpd	1.406e+44	8.59	8.59	7.783e+37	8.55e-05
12900	triHPacyl.pmtptmtpd	1.268e+44	8.53	8.53	7.712e+37	8.47e-05
12901	triHPacyl.tptmpmmnd	1.784e+44	8.74	8.74	7.711e+37	8.47e-05
12902	triHPacyl.pmtptmtpd	3.118e+43	7.70	7.70	7.710e+37	8.47e-05
12903	triHPacyl.tmpmtmpmpd	2.708e+43	7.62	7.62	7.630e+37	8.38e-05
12904	triHPacyl.pttmtmtpd	2.168e+44	8.86	8.86	7.628e+37	8.38e-05
12905	triHPacyl.ttptppmnd	1.027e+44	8.41	8.41	7.625e+37	8.38e-05
12906	triHPacyl.tmpmmpmnd	5.502e+43	8.04	8.04	7.616e+37	8.37e-05
12907	triHPacyl.mptmmtmpd	8.418e+43	8.30	8.30	7.582e+37	8.33e-05
12908	triHPacyl.tpmtptmpmd	1.120e+44	8.47	8.47	7.544e+37	8.29e-05
12909	triHPacyl.pmtpttppd	4.673e+44	9.33	9.33	7.447e+37	8.18e-05
12910	triHPacyl.mttmmtppd	1.860e+44	8.78	8.78	7.443e+37	8.18e-05
12911	triHPacyl.mtttptppd	1.188e+44	8.52	8.52	7.412e+37	8.14e-05
12912	triHPacyl.ptmmmpmnd	3.082e+44	9.09	9.09	7.407e+37	8.14e-05
12913	triHPacyl.ttpmptmnd	1.358e+43	7.23	7.23	7.366e+37	8.09e-05
12914	triHPacyl.pmtmtpmnd	5.319e+43	8.05	8.05	7.328e+37	8.05e-05
12915	triHPacyl.ttppptppd	2.027e+43	7.47	7.47	7.278e+37	8e-05
12916	triHPacyl.mtmmpmmpd	4.504e+43	7.95	7.95	7.272e+37	7.99e-05
12917	triHPacyl.mtttmtmpmd	1.102e+44	8.49	8.49	7.235e+37	7.95e-05
12918	triHPacyl.mptpmmmnd	7.447e+43	8.25	8.25	7.230e+37	7.94e-05
12919	triHPacyl.ptppmtmnd	2.439e+43	7.59	7.59	7.202e+37	7.91e-05
12920	triHPacyl.mptpmtppd	1.275e+44	8.58	8.58	7.165e+37	7.87e-05
12921	triHPacyl.ttpmmmmnd	2.363e+43	7.58	7.58	7.134e+37	7.84e-05
12922	triHPacyl.ttmtmtpmd	7.053e+44	9.60	9.60	7.120e+37	7.82e-05
12923	triHPacyl.tmmpmtmpd	7.285e+43	8.25	8.25	7.111e+37	7.81e-05
12924	triHPacyl.tmtpttppd	5.062e+44	9.41	9.41	7.072e+37	7.77e-05
12925	triHPacyl.ttmtmpmnd	3.785e+44	9.24	9.24	7.044e+37	7.74e-05
12926	triHPacyl.mtpmptppd	3.239e+43	7.77	7.77	7.025e+37	7.72e-05
12927	triHPacyl.mmpmmtmnd	2.219e+43	7.55	7.55	7.008e+37	7.7e-05
12928	triHPacyl.pmmmmpppd	4.119e+43	7.92	7.92	6.995e+37	7.69e-05
12929	triHPacyl.ttmtmmpmd	3.720e+44	9.23	9.23	6.991e+37	7.68e-05
12930	triHPacyl.pttpmtmpd	1.584e+44	8.73	8.73	6.942e+37	7.63e-05
12931	triHPacyl.ptmtmtpmnd	2.265e+45	10.32	10.32	6.923e+37	7.61e-05
12932	triHPacyl.tppttppd	2.891e+44	9.09	9.09	6.908e+37	7.59e-05
12933	triHPacyl.pmpptmpmd	5.580e+44	9.48	9.48	6.887e+37	7.57e-05
12934	triHPacyl.tpttptmnd	7.723e+44	9.69	9.69	6.778e+37	7.45e-05
12935	triHPacyl.tptmmpmnd	5.923e+43	8.16	8.16	6.756e+37	7.42e-05

12936	triHPacyl.tpttpttppd	5.091e+44	9.44	9.44	6.725e+37	7.39e-05
12937	triHPacyl.mtttmmpppd	1.059e+44	8.51	8.51	6.696e+37	7.36e-05
12938	triHPacyl.mtppmppppd	3.359e+43	7.83	7.83	6.687e+37	7.35e-05
12939	triHPacyl.pmpppmmpmd	1.515e+43	7.35	7.35	6.649e+37	7.31e-05
12940	triHPacyl.tmppnmppmd	2.859e+43	7.73	7.73	6.634e+37	7.29e-05
12941	triHPacyl.tpmmpptmmd	1.060e+44	8.52	8.52	6.584e+37	7.23e-05
12942	triHPacyl.tmtmtttmpd	4.978e+44	9.44	9.44	6.571e+37	7.22e-05
12943	triHPacyl.mmtptttmpd	2.000e+44	8.90	8.90	6.571e+37	7.22e-05
12944	triHPacyl.tttppmmmd	3.809e+43	7.92	7.92	6.515e+37	7.16e-05
12945	triHPacyl.pmmtpmpppd	1.531e+44	8.75	8.75	6.481e+37	7.12e-05
12946	triHPacyl.ttptmtttmpd	2.666e+44	9.08	9.08	6.438e+37	7.07e-05
12947	triHPacyl.mmtptttmpd	2.994e+44	9.15	9.15	6.437e+37	7.07e-05
12948	triHPacyl.mttmpmpppd	6.344e+43	8.23	8.23	6.410e+37	7.04e-05
12949	triHPacyl.pmmtpmtmpd	2.421e+44	9.03	9.03	6.389e+37	7.02e-05
12950	triHPacyl.tmpmmtpmmd	2.761e+43	7.74	7.74	6.364e+37	6.99e-05
12951	triHPacyl.mmmptmmpmd	9.015e+43	8.45	8.45	6.343e+37	6.97e-05
12952	triHPacyl.tttpttppd	1.148e+44	8.59	8.59	6.328e+37	6.95e-05
12953	triHPacyl.ptpmmpppd	3.596e+43	7.90	7.90	6.323e+37	6.95e-05
12954	triHPacyl.pmpptmmpmd	5.177e+43	8.12	8.12	6.306e+37	6.93e-05
12955	triHPacyl.ttptmmpppd	4.504e+43	8.04	8.04	6.298e+37	6.92e-05
12956	triHPacyl.mmtppmmpmd	2.017e+44	8.93	8.93	6.266e+37	6.89e-05
12957	triHPacyl.tpmppptmpd	1.049e+44	8.55	8.55	6.214e+37	6.83e-05
12958	triHPacyl.pttptmmpmd	8.319e+43	8.41	8.41	6.204e+37	6.82e-05
12959	triHPacyl.ttmppptmmd	4.558e+43	8.06	8.06	6.174e+37	6.78e-05
12960	triHPacyl.mmmptmmpmd	8.657e+43	8.44	8.44	6.115e+37	6.72e-05
12961	triHPacyl.ppmtpmtmmd	3.108e+44	9.21	9.21	6.030e+37	6.63e-05
12962	triHPacyl.tpttptmpmd	4.667e+44	9.46	9.46	5.982e+37	6.57e-05
12963	triHPacyl.tmpmptmpmd	3.905e+43	7.98	7.98	5.979e+37	6.57e-05
12964	triHPacyl.pmpptppmmd	3.995e+43	8.00	8.00	5.961e+37	6.55e-05
12965	triHPacyl.pttmtptmmd	1.793e+44	8.89	8.89	5.960e+37	6.55e-05
12966	triHPacyl.mptppptmmd	5.610e+43	8.20	8.20	5.951e+37	6.54e-05
12967	triHPacyl.pmmtpmmpmd	3.167e+43	7.87	7.87	5.904e+37	6.49e-05
12968	triHPacyl.pmtmppmmd	7.741e+43	8.40	8.40	5.888e+37	6.47e-05
12969	triHPacyl.tptmptmpd	2.149e+44	9.01	9.01	5.871e+37	6.45e-05
12970	triHPacyl.mmmmmmtmpd	3.822e+44	9.36	9.36	5.845e+37	6.42e-05
12971	triHPacyl.pmpptmmpd	2.417e+43	7.71	7.71	5.821e+37	6.4e-05
12972	triHPacyl.pttppppmmd	1.341e+44	8.73	8.73	5.818e+37	6.39e-05
12973	triHPacyl.tttptttmpd	4.076e+44	9.40	9.40	5.802e+37	6.38e-05
12974	triHPacyl.pmmmtmpmpd	9.839e+43	8.55	8.55	5.793e+37	6.37e-05
12975	triHPacyl.tpmmpptppd	1.922e+44	8.95	8.95	5.778e+37	6.35e-05
12976	triHPacyl.mtmtmmpmmd	3.558e+44	9.32	9.32	5.745e+37	6.31e-05
12977	triHPacyl.mmpptmmpmd	3.466e+43	7.94	7.94	5.719e+37	6.28e-05
12978	triHPacyl.tptmpppppd	1.127e+44	8.64	8.64	5.682e+37	6.24e-05
12979	triHPacyl.mtttptmpmd	1.391e+44	8.77	8.77	5.680e+37	6.24e-05
12980	triHPacyl.ttmtmmpmmd	3.145e+43	7.89	7.89	5.616e+37	6.17e-05
12981	triHPacyl.pttptttmpd	1.139e+44	8.66	8.66	5.607e+37	6.16e-05
12982	triHPacyl.ppmtpmtmpd	6.754e+44	9.72	9.72	5.602e+37	6.16e-05
12983	triHPacyl.tpmppppppd	4.929e+43	8.16	8.16	5.572e+37	6.12e-05
12984	triHPacyl.tpmppmmpmd	4.830e+43	8.15	8.15	5.558e+37	6.11e-05
12985	triHPacyl.mtppmmpppd	4.176e+43	8.07	8.07	5.557e+37	6.11e-05
12986	triHPacyl.ptpmmtpppd	4.561e+43	8.12	8.12	5.556e+37	6.11e-05
12987	triHPacyl.pmpppmtppd	2.908e+43	7.85	7.85	5.550e+37	6.1e-05
12988	triHPacyl.ptptmmpmmd	7.161e+43	8.40	8.40	5.474e+37	6.02e-05
12989	triHPacyl.tmtptmmpmd	2.105e+44	9.04	9.04	5.462e+37	6e-05
12990	triHPacyl.tttptttmpd	6.674e+43	8.36	8.36	5.437e+37	5.97e-05
12991	triHPacyl.tmtmpppppd	2.354e+44	9.11	9.11	5.432e+37	5.97e-05
12992	triHPacyl.pppmmppppd	1.171e+44	8.70	8.70	5.425e+37	5.96e-05
12993	triHPacyl.mptppmmpmd	1.015e+44	8.61	8.61	5.420e+37	5.96e-05
12994	triHPacyl.ptpppmpppd	3.093e+43	7.90	7.90	5.403e+37	5.94e-05
12995	triHPacyl.mmmptmmpmd	1.014e+44	8.61	8.61	5.387e+37	5.92e-05
12996	triHPacyl.tmppppmmpd	4.749e+43	8.16	8.16	5.378e+37	5.91e-05
12997	triHPacyl.mptptmmpmd	3.453e+43	7.98	7.98	5.343e+37	5.87e-05
12998	triHPacyl.mmpmmttppd	9.532e+43	8.58	8.58	5.340e+37	5.87e-05
12999	triHPacyl.tmpmptmpd	1.246e+44	8.74	8.74	5.334e+37	5.86e-05
13000	triHPacyl.tpmppmtmpd	1.331e+43	7.41	7.41	5.328e+37	5.85e-05
13001	triHPacyl.tmtmmpmmd	1.779e+43	7.58	7.58	5.321e+37	5.85e-05
13002	triHPacyl.ttmppmmppd	6.002e+43	8.31	8.31	5.280e+37	5.8e-05
13003	triHPacyl.mtppmmtmmpd	1.271e+43	7.39	7.39	5.226e+37	5.74e-05
13004	triHPacyl.mtttppppmd	2.380e+44	9.14	9.14	5.201e+37	5.71e-05
13005	triHPacyl.tppppmmpmd	8.511e+43	8.53	8.53	5.179e+37	5.69e-05
13006	triHPacyl.ttttppmmpd	1.036e+44	8.65	8.65	5.174e+37	5.69e-05
13007	triHPacyl.tmtpttppd	1.327e+45	10.17	10.17	5.171e+37	5.68e-05

13008	triHPacyl.tpptmmpmd	2.616e+44	9.20	9.20	5.162e+37	5.67e-05
13009	triHPacyl.pttpttppd	7.194e+43	8.44	8.44	5.147e+37	5.66e-05
13010	triHPacyl.tpttptmmd	1.676e+44	8.94	8.94	5.106e+37	5.61e-05
13011	triHPacyl.tmptppmmd	1.154e+44	8.72	8.72	5.103e+37	5.61e-05
13012	triHPacyl.pttpttppd	6.921e+43	8.42	8.42	5.093e+37	5.6e-05
13013	triHPacyl.ptmtptmmd	3.029e+44	9.31	9.31	5.013e+37	5.51e-05
13014	triHPacyl.ptptmmpmd	6.496e+43	8.39	8.39	4.996e+37	5.49e-05
13015	triHPacyl.tpmptpmpd	5.058e+43	8.25	8.25	4.975e+37	5.47e-05
13016	triHPacyl.mtpmmtmmd	3.744e+43	8.07	8.07	4.969e+37	5.46e-05
13017	triHPacyl.mtmtmmpmd	8.261e+43	8.54	8.54	4.956e+37	5.45e-05
13018	triHPacyl.tpttmtmmd	4.113e+44	9.50	9.50	4.927e+37	5.41e-05
13019	triHPacyl.pmmmpmmpmd	4.626e+44	9.58	9.58	4.885e+37	5.37e-05
13020	triHPacyl.mttmmtmmd	1.401e+44	8.87	8.87	4.812e+37	5.29e-05
13021	triHPacyl.tppptpppd	1.426e+44	8.88	8.88	4.804e+37	5.28e-05
13022	triHPacyl.pmttppmmd	1.516e+44	8.92	8.92	4.786e+37	5.26e-05
13023	triHPacyl.pmtmtmmd	6.607e+44	9.80	9.80	4.766e+37	5.24e-05
13024	triHPacyl.mptmmtmmd	9.952e+43	8.68	8.68	4.744e+37	5.21e-05
13025	triHPacyl.mtmtptmmd	1.671e+44	8.99	8.99	4.697e+37	5.16e-05
13026	triHPacyl.mttpttmd	9.374e+43	8.66	8.66	4.637e+37	5.09e-05
13027	triHPacyl.mmpmmtmmd	1.114e+44	8.77	8.77	4.587e+37	5.04e-05
13028	triHPacyl.mtmtptppd	1.935e+44	9.10	9.10	4.528e+37	4.98e-05
13029	triHPacyl.tpmmpmmpmd	2.104e+44	9.15	9.15	4.522e+37	4.97e-05
13030	triHPacyl.pmtmtmmd	1.609e+45	10.37	10.37	4.513e+37	4.96e-05
13031	triHPacyl.mppmmpmd	3.706e+43	8.12	8.12	4.513e+37	4.96e-05
13032	triHPacyl.ttttmtppmd	1.173e+45	10.19	10.19	4.465e+37	4.91e-05
13033	triHPacyl.pmtmmtmmd	5.307e+43	8.34	8.34	4.455e+37	4.89e-05
13034	triHPacyl.pmttmmpmd	1.333e+44	8.89	8.89	4.433e+37	4.87e-05
13035	triHPacyl.mptmmtmmd	3.346e+43	8.07	8.07	4.407e+37	4.84e-05
13036	triHPacyl.pmtmptmmd	8.130e+43	8.60	8.60	4.385e+37	4.82e-05
13037	triHPacyl.pppppmmpd	4.041e+43	8.19	8.19	4.375e+37	4.81e-05
13038	triHPacyl.tptppmmpd	2.641e+44	9.31	9.31	4.361e+37	4.79e-05
13039	triHPacyl.mmtmmtmmd	6.120e+43	8.44	8.44	4.334e+37	4.76e-05
13040	triHPacyl.mmpmmpmmd	5.358e+43	8.36	8.36	4.333e+37	4.76e-05
13041	triHPacyl.pmptppmmd	4.157e+43	8.21	8.21	4.314e+37	4.74e-05
13042	triHPacyl.mtptmtmmd	4.740e+44	9.67	9.67	4.282e+37	4.71e-05
13043	triHPacyl.mmtmmpmmd	5.580e+43	8.40	8.40	4.273e+37	4.7e-05
13044	triHPacyl.ttpmmtmmd	8.720e+43	8.66	8.66	4.253e+37	4.67e-05
13045	triHPacyl.ppmtptmmd	4.412e+44	9.63	9.63	4.244e+37	4.66e-05
13046	triHPacyl.mtttppmmd	1.203e+44	8.86	8.86	4.242e+37	4.66e-05
13047	triHPacyl.tmtmtppmd	2.311e+43	7.87	7.87	4.242e+37	4.66e-05
13048	triHPacyl.ptptptmmd	2.302e+43	7.87	7.87	4.241e+37	4.66e-05
13049	triHPacyl.tpptpmpmd	3.338e+44	9.47	9.47	4.237e+37	4.66e-05
13050	triHPacyl.mttmtmmd	2.198e+44	9.22	9.22	4.236e+37	4.65e-05
13051	triHPacyl.pmtmmtmmd	9.963e+43	8.75	8.75	4.221e+37	4.64e-05
13052	triHPacyl.ttmtmmpmd	3.479e+44	9.49	9.49	4.217e+37	4.63e-05
13053	triHPacyl.mmtmtpppd	9.508e+43	8.72	8.72	4.199e+37	4.61e-05
13054	triHPacyl.ttttmtppmd	4.036e+44	9.59	9.59	4.186e+37	4.6e-05
13055	triHPacyl.ptptptmmd	1.069e+44	8.80	8.80	4.174e+37	4.59e-05
13056	triHPacyl.ptmtmtmmd	4.302e+44	9.63	9.63	4.130e+37	4.54e-05
13057	triHPacyl.pttpttmd	7.301e+43	8.58	8.58	4.100e+37	4.51e-05
13058	triHPacyl.mttmmpmmd	2.879e+44	9.40	9.40	4.087e+37	4.49e-05
13059	triHPacyl.mtmtmmpmd	3.699e+43	8.18	8.18	4.056e+37	4.46e-05
13060	triHPacyl.tttmptmmd	1.127e+44	8.85	8.85	4.008e+37	4.4e-05
13061	triHPacyl.pmptmmpmd	6.358e+43	8.51	8.51	3.987e+37	4.38e-05
13062	triHPacyl.ptmtmmpmd	3.381e+44	9.51	9.51	3.959e+37	4.35e-05
13063	triHPacyl.ttttmtppd	4.889e+44	9.74	9.74	3.912e+37	4.3e-05
13064	triHPacyl.tmmtptmmd	6.117e+44	9.88	9.88	3.905e+37	4.29e-05
13065	triHPacyl.pmptmtpmd	1.489e+44	9.03	9.03	3.903e+37	4.29e-05
13066	triHPacyl.pmmmpmmpmd	1.099e+44	8.86	8.86	3.879e+37	4.26e-05
13067	triHPacyl.mtppmtmmd	1.399e+43	7.63	7.63	3.864e+37	4.25e-05
13068	triHPacyl.ptmtmmpmd	1.719e+44	9.13	9.13	3.864e+37	4.25e-05
13069	triHPacyl.pttptmmd	1.953e+44	9.21	9.21	3.822e+37	4.2e-05
13070	triHPacyl.ptmtmmpmd	1.995e+44	9.22	9.22	3.818e+37	4.19e-05
13071	triHPacyl.mtmtmmpmd	1.083e+44	8.86	8.86	3.790e+37	4.16e-05
13072	triHPacyl.tmmpmtmmd	7.120e+43	8.61	8.61	3.787e+37	4.16e-05
13073	triHPacyl.pmmmpmmpmd	7.632e+43	8.66	8.66	3.767e+37	4.14e-05
13074	triHPacyl.mptmptmmd	2.552e+44	9.38	9.38	3.758e+37	4.13e-05
13075	triHPacyl.mptmmtmmd	7.133e+43	8.62	8.62	3.754e+37	4.13e-05
13076	triHPacyl.mmpmmpmmd	1.492e+43	7.69	7.69	3.738e+37	4.11e-05
13077	triHPacyl.pmtmmpmmd	6.439e+43	8.57	8.57	3.693e+37	4.06e-05
13078	triHPacyl.ptmtmtmmd	3.493e+44	9.58	9.58	3.690e+37	4.05e-05
13079	triHPacyl.tmmmpmtmmd	3.988e+44	9.66	9.66	3.670e+37	4.03e-05

13080	triHPacyl.mmmtpptpmd	6.030e+44	9.91	9.91	3.655e+37	4.02e-05
13081	triHPacyl.ptmtpttppd	3.900e+44	9.65	9.65	3.631e+37	3.99e-05
13082	triHPacyl.tptppptppd	1.899e+44	9.22	9.22	3.617e+37	3.97e-05
13083	triHPacyl.tptmmmtmmd	1.341e+44	9.02	9.02	3.601e+37	3.96e-05
13084	triHPacyl.mtptptmmmd	5.051e+43	8.44	8.44	3.578e+37	3.93e-05
13085	triHPacyl.tttppmtppd	4.388e+43	8.36	8.36	3.572e+37	3.93e-05
13086	triHPacyl.mmttmmtppd	2.208e+44	9.33	9.33	3.549e+37	3.9e-05
13087	triHPacyl.tptpttppd	1.109e+44	8.92	8.92	3.542e+37	3.89e-05
13088	triHPacyl.mppmppppmd	5.022e+43	8.44	8.44	3.541e+37	3.89e-05
13089	triHPacyl.ptptptmmpd	1.121e+44	8.92	8.92	3.536e+37	3.89e-05
13090	triHPacyl.mtmmmtmmd	3.018e+44	9.52	9.52	3.507e+37	3.85e-05
13091	triHPacyl.ptppmmmpd	1.725e+43	7.81	7.81	3.505e+37	3.85e-05
13092	triHPacyl.tmppptppd	1.059e+44	8.90	8.90	3.500e+37	3.85e-05
13093	triHPacyl.mpmptmpmd	5.678e+43	8.53	8.53	3.482e+37	3.83e-05
13094	triHPacyl.ttmtpmmpd	9.789e+43	8.85	8.85	3.479e+37	3.82e-05
13095	triHPacyl.mtppmmpmd	1.186e+44	8.97	8.97	3.477e+37	3.82e-05
13096	triHPacyl.mmtmmtppd	3.731e+43	8.28	8.28	3.456e+37	3.8e-05
13097	triHPacyl.ptmtptmmd	5.450e+44	9.88	9.88	3.440e+37	3.78e-05
13098	triHPacyl.mmtppptppd	1.770e+44	9.21	9.21	3.439e+37	3.78e-05
13099	triHPacyl.ttpmptppd	3.911e+43	8.31	8.31	3.433e+37	3.77e-05
13100	triHPacyl.mmtppmmpd	1.671e+44	9.18	9.18	3.430e+37	3.77e-05
13101	triHPacyl.mptmmpmpd	6.156e+43	8.59	8.59	3.419e+37	3.76e-05
13102	triHPacyl.mttmmmpmd	8.775e+43	8.80	8.80	3.408e+37	3.75e-05
13103	triHPacyl.tmmptmmpd	7.658e+43	8.72	8.72	3.398e+37	3.73e-05
13104	triHPacyl.tppmpmmpd	4.319e+43	8.38	8.38	3.389e+37	3.72e-05
13105	triHPacyl.tppptmmpd	1.884e+43	7.89	7.89	3.386e+37	3.72e-05
13106	triHPacyl.pmtmmtmmd	9.072e+43	8.83	8.83	3.370e+37	3.7e-05
13107	triHPacyl.tpttmmtmmd	4.911e+44	9.84	9.84	3.358e+37	3.69e-05
13108	triHPacyl.ttttptmmd	4.559e+44	9.80	9.80	3.319e+37	3.65e-05
13109	triHPacyl.pmpptppd	1.711e+43	7.84	7.84	3.313e+37	3.64e-05
13110	triHPacyl.mtppmmpd	7.575e+43	8.73	8.73	3.291e+37	3.62e-05
13111	triHPacyl.tmtppppmd	5.315e+44	9.90	9.90	3.285e+37	3.61e-05
13112	triHPacyl.pmttmmpmd	1.947e+44	9.30	9.30	3.279e+37	3.6e-05
13113	triHPacyl.tppppppmd	5.475e+43	8.54	8.54	3.263e+37	3.59e-05
13114	triHPacyl.ttttmppmd	6.331e+44	10.01	10.01	3.248e+37	3.57e-05
13115	triHPacyl.ptttppmmd	5.025e+43	8.50	8.50	3.241e+37	3.56e-05
13116	triHPacyl.ttpmptmpd	8.105e+43	8.79	8.79	3.218e+37	3.54e-05
13117	triHPacyl.tttmptmpd	8.795e+43	8.84	8.84	3.210e+37	3.53e-05
13118	triHPacyl.tmpmmtmmd	6.053e+43	8.62	8.62	3.188e+37	3.5e-05
13119	triHPacyl.mmtmtppd	3.667e+44	9.70	9.70	3.166e+37	3.48e-05
13120	triHPacyl.mtptmtmmpd	7.118e+43	8.72	8.72	3.155e+37	3.47e-05
13121	triHPacyl.tmpmmpppd	1.057e+44	8.96	8.96	3.146e+37	3.46e-05
13122	triHPacyl.ptptmmmpd	5.123e+43	8.53	8.53	3.135e+37	3.44e-05
13123	triHPacyl.pmttptmmpd	4.612e+44	9.84	9.84	3.132e+37	3.44e-05
13124	triHPacyl.tmtmmpppd	1.739e+44	9.26	9.26	3.128e+37	3.44e-05
13125	triHPacyl.mmmtpptmpd	3.469e+44	9.67	9.67	3.125e+37	3.43e-05
13126	triHPacyl.tmmppmmpd	6.438e+43	8.67	8.67	3.124e+37	3.43e-05
13127	triHPacyl.ptppmmpmd	8.423e+43	8.83	8.83	3.105e+37	3.41e-05
13128	triHPacyl.mmpptpmpd	5.918e+43	8.63	8.63	3.080e+37	3.38e-05
13129	triHPacyl.pmttmmtppd	1.408e+44	9.14	9.14	3.077e+37	3.38e-05
13130	triHPacyl.mppppppmd	4.027e+43	8.40	8.40	3.047e+37	3.35e-05
13131	triHPacyl.ptttmmmpd	9.263e+43	8.90	8.90	3.035e+37	3.34e-05
13132	triHPacyl.mtptmtmmpd	4.163e+44	9.80	9.80	3.034e+37	3.33e-05
13133	triHPacyl.tptmmpppd	4.709e+44	9.87	9.87	3.015e+37	3.31e-05
13134	triHPacyl.mmttmmpd	4.702e+44	9.88	9.88	3.007e+37	3.3e-05
13135	triHPacyl.tptmptmmd	2.750e+44	9.56	9.56	3.003e+37	3.3e-05
13136	triHPacyl.pmpmmpmpd	1.489e+43	7.82	7.82	2.995e+37	3.29e-05
13137	triHPacyl.tpmmtmmd	3.567e+44	9.71	9.71	2.993e+37	3.29e-05
13138	triHPacyl.tppmppppd	6.689e+43	8.72	8.72	2.992e+37	3.29e-05
13139	triHPacyl.ptttptmmpd	9.506e+43	8.93	8.93	2.953e+37	3.25e-05
13140	triHPacyl.pmpptppmd	8.684e+43	8.88	8.88	2.952e+37	3.24e-05
13141	triHPacyl.ptttptppd	9.359e+43	8.93	8.93	2.946e+37	3.24e-05
13142	triHPacyl.mmttmtpmd	4.455e+44	9.86	9.86	2.945e+37	3.24e-05
13143	triHPacyl.tppppmpmd	2.524e+43	8.16	8.16	2.884e+37	3.17e-05
13144	triHPacyl.ptmmmpmd	8.005e+43	8.85	8.85	2.879e+37	3.16e-05
13145	triHPacyl.ptmtptppd	4.103e+44	9.83	9.83	2.840e+37	3.12e-05
13146	triHPacyl.tppptppmd	2.808e+44	9.61	9.61	2.816e+37	3.09e-05
13147	triHPacyl.pmmmmmtmmd	4.779e+43	8.55	8.55	2.809e+37	3.09e-05
13148	triHPacyl.tmpmmmmmd	6.176e+43	8.71	8.71	2.803e+37	3.08e-05
13149	triHPacyl.pmmmtmmpd	3.316e+44	9.71	9.71	2.802e+37	3.08e-05
13150	triHPacyl.ptmptmmpd	2.745e+44	9.60	9.60	2.801e+37	3.08e-05
13151	triHPacyl.tmmppptppd	1.251e+44	9.13	9.13	2.794e+37	3.07e-05

13152	triHPacyl.mmmtpptmmd	6.978e+43	8.78	8.78	2.789e+37	3.06e-05
13153	triHPacyl.pmmppmtppd	2.429e+43	8.16	8.16	2.783e+37	3.06e-05
13154	triHPacyl.mppmpmpmpmd	6.578e+43	8.75	8.75	2.783e+37	3.06e-05
13155	triHPacyl.ptmpmttmd	5.021e+44	9.96	9.96	2.780e+37	3.05e-05
13156	triHPacyl.pmmppptmmd	9.451e+43	8.97	8.97	2.751e+37	3.02e-05
13157	triHPacyl.ptmtmtmpmd	4.809e+44	9.94	9.94	2.750e+37	3.02e-05
13158	triHPacyl.tptmptmpmd	1.052e+44	9.04	9.04	2.749e+37	3.02e-05
13159	triHPacyl.pmmmmptmmd	2.124e+44	9.46	9.46	2.719e+37	2.99e-05
13160	triHPacyl.mmttmtmpmd	3.480e+44	9.76	9.76	2.715e+37	2.98e-05
13161	triHPacyl.mtmtmpmppd	2.216e+44	9.49	9.49	2.703e+37	2.97e-05
13162	triHPacyl.mttptmtpd	1.118e+44	9.08	9.08	2.699e+37	2.97e-05
13163	triHPacyl.ttpptmpmd	6.476e+43	8.77	8.77	2.660e+37	2.92e-05
13164	triHPacyl.ptmtmmmmmd	1.641e+44	9.32	9.32	2.653e+37	2.92e-05
13165	triHPacyl.ppmtpppppd	2.254e+44	9.51	9.51	2.644e+37	2.9e-05
13166	triHPacyl.mmmppmpmpmd	3.098e+43	8.33	8.33	2.641e+37	2.9e-05
13167	triHPacyl.pmmppmmmmmd	7.779e+43	8.88	8.88	2.640e+37	2.9e-05
13168	triHPacyl.mtppmpmpmd	9.544e+43	9.00	9.00	2.640e+37	2.9e-05
13169	triHPacyl.tpptmmpmd	2.078e+44	9.47	9.47	2.640e+37	2.9e-05
13170	triHPacyl.pmpmtmmpmd	1.859e+44	9.40	9.40	2.636e+37	2.9e-05
13171	triHPacyl.tmmppmpmd	6.700e+43	8.80	8.80	2.624e+37	2.88e-05
13172	triHPacyl.mmtpmmtmmd	1.240e+44	9.16	9.16	2.618e+37	2.88e-05
13173	triHPacyl.mmpppmmmmmd	5.865e+43	8.72	8.72	2.593e+37	2.85e-05
13174	triHPacyl.mptmmmmppd	5.145e+43	8.65	8.65	2.587e+37	2.84e-05
13175	triHPacyl.mtmmmmtpd	3.357e+45	11.14	11.14	2.584e+37	2.84e-05
13176	triHPacyl.mtmpmtmpmd	3.637e+43	8.45	8.45	2.560e+37	2.81e-05
13177	triHPacyl.tpptptmpd	3.054e+44	9.72	9.72	2.526e+37	2.78e-05
13178	triHPacyl.mtptmpmpmd	1.286e+44	9.21	9.21	2.522e+37	2.77e-05
13179	triHPacyl.pmmppmtmmd	7.732e+43	8.91	8.91	2.514e+37	2.76e-05
13180	triHPacyl.mtttptmpd	1.500e+44	9.30	9.30	2.498e+37	2.75e-05
13181	triHPacyl.tmpmmmtmpd	7.372e+43	8.88	8.88	2.496e+37	2.74e-05
13182	triHPacyl.mpmtpppppd	1.000e+44	9.06	9.06	2.494e+37	2.74e-05
13183	triHPacyl.tppmpmpmpmd	1.074e+44	9.11	9.11	2.481e+37	2.73e-05
13184	triHPacyl.mmmmmmtmmd	2.892e+44	9.70	9.70	2.468e+37	2.71e-05
13185	triHPacyl.pmpppptppd	7.714e+44	10.29	10.29	2.463e+37	2.71e-05
13186	triHPacyl.tttmpmmpmd	7.568e+43	8.91	8.91	2.463e+37	2.71e-05
13187	triHPacyl.mptmtpmpd	1.011e+44	9.08	9.08	2.459e+37	2.7e-05
13188	triHPacyl.mptmmmmmmmd	9.784e+43	9.06	9.06	2.447e+37	2.69e-05
13189	triHPacyl.tmpmmmtmmd	5.924e+43	8.77	8.77	2.439e+37	2.68e-05
13190	triHPacyl.mmtppmpmpmd	4.849e+43	8.65	8.65	2.439e+37	2.68e-05
13191	triHPacyl.tppmpptppd	3.714e+44	9.86	9.86	2.437e+37	2.68e-05
13192	triHPacyl.ttmmpmtmmd	2.647e+44	9.67	9.67	2.398e+37	2.64e-05
13193	triHPacyl.pmmmtmtmmd	2.745e+44	9.69	9.69	2.388e+37	2.62e-05
13194	triHPacyl.ptppmmppd	1.052e+44	9.12	9.12	2.373e+37	2.61e-05
13195	triHPacyl.mtmtptppmd	2.928e+43	8.36	8.36	2.370e+37	2.6e-05
13196	triHPacyl.pmttptmpd	2.935e+44	9.75	9.75	2.316e+37	2.54e-05
13197	triHPacyl.pmttmppmd	5.860e+44	10.17	10.17	2.303e+37	2.53e-05
13198	triHPacyl.mttmmmmmmmd	8.525e+43	9.02	9.02	2.298e+37	2.53e-05
13199	triHPacyl.mptpmtpd	1.849e+44	9.48	9.48	2.298e+37	2.53e-05
13200	triHPacyl.mtptmmpmpmd	2.574e+44	9.68	9.68	2.298e+37	2.52e-05
13201	triHPacyl.mmpptppmmmd	4.544e+43	8.64	8.64	2.295e+37	2.52e-05
13202	triHPacyl.ptmtmmtmpd	4.192e+44	9.97	9.97	2.291e+37	2.52e-05
13203	triHPacyl.mtptmtpd	6.915e+43	8.90	8.90	2.262e+37	2.49e-05
13204	triHPacyl.mpmtpmtmmd	1.377e+44	9.32	9.32	2.245e+37	2.47e-05
13205	triHPacyl.mmtmmmtmpd	1.819e+44	9.48	9.48	2.243e+37	2.46e-05
13206	triHPacyl.tpptmmpmd	9.015e+43	9.07	9.07	2.243e+37	2.46e-05
13207	triHPacyl.pttptppd	7.180e+43	8.93	8.93	2.234e+37	2.45e-05
13208	triHPacyl.mmmppmtmpd	3.496e+43	8.50	8.50	2.231e+37	2.45e-05
13209	triHPacyl.mttmmmtmpd	2.494e+44	9.68	9.68	2.205e+37	2.42e-05
13210	triHPacyl.pmmppmtmpd	2.126e+43	8.22	8.22	2.190e+37	2.41e-05
13211	triHPacyl.pmmppptppd	4.605e+43	8.68	8.68	2.189e+37	2.41e-05
13212	triHPacyl.tpptptmpd	7.340e+44	10.33	10.33	2.179e+37	2.39e-05
13213	triHPacyl.mpmtpmtmpd	1.591e+44	9.42	9.42	2.169e+37	2.38e-05
13214	triHPacyl.pmtpmmtmpd	1.260e+44	9.29	9.29	2.148e+37	2.36e-05
13215	triHPacyl.tpttpmpmpd	3.883e+44	9.96	9.96	2.144e+37	2.36e-05
13216	triHPacyl.tpmmpmtmpd	9.753e+43	9.14	9.14	2.138e+37	2.35e-05
13217	triHPacyl.pmmtpmpmd	1.090e+43	7.84	7.84	2.137e+37	2.35e-05
13218	triHPacyl.mmpppppmpd	9.882e+43	9.16	9.16	2.085e+37	2.29e-05
13219	triHPacyl.mtmmmtppd	5.795e+44	10.22	10.22	2.084e+37	2.29e-05
13220	triHPacyl.tppmmmmmmmd	5.689e+43	8.84	8.84	2.074e+37	2.28e-05
13221	triHPacyl.tpmppptmmd	1.265e+44	9.32	9.32	2.067e+37	2.27e-05
13222	triHPacyl.ptptptppd	1.488e+44	9.41	9.41	2.063e+37	2.27e-05
13223	triHPacyl.ttpmpmtmpd	9.191e+43	9.13	9.13	2.062e+37	2.27e-05

13224	triHPacyl.tpmppmpmpd	3.416e+43	8.54	8.54	2.055e+37	2.26e-05
13225	triHPacyl.mtmtpmppmd	2.188e+44	9.65	9.65	2.053e+37	2.26e-05
13226	triHPacyl.tpttpmpppd	4.707e+44	10.10	10.10	2.051e+37	2.25e-05
13227	triHPacyl.tpttptpppd	4.691e+44	10.11	10.11	2.038e+37	2.24e-05
13228	triHPacyl.tpmtmmtmpd	5.305e+44	10.18	10.18	2.029e+37	2.23e-05
13229	triHPacyl.ptttmmpppd	1.999e+44	9.60	9.60	2.027e+37	2.23e-05
13230	triHPacyl.tptppmppmd	1.551e+44	9.45	9.45	2.010e+37	2.21e-05
13231	triHPacyl.ptptpmmmmd	8.378e+43	9.09	9.09	1.988e+37	2.18e-05
13232	triHPacyl.ttpmnmppd	3.596e+43	8.59	8.59	1.986e+37	2.18e-05
13233	triHPacyl.pmmptmpmd	2.469e+44	9.75	9.75	1.964e+37	2.16e-05
13234	triHPacyl.pmttmtmmd	4.362e+44	10.09	10.09	1.957e+37	2.15e-05
13235	triHPacyl.mtmtpmmmmd	1.127e+44	9.28	9.28	1.941e+37	2.13e-05
13236	triHPacyl.mmpmmmtppd	1.600e+44	9.50	9.50	1.918e+37	2.11e-05
13237	triHPacyl.mmpmmtmpd	1.856e+44	9.59	9.59	1.906e+37	2.09e-05
13238	triHPacyl.mpppmmtmmd	1.610e+44	9.51	9.51	1.899e+37	2.09e-05
13239	triHPacyl.mpppmppmd	4.191e+43	8.71	8.71	1.890e+37	2.08e-05
13240	triHPacyl.mtpmmtmpd	1.135e+44	9.31	9.31	1.873e+37	2.06e-05
13241	triHPacyl.mpppmmtmpd	8.314e+43	9.12	9.12	1.873e+37	2.06e-05
13242	triHPacyl.ttmtptmpd	3.505e+44	9.99	9.99	1.865e+37	2.05e-05
13243	triHPacyl.mpmmpmmpmd	2.268e+44	9.73	9.73	1.849e+37	2.03e-05
13244	triHPacyl.ttmtmmmmmd	5.768e+43	8.92	8.92	1.842e+37	2.02e-05
13245	triHPacyl.pttmmpppd	7.528e+43	9.08	9.08	1.839e+37	2.02e-05
13246	triHPacyl.mmtmpmpppd	1.409e+44	9.46	9.46	1.821e+37	2e-05
13247	triHPacyl.tmttppmpd	3.950e+44	10.07	10.07	1.815e+37	1.99e-05
13248	triHPacyl.ttttppmpd	3.844e+44	10.06	10.06	1.811e+37	1.99e-05
13249	triHPacyl.mmtmptppd	1.501e+44	9.50	9.50	1.806e+37	1.98e-05
13250	triHPacyl.mpttppmpd	3.255e+44	9.96	9.96	1.803e+37	1.98e-05
13251	triHPacyl.tmttppppd	3.923e+44	10.07	10.07	1.798e+37	1.98e-05
13252	triHPacyl.tpttptppmd	5.880e+44	10.32	10.32	1.788e+37	1.96e-05
13253	triHPacyl.tptppmmpd	1.109e+44	9.33	9.33	1.779e+37	1.95e-05
13254	triHPacyl.pmpptpppd	2.583e+43	8.46	8.46	1.771e+37	1.95e-05
13255	triHPacyl.mpptptmmd	1.691e+44	9.59	9.59	1.733e+37	1.9e-05
13256	triHPacyl.pmmptmpd	3.276e+43	8.62	8.62	1.728e+37	1.9e-05
13257	triHPacyl.tmptptmpd	1.476e+44	9.52	9.52	1.725e+37	1.9e-05
13258	triHPacyl.ttptmmpmd	1.155e+44	9.37	9.37	1.720e+37	1.89e-05
13259	triHPacyl.mmmptmpd	2.977e+43	8.56	8.56	1.719e+37	1.89e-05
13260	triHPacyl.mpppmtpmd	7.110e+43	9.09	9.09	1.702e+37	1.87e-05
13261	triHPacyl.pmtmmmpmd	6.829e+43	9.07	9.07	1.698e+37	1.87e-05
13262	triHPacyl.ptmmppmmd	1.180e+44	9.39	9.39	1.697e+37	1.86e-05
13263	triHPacyl.ptptmmtmpd	3.153e+44	9.98	9.98	1.693e+37	1.86e-05
13264	triHPacyl.mptpmmmmd	1.442e+44	9.52	9.52	1.684e+37	1.85e-05
13265	triHPacyl.mtmtptppd	7.879e+44	10.53	10.53	1.674e+37	1.84e-05
13266	triHPacyl.mmmmmmmmd	1.173e+44	9.40	9.40	1.664e+37	1.83e-05
13267	triHPacyl.pmpppmpmpd	1.523e+43	8.18	8.18	1.661e+37	1.82e-05
13268	triHPacyl.tpttptmmpd	2.629e+44	9.88	9.88	1.657e+37	1.82e-05
13269	triHPacyl.mtmptmmpd	6.990e+43	9.10	9.10	1.644e+37	1.81e-05
13270	triHPacyl.tpmtmmmpd	3.065e+44	9.98	9.98	1.644e+37	1.81e-05
13271	triHPacyl.tptppmmpd	8.331e+43	9.21	9.21	1.640e+37	1.8e-05
13272	triHPacyl.mmttppppd	4.318e+44	10.19	10.19	1.638e+37	1.8e-05
13273	triHPacyl.mmmtpmtmpd	9.445e+44	10.65	10.65	1.636e+37	1.8e-05
13274	triHPacyl.mtmtmtmpd	3.401e+44	10.05	10.05	1.630e+37	1.79e-05
13275	triHPacyl.tmpmptmmd	2.750e+44	9.92	9.92	1.619e+37	1.78e-05
13276	triHPacyl.tmpppmmpmd	1.496e+44	9.56	9.56	1.616e+37	1.78e-05
13277	triHPacyl.pttmmmtmmd	1.222e+44	9.44	9.44	1.616e+37	1.78e-05
13278	triHPacyl.tpmmpmtmmd	2.217e+44	9.80	9.80	1.605e+37	1.76e-05
13279	triHPacyl.ptmtptmpd	3.285e+44	10.04	10.04	1.594e+37	1.75e-05
13280	triHPacyl.tmpppmmtmmd	1.401e+44	9.53	9.53	1.589e+37	1.75e-05
13281	triHPacyl.mmmmmmpmpd	2.223e+43	8.44	8.44	1.579e+37	1.73e-05
13282	triHPacyl.tptppppppd	2.856e+44	9.96	9.96	1.576e+37	1.73e-05
13283	triHPacyl.ttttppmmpd	1.483e+44	9.58	9.58	1.567e+37	1.72e-05
13284	triHPacyl.tmmtpmppd	2.070e+44	9.78	9.78	1.565e+37	1.72e-05
13285	triHPacyl.ptpmmmmmmd	3.904e+43	8.78	8.78	1.564e+37	1.72e-05
13286	triHPacyl.mtptpmmmmd	6.326e+43	9.07	9.07	1.555e+37	1.71e-05
13287	triHPacyl.mtppppmmd	1.154e+43	8.06	8.06	1.543e+37	1.7e-05
13288	triHPacyl.tppmpmmpmd	6.828e+43	9.12	9.12	1.542e+37	1.69e-05
13289	triHPacyl.mppptptmmd	1.175e+44	9.45	9.45	1.542e+37	1.69e-05
13290	triHPacyl.tpmtmtmpd	7.168e+44	10.53	10.53	1.534e+37	1.69e-05
13291	triHPacyl.pmpptmpd	2.844e+44	9.98	9.98	1.516e+37	1.67e-05
13292	triHPacyl.pmtmptmmd	2.455e+44	9.90	9.90	1.511e+37	1.66e-05
13293	triHPacyl.mmmmmmpmmpd	1.724e+44	9.69	9.69	1.508e+37	1.66e-05
13294	triHPacyl.pppmpmmpd	8.123e+43	9.24	9.24	1.500e+37	1.65e-05
13295	triHPacyl.mttmmtmpd	1.006e+44	9.37	9.37	1.500e+37	1.65e-05

13296	triHPacyl.tpppppppppd	1.456e+44	9.59	9.59	1.491e+37	1.64e-05
13297	triHPacyl.mmttmtmmmd	1.511e+44	9.62	9.62	1.489e+37	1.64e-05
13298	triHPacyl.tmtptmmmpd	2.040e+44	9.80	9.80	1.484e+37	1.63e-05
13299	triHPacyl.tmpptppmd	9.289e+43	9.34	9.34	1.466e+37	1.61e-05
13300	triHPacyl.mmttppppmd	3.595e+44	10.15	10.15	1.456e+37	1.6e-05
13301	triHPacyl.mmmtpppppmd	5.659e+43	9.05	9.05	1.446e+37	1.59e-05
13302	triHPacyl.pmmppppmd	1.251e+44	9.53	9.53	1.438e+37	1.58e-05
13303	triHPacyl.mmpmmmpmd	1.468e+43	8.25	8.25	1.434e+37	1.58e-05
13304	triHPacyl.mmptptpmd	5.431e+43	9.03	9.03	1.425e+37	1.57e-05
13305	triHPacyl.pmpmtppmd	1.425e+44	9.61	9.61	1.420e+37	1.56e-05
13306	triHPacyl.mtptppppmd	1.095e+45	10.83	10.83	1.419e+37	1.56e-05
13307	triHPacyl.mmmppmmmd	6.994e+43	9.19	9.19	1.418e+37	1.56e-05
13308	triHPacyl.tmppppmpmd	2.101e+43	8.48	8.48	1.394e+37	1.53e-05
13309	triHPacyl.tmtpttppmd	5.920e+44	10.48	10.48	1.379e+37	1.52e-05
13310	triHPacyl.tmpppmmppd	2.723e+43	8.66	8.66	1.348e+37	1.48e-05
13311	triHPacyl.mtttmtppmd	3.232e+44	10.13	10.13	1.342e+37	1.48e-05
13312	triHPacyl.pmmtmppmd	1.252e+44	9.57	9.57	1.337e+37	1.47e-05
13313	triHPacyl.mmptppppmd	2.161e+44	9.90	9.90	1.319e+37	1.45e-05
13314	triHPacyl.tmpmmmpmd	2.447e+43	8.61	8.61	1.307e+37	1.44e-05
13315	triHPacyl.mmtptpmpd	3.852e+43	8.88	8.88	1.299e+37	1.43e-05
13316	triHPacyl.tppmmtppmd	2.173e+44	9.92	9.92	1.291e+37	1.42e-05
13317	triHPacyl.ptpmpptmd	2.678e+43	8.67	8.67	1.289e+37	1.42e-05
13318	triHPacyl.mmtmmmpmd	5.451e+43	9.10	9.10	1.284e+37	1.41e-05
13319	triHPacyl.mtmtmtmmmd	4.494e+44	10.36	10.36	1.280e+37	1.41e-05
13320	triHPacyl.pmttmpppd	7.960e+44	10.71	10.71	1.257e+37	1.38e-05
13321	triHPacyl.ptmtmmppd	2.508e+44	10.03	10.03	1.243e+37	1.37e-05
13322	triHPacyl.tppmmtmmmd	3.349e+43	8.83	8.83	1.236e+37	1.36e-05
13323	triHPacyl.mptptppmd	1.013e+44	9.49	9.49	1.231e+37	1.35e-05
13324	triHPacyl.mtmtmtppd	1.135e+45	10.94	10.94	1.209e+37	1.33e-05
13325	triHPacyl.pmpmmtpmd	1.360e+44	9.68	9.68	1.209e+37	1.33e-05
13326	triHPacyl.tppttmmmd	1.754e+44	9.84	9.84	1.181e+37	1.3e-05
13327	triHPacyl.ttptpmtmd	7.114e+43	9.31	9.31	1.177e+37	1.29e-05
13328	triHPacyl.tmtppmmppd	5.993e+44	10.58	10.58	1.173e+37	1.29e-05
13329	triHPacyl.mmpmmppmd	2.547e+43	8.70	8.70	1.173e+37	1.29e-05
13330	triHPacyl.ptttmmpmd	2.048e+44	9.94	9.94	1.172e+37	1.29e-05
13331	triHPacyl.tpmtptppd	1.730e+44	9.84	9.84	1.169e+37	1.28e-05
13332	triHPacyl.mmpmmtppd	1.666e+44	9.82	9.82	1.169e+37	1.28e-05
13333	triHPacyl.ptmptppmd	4.477e+43	9.04	9.04	1.165e+37	1.28e-05
13334	triHPacyl.tptppmmppd	1.355e+44	9.70	9.70	1.162e+37	1.28e-05
13335	triHPacyl.pmpptppmd	1.364e+43	8.34	8.34	1.155e+37	1.27e-05
13336	triHPacyl.ptpmmtpmd	6.431e+43	9.26	9.26	1.150e+37	1.26e-05
13337	triHPacyl.mmpmptpmd	2.339e+43	8.66	8.66	1.145e+37	1.26e-05
13338	triHPacyl.mmttptppd	3.311e+44	10.24	10.24	1.145e+37	1.26e-05
13339	triHPacyl.ttmmpppmd	4.821e+44	10.47	10.47	1.133e+37	1.25e-05
13340	triHPacyl.tpmtppppd	1.012e+44	9.55	9.55	1.125e+37	1.24e-05
13341	triHPacyl.pttmppppd	2.839e+43	8.79	8.79	1.118e+37	1.23e-05
13342	triHPacyl.tpptppppd	5.747e+44	10.59	10.59	1.113e+37	1.22e-05
13343	triHPacyl.tppptppppd	2.219e+44	10.02	10.02	1.113e+37	1.22e-05
13344	triHPacyl.mmmppmmppd	3.579e+43	8.94	8.94	1.104e+37	1.21e-05
13345	triHPacyl.ptptmtmmmd	9.038e+43	9.49	9.49	1.102e+37	1.21e-05
13346	triHPacyl.tpppmtppd	4.536e+43	9.09	9.09	1.092e+37	1.2e-05
13347	triHPacyl.tmpptpmpd	1.068e+44	9.60	9.60	1.090e+37	1.2e-05
13348	triHPacyl.tmttppppd	3.567e+44	10.32	10.32	1.090e+37	1.2e-05
13349	triHPacyl.tmttptppd	8.442e+44	10.83	10.83	1.088e+37	1.2e-05
13350	triHPacyl.mmmppptppd	6.864e+43	9.33	9.33	1.087e+37	1.19e-05
13351	triHPacyl.mptpmtppd	4.251e+44	10.42	10.42	1.084e+37	1.19e-05
13352	triHPacyl.tppppppmpd	8.572e+43	9.47	9.47	1.083e+37	1.19e-05
13353	triHPacyl.ppttmmppd	1.304e+44	9.72	9.72	1.080e+37	1.19e-05
13354	triHPacyl.mmttmmpmd	7.834e+44	10.79	10.79	1.079e+37	1.19e-05
13355	triHPacyl.tmtmpttmd	2.929e+44	10.21	10.21	1.069e+37	1.17e-05
13356	triHPacyl.pmpptppmd	4.204e+43	9.06	9.06	1.052e+37	1.16e-05
13357	triHPacyl.pppppppmd	1.487e+44	9.82	9.82	1.050e+37	1.15e-05
13358	triHPacyl.mppmmppmd	1.536e+44	9.84	9.84	1.044e+37	1.15e-05
13359	triHPacyl.mpttppppd	8.692e+43	9.51	9.51	1.028e+37	1.13e-05
13360	triHPacyl.mtppmtppd	6.335e+43	9.32	9.32	1.024e+37	1.12e-05
13361	triHPacyl.mppppppmd	2.999e+43	8.88	8.88	1.023e+37	1.12e-05
13362	triHPacyl.mmttppptppd	7.231e+43	9.40	9.40	1.020e+37	1.12e-05
13363	triHPacyl.ptptmtppmd	1.827e+44	9.96	9.96	1.017e+37	1.12e-05
13364	triHPacyl.mmtmmtppmd	6.886e+43	9.38	9.38	1.011e+37	1.11e-05
13365	triHPacyl.mpttmtppd	1.758e+44	9.94	9.94	1.005e+37	1.1e-05
13366	triHPacyl.mptpmtppd	1.699e+44	9.92	9.92	1.004e+37	1.1e-05
13367	triHPacyl.tpptppppmd	4.281e+44	10.47	10.47	1.003e+37	1.1e-05

13368	triHPacyl.mmttptpmnd	4.672e+44	10.53	10.53	9.892e+36	1.09e-05
13369	triHPacyl.tpptpmpmpd	4.336e+44	10.49	10.49	9.821e+36	1.08e-05
13370	triHPacyl.pmtmtttmpd	2.725e+44	10.22	10.22	9.818e+36	1.08e-05
13371	triHPacyl.pmpmpmmpmpd	1.631e+44	9.91	9.91	9.787e+36	1.08e-05
13372	triHPacyl.ptmpmtpppd	4.489e+43	9.15	9.15	9.702e+36	1.07e-05
13373	triHPacyl.mptppmmppd	4.782e+43	9.19	9.19	9.585e+36	1.05e-05
13374	triHPacyl.mpptmttppd	1.698e+44	9.96	9.96	9.496e+36	1.04e-05
13375	triHPacyl.mpttmtmmnd	1.151e+44	9.73	9.73	9.402e+36	1.03e-05
13376	triHPacyl.mmmppmtttmpd	4.441e+43	9.17	9.17	9.347e+36	1.03e-05
13377	triHPacyl.tpmtpmpmpd	2.494e+44	10.20	10.20	9.293e+36	1.02e-05
13378	triHPacyl.mmttpttmmnd	3.822e+44	10.45	10.45	9.264e+36	1.02e-05
13379	triHPacyl.pmpptppppd	4.349e+43	9.16	9.16	9.178e+36	1.01e-05
13380	triHPacyl.mmpmttppd	7.751e+43	9.51	9.51	9.145e+36	1e-05
13381	triHPacyl.pmtmptmnd	8.551e+43	9.57	9.57	9.105e+36	1e-05
13382	triHPacyl.mmttmppmpd	7.952e+44	10.91	10.91	8.988e+36	9.88e-06
13383	triHPacyl.mptmmppppd	8.680e+43	9.59	9.59	8.983e+36	9.87e-06
13384	triHPacyl.tppmptpmd	1.199e+44	9.78	9.78	8.971e+36	9.86e-06
13385	triHPacyl.mmtppmpmpd	2.485e+44	10.22	10.22	8.938e+36	9.82e-06
13386	triHPacyl.mptpmmppmd	1.431e+44	9.89	9.89	8.929e+36	9.81e-06
13387	triHPacyl.mtppmmmmnd	1.405e+44	9.88	9.88	8.929e+36	9.81e-06
13388	triHPacyl.pttpmmtmpd	2.560e+44	10.24	10.24	8.924e+36	9.81e-06
13389	triHPacyl.mmpmmmmmpd	1.268e+44	9.82	9.82	8.852e+36	9.73e-06
13390	triHPacyl.mptmmppppd	6.334e+43	9.41	9.41	8.810e+36	9.68e-06
13391	triHPacyl.mmmtpptpmnd	6.123e+43	9.39	9.39	8.775e+36	9.64e-06
13392	triHPacyl.tpmtmmtmpd	3.859e+44	10.49	10.49	8.764e+36	9.63e-06
13393	triHPacyl.mtppmmmmnd	4.174e+43	9.17	9.17	8.714e+36	9.58e-06
13394	triHPacyl.tpptptpmd	3.138e+44	10.38	10.38	8.568e+36	9.42e-06
13395	triHPacyl.ttmtpttmmnd	2.872e+44	10.33	10.33	8.539e+36	9.38e-06
13396	triHPacyl.mmpmptmnd	1.398e+44	9.91	9.91	8.469e+36	9.31e-06
13397	triHPacyl.pmpmmmpmpd	3.438e+43	9.07	9.07	8.440e+36	9.27e-06
13398	triHPacyl.mmtmmppppd	1.522e+44	9.96	9.96	8.377e+36	9.21e-06
13399	triHPacyl.tmtmmpmpd	6.046e+44	10.79	10.79	8.375e+36	9.2e-06
13400	triHPacyl.mpmtpmmppd	3.750e+44	10.51	10.51	8.215e+36	9.03e-06
13401	triHPacyl.mmmmmmpmnd	1.098e+44	9.78	9.78	8.206e+36	9.02e-06
13402	triHPacyl.tmppttppmd	1.074e+45	11.14	11.14	8.196e+36	9.01e-06
13403	triHPacyl.mmpmpmpmpd	5.759e+43	9.40	9.40	8.186e+36	8.99e-06
13404	triHPacyl.tpptppppmd	2.807e+44	10.34	10.34	8.184e+36	8.99e-06
13405	triHPacyl.tttptpppd	8.302e+44	10.99	10.99	8.177e+36	8.98e-06
13406	triHPacyl.ppmtptpppd	2.961e+44	10.38	10.38	8.167e+36	8.97e-06
13407	triHPacyl.mmpppmmpd	3.109e+43	9.03	9.03	8.153e+36	8.96e-06
13408	triHPacyl.mmtmmtmnd	2.285e+45	11.60	11.60	8.152e+36	8.96e-06
13409	triHPacyl.mmpmmmmmpd	5.492e+43	9.37	9.37	8.139e+36	8.94e-06
13410	triHPacyl.mmmmttppd	2.860e+44	10.36	10.36	8.099e+36	8.9e-06
13411	triHPacyl.tppmmmpmpd	4.603e+43	9.28	9.28	8.041e+36	8.84e-06
13412	triHPacyl.tmmppttmpd	8.555e+43	9.66	9.66	7.821e+36	8.59e-06
13413	triHPacyl.mmtppptmpd	8.036e+43	9.63	9.63	7.813e+36	8.59e-06
13414	triHPacyl.tmtppptmpd	2.121e+44	10.21	10.21	7.749e+36	8.51e-06
13415	triHPacyl.tppmmmmmpd	5.040e+44	10.73	10.73	7.654e+36	8.41e-06
13416	triHPacyl.mmpmpttppd	4.468e+43	9.29	9.29	7.605e+36	8.36e-06
13417	triHPacyl.tppmppppmd	4.197e+43	9.26	9.26	7.597e+36	8.35e-06
13418	triHPacyl.ptpmmmtmnd	5.779e+43	9.45	9.45	7.579e+36	8.33e-06
13419	triHPacyl.ptptmmmmnd	8.825e+43	9.70	9.70	7.513e+36	8.26e-06
13420	triHPacyl.pmpppttmnd	4.656e+43	9.32	9.32	7.501e+36	8.24e-06
13421	triHPacyl.pmtmmmtmnd	7.400e+43	9.61	9.61	7.442e+36	8.18e-06
13422	triHPacyl.ptpmmppmpd	1.313e+43	8.58	8.58	7.388e+36	8.12e-06
13423	triHPacyl.tpmtmmtppd	7.069e+44	10.96	10.96	7.276e+36	7.99e-06
13424	triHPacyl.tppmpmpmpd	1.582e+44	10.08	10.08	7.224e+36	7.94e-06
13425	triHPacyl.pmpmptpppd	3.870e+43	9.24	9.24	7.190e+36	7.9e-06
13426	triHPacyl.tpmppmtmpd	1.071e+44	9.85	9.85	7.176e+36	7.88e-06
13427	triHPacyl.mmpptpmpmpd	9.235e+43	9.76	9.76	7.125e+36	7.83e-06
13428	triHPacyl.tmpmtttmpd	3.859e+44	10.62	10.62	7.100e+36	7.8e-06
13429	triHPacyl.tpmtmptppd	7.747e+44	11.04	11.04	7.043e+36	7.74e-06
13430	triHPacyl.mtmmmpmnd	2.525e+44	10.37	10.37	7.021e+36	7.71e-06
13431	triHPacyl.tmttppmmpd	6.250e+44	10.91	10.91	7.019e+36	7.71e-06
13432	triHPacyl.mppppmmpmpd	1.406e+44	10.03	10.03	6.965e+36	7.65e-06
13433	triHPacyl.mpmmmmtmpd	7.208e+43	9.63	9.63	6.919e+36	7.6e-06
13434	triHPacyl.tttppmtppd	1.589e+44	10.11	10.11	6.875e+36	7.55e-06
13435	triHPacyl.ptttmmtmpd	2.180e+44	10.30	10.30	6.844e+36	7.52e-06
13436	triHPacyl.tmmppttppd	1.158e+44	9.93	9.93	6.808e+36	7.48e-06
13437	triHPacyl.tmpmptmpmd	2.679e+43	9.05	9.05	6.799e+36	7.47e-06
13438	triHPacyl.mmpptmmmmnd	1.966e+44	10.24	10.24	6.767e+36	7.44e-06
13439	triHPacyl.mtmtpttppd	4.280e+43	9.34	9.34	6.739e+36	7.41e-06

13440	triHPacyl.mpptmtpmnd	1.783e+44	10.19	10.19	6.689e+36	7.35e-06
13441	triHPacyl.tpmtmptmpd	4.764e+44	10.78	10.78	6.678e+36	7.34e-06
13442	triHPacyl.tptmpmpmnd	3.305e+44	10.56	10.56	6.674e+36	7.33e-06
13443	triHPacyl.mppptpppmd	9.308e+43	9.81	9.81	6.656e+36	7.31e-06
13444	triHPacyl.mtmmmtppmd	3.896e+44	10.67	10.67	6.612e+36	7.27e-06
13445	triHPacyl.mttppmmmpd	1.164e+44	9.95	9.95	6.599e+36	7.25e-06
13446	triHPacyl.ptptmttppd	2.093e+44	10.31	10.31	6.483e+36	7.12e-06
13447	triHPacyl.ttmppppmnd	1.269e+44	10.01	10.01	6.480e+36	7.12e-06
13448	triHPacyl.ptmtmmtmpd	3.459e+44	10.61	10.61	6.401e+36	7.03e-06
13449	triHPacyl.ptptmmpmpd	3.120e+44	10.55	10.55	6.391e+36	7.02e-06
13450	triHPacyl.ptmtmmtmnd	5.658e+44	10.91	10.91	6.362e+36	6.99e-06
13451	triHPacyl.tttmppmmnd	5.390e+43	9.51	9.51	6.356e+36	6.98e-06
13452	triHPacyl.tmpptpppd	1.906e+44	10.26	10.26	6.353e+36	6.98e-06
13453	triHPacyl.pttmmmtmpd	1.418e+44	10.10	10.10	6.241e+36	6.86e-06
13454	triHPacyl.mpttptmpd	1.317e+44	10.05	10.05	6.240e+36	6.86e-06
13455	triHPacyl.mmttmppppd	5.006e+44	10.85	10.85	6.222e+36	6.84e-06
13456	triHPacyl.mpmtpmmpmd	2.702e+44	10.49	10.49	6.210e+36	6.82e-06
13457	triHPacyl.pmpptppmd	5.366e+43	9.53	9.53	6.113e+36	6.72e-06
13458	triHPacyl.mptmtmmpd	1.478e+44	10.14	10.14	6.082e+36	6.68e-06
13459	triHPacyl.tpmmpmtmnd	3.096e+44	10.58	10.58	6.070e+36	6.67e-06
13460	triHPacyl.mmttptmpd	2.240e+44	10.40	10.40	5.943e+36	6.53e-06
13461	triHPacyl.mmttpppmd	2.020e+43	8.97	8.97	5.898e+36	6.48e-06
13462	triHPacyl.mtmppmmmpd	6.622e+43	9.69	9.69	5.766e+36	6.34e-06
13463	triHPacyl.ttttptmnd	1.061e+44	9.98	9.98	5.727e+36	6.29e-06
13464	triHPacyl.mptppmtmnd	2.361e+44	10.46	10.46	5.697e+36	6.26e-06
13465	triHPacyl.pmmmttppd	1.116e+44	10.02	10.02	5.631e+36	6.19e-06
13466	triHPacyl.mpttmtmpd	1.170e+45	11.42	11.42	5.620e+36	6.18e-06
13467	triHPacyl.tpttppmnd	6.236e+43	9.68	9.68	5.571e+36	6.12e-06
13468	triHPacyl.tpttptmpd	9.231e+44	11.28	11.28	5.552e+36	6.1e-06
13469	triHPacyl.mttppmtmpd	2.900e+44	10.60	10.60	5.538e+36	6.09e-06
13470	triHPacyl.mmttmtmmpd	2.419e+44	10.49	10.49	5.530e+36	6.08e-06
13471	triHPacyl.pmmmtttmpd	9.220e+43	9.92	9.92	5.450e+36	5.99e-06
13472	triHPacyl.mppppmmpmd	7.209e+43	9.78	9.78	5.417e+36	5.95e-06
13473	triHPacyl.mpptmtmpd	6.276e+43	9.70	9.70	5.403e+36	5.94e-06
13474	triHPacyl.ttptmtppmd	1.178e+44	10.08	10.08	5.368e+36	5.9e-06
13475	triHPacyl.tpmppptpmd	1.553e+44	10.25	10.25	5.338e+36	5.87e-06
13476	triHPacyl.mptppmpmnd	1.715e+44	10.31	10.31	5.317e+36	5.84e-06
13477	triHPacyl.mmttmppmnd	3.514e+44	10.74	10.74	5.308e+36	5.83e-06
13478	triHPacyl.pmmppppppd	1.783e+43	8.96	8.96	5.269e+36	5.79e-06
13479	triHPacyl.pmpppmmmpd	1.800e+43	8.97	8.97	5.255e+36	5.77e-06
13480	triHPacyl.tptpppppmd	1.432e+44	10.22	10.22	5.176e+36	5.69e-06
13481	triHPacyl.ttmpttppmd	4.911e+44	10.95	10.95	5.166e+36	5.68e-06
13482	triHPacyl.mmtppmtmpd	5.358e+44	11.01	11.01	5.153e+36	5.66e-06
13483	triHPacyl.mmtmttpppd	3.111e+44	10.69	10.69	5.102e+36	5.61e-06
13484	triHPacyl.tpmmpmpmd	3.576e+44	10.78	10.78	5.055e+36	5.55e-06
13485	triHPacyl.ptmtmtmnd	3.753e+43	9.43	9.43	5.047e+36	5.55e-06
13486	triHPacyl.tpttppmmnd	1.715e+44	10.34	10.34	4.996e+36	5.49e-06
13487	triHPacyl.mmpmpmtppd	2.062e+44	10.46	10.46	4.948e+36	5.44e-06
13488	triHPacyl.mppmmmtppd	3.897e+43	9.47	9.47	4.928e+36	5.42e-06
13489	triHPacyl.mtmtmmtmpd	4.644e+44	10.95	10.95	4.926e+36	5.41e-06
13490	triHPacyl.mttmtmmpd	1.083e+44	10.08	10.08	4.915e+36	5.4e-06
13491	triHPacyl.ttmptmtmnd	1.312e+44	10.20	10.20	4.896e+36	5.38e-06
13492	triHPacyl.mmmmtttmpd	3.230e+44	10.73	10.73	4.887e+36	5.37e-06
13493	triHPacyl.tmmtpptmpd	4.026e+44	10.87	10.87	4.866e+36	5.35e-06
13494	triHPacyl.tpmptttmpd	2.984e+44	10.69	10.69	4.828e+36	5.31e-06
13495	triHPacyl.pmtptttmpd	1.396e+44	10.24	10.24	4.821e+36	5.3e-06
13496	triHPacyl.mppmmmtppd	9.224e+43	10.00	10.00	4.796e+36	5.27e-06
13497	triHPacyl.mpmtppmnd	1.805e+44	10.41	10.41	4.748e+36	5.22e-06
13498	triHPacyl.ttptptppd	1.327e+44	10.22	10.22	4.739e+36	5.21e-06
13499	triHPacyl.tttmptmpd	1.042e+44	10.08	10.08	4.702e+36	5.17e-06
13500	triHPacyl.ptmppmmmmnd	8.094e+43	9.93	9.93	4.693e+36	5.16e-06
13501	triHPacyl.tpmmmtpmpd	1.616e+44	10.35	10.35	4.687e+36	5.15e-06
13502	triHPacyl.mmmmmptmnd	4.699e+45	12.36	12.36	4.641e+36	5.1e-06
13503	triHPacyl.mmmppmmmpd	4.772e+43	9.63	9.63	4.641e+36	5.1e-06
13504	triHPacyl.mppppmtmpd	4.500e+44	10.96	10.96	4.633e+36	5.09e-06
13505	triHPacyl.mttppmtppd	1.393e+44	10.27	10.27	4.608e+36	5.06e-06
13506	triHPacyl.mtmppptppd	2.404e+44	10.60	10.60	4.582e+36	5.03e-06
13507	triHPacyl.ttpmmmmmmnd	2.342e+43	9.21	9.21	4.581e+36	5.03e-06
13508	triHPacyl.tmpmtmpppd	6.447e+44	11.19	11.19	4.570e+36	5.02e-06
13509	triHPacyl.tpmtppmnd	5.111e+44	11.05	11.05	4.567e+36	5.02e-06
13510	triHPacyl.tmpmtmtmnd	3.812e+44	10.89	10.89	4.462e+36	4.9e-06
13511	triHPacyl.pmpmtmtmpd	3.314e+44	10.80	10.80	4.457e+36	4.9e-06

13512	triHPacyl.mtttmttppmd	1.881e+44	10.48	10.48	4.391e+36	4.83e-06
13513	triHPacyl.ptpmttppmd	5.960e+43	9.79	9.79	4.372e+36	4.8e-06
13514	triHPacyl.tpttpmmpd	1.825e+44	10.47	10.47	4.310e+36	4.74e-06
13515	triHPacyl.pmpmtppmd	3.773e+43	9.53	9.53	4.295e+36	4.72e-06
13516	triHPacyl.mptpnmmpmd	8.113e+43	9.99	9.99	4.267e+36	4.69e-06
13517	triHPacyl.ptttmttmd	4.299e+44	10.99	10.99	4.228e+36	4.65e-06
13518	triHPacyl.tpmpmmpd	3.386e+43	9.48	9.48	4.208e+36	4.62e-06
13519	triHPacyl.ttttpttmd	1.441e+44	10.35	10.35	4.169e+36	4.58e-06
13520	triHPacyl.pmpmmpmd	1.724e+44	10.46	10.46	4.169e+36	4.58e-06
13521	triHPacyl.tpmtppmmd	1.416e+44	10.34	10.34	4.152e+36	4.56e-06
13522	triHPacyl.pmtmmpmd	6.183e+43	9.85	9.85	4.150e+36	4.56e-06
13523	triHPacyl.mtppmmpmd	1.552e+44	10.40	10.40	4.135e+36	4.54e-06
13524	triHPacyl.tptmppppmd	3.253e+44	10.84	10.84	4.125e+36	4.53e-06
13525	triHPacyl.mmtppmmpmd	4.736e+43	9.69	9.69	4.104e+36	4.51e-06
13526	triHPacyl.pmpmmpd	2.014e+44	10.57	10.57	4.048e+36	4.45e-06
13527	triHPacyl.mptppmmpd	6.357e+43	9.88	9.88	4.035e+36	4.43e-06
13528	triHPacyl.mptppmmpd	2.789e+44	10.76	10.76	4.034e+36	4.43e-06
13529	triHPacyl.pmtmppppmd	2.416e+43	9.31	9.31	3.973e+36	4.37e-06
13530	triHPacyl.tmtppmmpd	1.337e+44	10.33	10.33	3.960e+36	4.35e-06
13531	triHPacyl.tptmpttmd	4.442e+44	11.05	11.05	3.954e+36	4.34e-06
13532	triHPacyl.mtppmtpd	1.022e+44	10.18	10.18	3.912e+36	4.3e-06
13533	triHPacyl.mmpmmpmmd	2.308e+43	9.30	9.30	3.901e+36	4.29e-06
13534	triHPacyl.ptptmtpd	2.175e+44	10.64	10.64	3.848e+36	4.23e-06
13535	triHPacyl.pmpmmtmmd	1.823e+44	10.54	10.54	3.837e+36	4.22e-06
13536	triHPacyl.ttptmtpd	1.564e+45	11.83	11.83	3.800e+36	4.18e-06
13537	triHPacyl.tttmtpppd	2.216e+44	10.66	10.66	3.800e+36	4.18e-06
13538	triHPacyl.tpmppppd	7.242e+44	11.37	11.37	3.799e+36	4.17e-06
13539	triHPacyl.pmttmmtmd	3.475e+44	10.94	10.94	3.715e+36	4.08e-06
13540	triHPacyl.mtppmmpd	1.096e+44	10.26	10.26	3.702e+36	4.07e-06
13541	triHPacyl.mppmmtmmd	3.749e+43	9.62	9.62	3.674e+36	4.04e-06
13542	triHPacyl.tptmtpd	4.322e+44	11.08	11.08	3.661e+36	4.02e-06
13543	triHPacyl.mmpmtmmd	5.585e+43	9.86	9.86	3.648e+36	4.01e-06
13544	triHPacyl.ttptppmmd	2.658e+44	10.81	10.81	3.569e+36	3.92e-06
13545	triHPacyl.pmpmttmd	5.239e+43	9.84	9.84	3.558e+36	3.91e-06
13546	triHPacyl.mtmtmtpd	3.385e+44	10.96	10.96	3.531e+36	3.88e-06
13547	triHPacyl.mmtptmtpd	1.305e+44	10.40	10.40	3.483e+36	3.83e-06
13548	triHPacyl.tpmtmmpd	3.393e+44	10.97	10.97	3.465e+36	3.81e-06
13549	triHPacyl.tppmmpmd	8.049e+43	10.12	10.12	3.419e+36	3.76e-06
13550	triHPacyl.ttmtmtpd	4.989e+44	11.21	11.21	3.398e+36	3.73e-06
13551	triHPacyl.mtmtmmtmd	6.431e+44	11.37	11.37	3.376e+36	3.71e-06
13552	triHPacyl.mttmmtmmd	1.420e+44	10.47	10.47	3.327e+36	3.66e-06
13553	triHPacyl.mptppmmpd	3.160e+44	10.95	10.95	3.322e+36	3.65e-06
13554	triHPacyl.mmpmmtmmd	1.923e+43	9.30	9.30	3.245e+36	3.57e-06
13555	triHPacyl.pppmmtmmd	2.495e+44	10.84	10.84	3.180e+36	3.49e-06
13556	triHPacyl.tptppppd	3.457e+44	11.03	11.03	3.169e+36	3.48e-06
13557	triHPacyl.mmpmtmmpd	2.598e+43	9.49	9.49	3.163e+36	3.48e-06
13558	triHPacyl.mppmtmmpd	3.621e+43	9.69	9.69	3.162e+36	3.47e-06
13559	triHPacyl.mtmtmtpd	5.565e+44	11.32	11.32	3.142e+36	3.45e-06
13560	triHPacyl.ptpmmmpd	2.225e+43	9.40	9.40	3.138e+36	3.45e-06
13561	triHPacyl.ptppmmpd	4.276e+43	9.80	9.80	3.099e+36	3.41e-06
13562	triHPacyl.mmtmtpmmd	1.673e+44	10.62	10.62	3.083e+36	3.39e-06
13563	triHPacyl.mpttmtpd	2.337e+44	10.82	10.82	3.054e+36	3.36e-06
13564	triHPacyl.tpptpmpd	4.803e+44	11.26	11.26	3.023e+36	3.32e-06
13565	triHPacyl.mmpmtpmmd	2.145e+43	9.41	9.41	2.998e+36	3.29e-06
13566	triHPacyl.tpmptmtpd	5.153e+44	11.31	11.31	2.992e+36	3.29e-06
13567	triHPacyl.mptmtpd	1.811e+44	10.68	10.68	2.989e+36	3.28e-06
13568	triHPacyl.pmpptmtpd	9.199e+43	10.28	10.28	2.968e+36	3.26e-06
13569	triHPacyl.tttppmmpd	8.262e+43	10.22	10.22	2.958e+36	3.25e-06
13570	triHPacyl.tttmtpmmd	1.158e+44	10.42	10.42	2.954e+36	3.25e-06
13571	triHPacyl.mtmmtppd	3.890e+44	11.15	11.15	2.951e+36	3.24e-06
13572	triHPacyl.tmtmtpd	7.053e+44	11.50	11.50	2.947e+36	3.24e-06
13573	triHPacyl.mmtmmpmmd	9.272e+43	10.30	10.30	2.930e+36	3.22e-06
13574	triHPacyl.mmpmmpd	3.847e+43	9.77	9.77	2.925e+36	3.21e-06
13575	triHPacyl.mttmptmmd	9.725e+43	10.33	10.33	2.922e+36	3.21e-06
13576	triHPacyl.mpttmmpd	1.785e+44	10.69	10.69	2.921e+36	3.21e-06
13577	triHPacyl.ttttpttppd	1.225e+44	10.46	10.46	2.921e+36	3.21e-06
13578	triHPacyl.mmtmmtppd	5.539e+44	11.37	11.37	2.896e+36	3.18e-06
13579	triHPacyl.mpmptmmd	2.887e+44	10.98	10.98	2.896e+36	3.18e-06
13580	triHPacyl.ptmtmmpd	5.859e+43	10.04	10.04	2.863e+36	3.15e-06
13581	triHPacyl.pmttmtpd	2.441e+44	10.89	10.89	2.858e+36	3.14e-06
13582	triHPacyl.pptmmpmmd	1.497e+44	10.60	10.60	2.858e+36	3.14e-06
13583	triHPacyl.mtppmmpmmd	3.768e+43	9.78	9.78	2.843e+36	3.12e-06

13584	triHPacyl.tmpppmtmpd	3.792e+43	9.78	9.78	2.833e+36	3.11e-06
13585	triHPacyl.mtptmpmpmd	2.356e+44	10.88	10.88	2.816e+36	3.09e-06
13586	triHPacyl.tmpmmtmpd	1.180e+44	10.47	10.47	2.793e+36	3.07e-06
13587	triHPacyl.mppmtpppd	4.797e+43	9.94	9.94	2.757e+36	3.03e-06
13588	triHPacyl.tpptppppd	2.212e+44	10.85	10.85	2.753e+36	3.02e-06
13589	triHPacyl.tpttpttmd	1.050e+45	11.78	11.78	2.749e+36	3.02e-06
13590	triHPacyl.mmtptmpd	3.966e+44	11.21	11.21	2.696e+36	2.96e-06
13591	triHPacyl.mtppmmmpd	4.234e+43	9.88	9.88	2.695e+36	2.96e-06
13592	triHPacyl.pmmtpmtmd	2.614e+43	9.59	9.59	2.692e+36	2.96e-06
13593	triHPacyl.mptmppppd	1.704e+44	10.71	10.71	2.675e+36	2.94e-06
13594	triHPacyl.mmpmtmpd	8.323e+43	10.29	10.29	2.664e+36	2.93e-06
13595	triHPacyl.mtptmpppd	1.693e+44	10.71	10.71	2.653e+36	2.92e-06
13596	triHPacyl.tpppmtppd	1.225e+44	10.52	10.52	2.646e+36	2.91e-06
13597	triHPacyl.mppmtmpmd	2.479e+44	10.95	10.95	2.626e+36	2.89e-06
13598	triHPacyl.pmpptmpd	3.222e+43	9.73	9.73	2.619e+36	2.88e-06
13599	triHPacyl.mtptmtmpd	2.120e+44	10.86	10.86	2.583e+36	2.84e-06
13600	triHPacyl.tpptppmpd	2.140e+44	10.88	10.88	2.537e+36	2.79e-06
13601	triHPacyl.mmtmpmpmd	7.100e+44	11.60	11.60	2.529e+36	2.78e-06
13602	triHPacyl.ttptpttmd	4.782e+44	11.36	11.36	2.524e+36	2.77e-06
13603	triHPacyl.ttmppmtmpd	7.994e+44	11.67	11.67	2.500e+36	2.75e-06
13604	triHPacyl.mtttmtppd	1.540e+44	10.70	10.70	2.476e+36	2.72e-06
13605	triHPacyl.tmmtmtmpd	1.221e+45	11.93	11.93	2.472e+36	2.72e-06
13606	triHPacyl.mtppmtmpd	3.013e+43	9.73	9.73	2.454e+36	2.7e-06
13607	triHPacyl.mptmpmpmd	8.623e+43	10.36	10.36	2.428e+36	2.67e-06
13608	triHPacyl.mmpmtmpmd	8.721e+43	10.37	10.37	2.422e+36	2.66e-06
13609	triHPacyl.tmpmpmpmd	3.976e+43	9.91	9.91	2.401e+36	2.64e-06
13610	triHPacyl.mppmtmpd	1.633e+44	10.76	10.76	2.383e+36	2.62e-06
13611	triHPacyl.mppmmtppd	2.494e+44	11.02	11.02	2.328e+36	2.56e-06
13612	triHPacyl.mtppmtmpd	3.360e+43	9.84	9.84	2.269e+36	2.49e-06
13613	triHPacyl.ptmpmtppd	5.832e+43	10.19	10.19	2.203e+36	2.42e-06
13614	triHPacyl.ttptppppd	3.666e+44	11.29	11.29	2.199e+36	2.42e-06
13615	triHPacyl.ttttptmpd	1.175e+44	10.61	10.61	2.196e+36	2.41e-06
13616	triHPacyl.ptmtmpmpmd	4.697e+44	11.44	11.44	2.186e+36	2.4e-06
13617	triHPacyl.tpmtptmpd	6.036e+44	11.59	11.59	2.179e+36	2.39e-06
13618	triHPacyl.mtptmtmpd	8.327e+44	11.78	11.78	2.179e+36	2.39e-06
13619	triHPacyl.mmpmpmtmpd	1.122e+44	10.59	10.59	2.160e+36	2.37e-06
13620	triHPacyl.ttmppmpmd	3.528e+44	11.28	11.28	2.156e+36	2.37e-06
13621	triHPacyl.mmtmpmpmd	2.166e+43	9.62	9.62	2.126e+36	2.34e-06
13622	triHPacyl.mptptmpd	2.231e+44	11.01	11.01	2.125e+36	2.33e-06
13623	triHPacyl.mptmtmpmd	1.482e+44	10.77	10.77	2.105e+36	2.31e-06
13624	triHPacyl.tpppmtmpd	6.123e+43	10.25	10.25	2.093e+36	2.3e-06
13625	triHPacyl.mmpmpmpmd	3.340e+43	9.89	9.89	2.080e+36	2.29e-06
13626	triHPacyl.mtppmtmpd	3.467e+44	11.30	11.30	2.046e+36	2.25e-06
13627	triHPacyl.mptmpmpmd	1.033e+44	10.58	10.58	2.029e+36	2.23e-06
13628	triHPacyl.pmpmpmpmd	6.381e+43	10.30	10.30	2.016e+36	2.22e-06
13629	triHPacyl.mptmpmpmd	2.006e+44	10.98	10.98	2.008e+36	2.21e-06
13630	triHPacyl.mmpmpmtmpd	5.663e+43	10.23	10.23	1.991e+36	2.19e-06
13631	triHPacyl.tpmtpttmd	1.298e+45	12.11	12.11	1.956e+36	2.15e-06
13632	triHPacyl.mppmtmpd	1.171e+44	10.68	10.68	1.951e+36	2.14e-06
13633	triHPacyl.ptptmtppd	2.260e+43	9.70	9.70	1.945e+36	2.14e-06
13634	triHPacyl.mmpmpmtppd	5.180e+43	10.19	10.19	1.944e+36	2.14e-06
13635	triHPacyl.mtppppmpd	3.445e+43	9.95	9.95	1.943e+36	2.14e-06
13636	triHPacyl.tmmpmpmpd	6.079e+43	10.29	10.29	1.938e+36	2.13e-06
13637	triHPacyl.ppppppppd	8.001e+43	10.46	10.46	1.932e+36	2.12e-06
13638	triHPacyl.tmtppmpmd	6.967e+44	11.75	11.75	1.932e+36	2.12e-06
13639	triHPacyl.mtptmpppd	5.575e+44	11.61	11.61	1.932e+36	2.12e-06
13640	triHPacyl.mmpmpmpmd	6.482e+43	10.34	10.34	1.909e+36	2.1e-06
13641	triHPacyl.mmtptmtmd	4.455e+44	11.49	11.49	1.899e+36	2.09e-06
13642	triHPacyl.mptmmtmpd	9.694e+43	10.59	10.59	1.868e+36	2.05e-06
13643	triHPacyl.mtptmmpmd	1.901e+44	10.99	10.99	1.866e+36	2.05e-06
13644	triHPacyl.mtmmpmpmd	5.550e+44	11.63	11.63	1.860e+36	2.04e-06
13645	triHPacyl.ttmppmtmpd	2.024e+44	11.03	11.03	1.857e+36	2.04e-06
13646	triHPacyl.mtmtmtmpd	1.553e+45	12.25	12.25	1.856e+36	2.04e-06
13647	triHPacyl.mmtmtmpd	4.533e+44	11.51	11.51	1.854e+36	2.04e-06
13648	triHPacyl.mtptmpppd	4.267e+44	11.48	11.48	1.842e+36	2.02e-06
13649	triHPacyl.mptptmpmd	2.123e+44	11.07	11.07	1.833e+36	2.01e-06
13650	triHPacyl.pmpmpmpmd	4.421e+43	10.14	10.14	1.825e+36	2.01e-06
13651	triHPacyl.tmtmpptmd	2.211e+44	11.10	11.10	1.808e+36	1.99e-06
13652	triHPacyl.mmpmpmpd	3.814e+43	10.07	10.07	1.768e+36	1.94e-06
13653	triHPacyl.mmtmtmpd	9.588e+44	11.99	11.99	1.756e+36	1.93e-06
13654	triHPacyl.ptmpmtmpd	3.046e+43	9.94	9.94	1.743e+36	1.91e-06
13655	triHPacyl.tpttppmpd	2.214e+44	11.13	11.13	1.725e+36	1.9e-06

13656	triHPacyl.tppmptmmnd	1.247e+44	10.79	10.79	1.722e+36	1.89e-06
13657	triHPacyl.pmmmtmtpmd	4.224e+43	10.16	10.16	1.689e+36	1.86e-06
13658	triHPacyl.mmmmtmtpmd	4.769e+43	10.23	10.23	1.679e+36	1.84e-06
13659	triHPacyl.pmmmpmtpmd	3.458e+43	10.04	10.04	1.671e+36	1.84e-06
13660	triHPacyl.mtptmmmpmd	3.013e+44	11.33	11.33	1.670e+36	1.83e-06
13661	triHPacyl.mpptmtmpmd	9.629e+43	10.66	10.66	1.653e+36	1.82e-06
13662	triHPacyl.ttmmpmppmd	5.752e+44	11.75	11.75	1.597e+36	1.75e-06
13663	triHPacyl.tmmppptppd	7.711e+43	10.55	10.55	1.589e+36	1.75e-06
13664	triHPacyl.mpptmmpmd	3.991e+44	11.53	11.53	1.580e+36	1.74e-06
13665	triHPacyl.mtttmtmmpd	1.245e+44	10.84	10.84	1.570e+36	1.72e-06
13666	triHPacyl.mptmmtmmpd	1.099e+45	12.15	12.15	1.546e+36	1.7e-06
13667	triHPacyl.mttmmtpppd	1.289e+44	10.88	10.88	1.540e+36	1.69e-06
13668	triHPacyl.mmpmtmtpd	1.363e+44	10.92	10.92	1.516e+36	1.67e-06
13669	triHPacyl.ttmtpmtmpd	1.178e+45	12.21	12.21	1.511e+36	1.66e-06
13670	triHPacyl.mtmptmtpmd	8.822e+44	12.04	12.04	1.504e+36	1.65e-06
13671	triHPacyl.mpttptmpd	5.234e+44	11.74	11.74	1.472e+36	1.62e-06
13672	triHPacyl.mpttmmmpd	5.730e+44	11.80	11.80	1.451e+36	1.59e-06
13673	triHPacyl.tmptppmpd	4.156e+43	10.24	10.24	1.430e+36	1.57e-06
13674	triHPacyl.mmttppmpd	2.909e+44	11.41	11.41	1.429e+36	1.57e-06
13675	triHPacyl.mppmtmpppd	4.630e+43	10.32	10.32	1.395e+36	1.53e-06
13676	triHPacyl.mmmtpppmpd	1.493e+44	11.03	11.03	1.381e+36	1.52e-06
13677	triHPacyl.tmttptmpd	6.784e+44	11.93	11.93	1.379e+36	1.52e-06
13678	triHPacyl.mmtmptmpd	9.411e+44	12.13	12.13	1.371e+36	1.51e-06
13679	triHPacyl.mpttmtmmpd	1.342e+44	10.97	10.97	1.358e+36	1.49e-06
13680	triHPacyl.mtmppmtpd	5.697e+43	10.47	10.47	1.339e+36	1.47e-06
13681	triHPacyl.mpptmtmpd	4.337e+44	11.69	11.69	1.331e+36	1.46e-06
13682	triHPacyl.ttmtpmtmnd	4.359e+44	11.69	11.69	1.324e+36	1.45e-06
13683	triHPacyl.mppmptmnd	1.300e+44	10.98	10.98	1.308e+36	1.44e-06
13684	triHPacyl.ttmtpmtpmd	8.494e+43	10.74	10.74	1.282e+36	1.41e-06
13685	triHPacyl.mpptmppmd	1.404e+44	11.05	11.05	1.259e+36	1.38e-06
13686	triHPacyl.ptppmppmd	1.295e+43	9.63	9.63	1.257e+36	1.38e-06
13687	triHPacyl.pmpmtmpppd	1.650e+44	11.15	11.15	1.242e+36	1.37e-06
13688	triHPacyl.mttmptmpd	1.100e+44	10.91	10.91	1.234e+36	1.36e-06
13689	triHPacyl.tmpmppmnd	1.347e+44	11.04	11.04	1.222e+36	1.34e-06
13690	triHPacyl.tpmtpmppmd	3.566e+44	11.62	11.62	1.217e+36	1.34e-06
13691	triHPacyl.mpttmtmnd	5.538e+44	11.89	11.89	1.210e+36	1.33e-06
13692	triHPacyl.mtmmtmmnd	3.035e+43	10.16	10.16	1.210e+36	1.33e-06
13693	triHPacyl.mmtmtpmnd	1.015e+44	10.88	10.88	1.204e+36	1.32e-06
13694	triHPacyl.ptmtmppmd	1.209e+44	10.99	10.99	1.187e+36	1.3e-06
13695	triHPacyl.ttmtpmtpmd	4.013e+43	10.34	10.34	1.182e+36	1.3e-06
13696	triHPacyl.mtttmmmmnd	1.640e+44	11.18	11.18	1.181e+36	1.3e-06
13697	triHPacyl.mtpmmpppd	1.286e+44	11.04	11.04	1.160e+36	1.27e-06
13698	triHPacyl.pmpmppppd	4.367e+43	10.40	10.40	1.155e+36	1.27e-06
13699	triHPacyl.tpmtpmpppd	6.598e+44	12.03	12.03	1.145e+36	1.26e-06
13700	triHPacyl.tpmppppmd	5.737e+43	10.57	10.57	1.143e+36	1.26e-06
13701	triHPacyl.tpptppmnd	1.859e+44	11.27	11.27	1.143e+36	1.26e-06
13702	triHPacyl.ttmtpmtpd	8.942e+44	12.21	12.21	1.138e+36	1.25e-06
13703	triHPacyl.mmtmmpmnd	1.725e+45	12.60	12.60	1.135e+36	1.25e-06
13704	triHPacyl.tpmtpmtpd	8.299e+44	12.17	12.17	1.129e+36	1.24e-06
13705	triHPacyl.ptptmmtmnd	1.764e+44	11.25	11.25	1.129e+36	1.24e-06
13706	triHPacyl.mtptmmtmpd	8.624e+44	12.19	12.19	1.127e+36	1.24e-06
13707	triHPacyl.tpmmpmtpmd	4.777e+44	11.85	11.85	1.105e+36	1.21e-06
13708	triHPacyl.mtpmptppd	7.391e+43	10.74	10.74	1.101e+36	1.21e-06
13709	triHPacyl.mpmtpppmd	9.195e+43	10.87	10.87	1.101e+36	1.21e-06
13710	triHPacyl.tmpmptppd	7.764e+43	10.77	10.77	1.101e+36	1.21e-06
13711	triHPacyl.tpppmtppd	7.073e+43	10.72	10.72	1.099e+36	1.21e-06
13712	triHPacyl.mptmmpmnd	1.473e+44	11.16	11.16	1.099e+36	1.21e-06
13713	triHPacyl.mppmmmpmnd	2.231e+44	11.41	11.41	1.096e+36	1.2e-06
13714	triHPacyl.mppmmtmmpd	5.205e+43	10.55	10.55	1.077e+36	1.18e-06
13715	triHPacyl.tpmmtmtpd	3.278e+44	11.65	11.65	1.074e+36	1.18e-06
13716	triHPacyl.mpptmmtmpd	1.967e+44	11.34	11.34	1.073e+36	1.18e-06
13717	triHPacyl.tttppmppd	1.050e+45	12.34	12.34	1.068e+36	1.17e-06
13718	triHPacyl.mttmmpmnd	1.400e+45	12.52	12.52	1.059e+36	1.16e-06
13719	triHPacyl.mpttmtmtpd	2.658e+44	11.54	11.54	1.048e+36	1.15e-06
13720	triHPacyl.ptmtmmpmnd	1.867e+44	11.33	11.33	1.048e+36	1.15e-06
13721	triHPacyl.mtttptmtpd	1.993e+44	11.37	11.37	1.043e+36	1.15e-06
13722	triHPacyl.pttmtmtpmd	1.719e+44	11.28	11.28	1.041e+36	1.14e-06
13723	triHPacyl.mppmtmmpd	1.276e+44	11.10	11.10	1.038e+36	1.14e-06
13724	triHPacyl.mmtmmtppd	3.205e+44	11.67	11.67	1.015e+36	1.12e-06
13725	triHPacyl.mppmmpmnd	1.549e+44	11.24	11.24	1.002e+36	1.1e-06
13726	triHPacyl.tmmtpmmpd	1.013e+45	12.36	12.36	1.000e+36	1.1e-06
13727	triHPacyl.mmmmtmtpmd	1.102e+44	11.04	11.04	9.951e+35	1.09e-06

13728	triHPacyl.tmptpnmmpmd	1.299e+44	11.14	11.14	9.931e+35	1.09e-06
13729	triHPacyl.pmmtnmtmpd	2.520e+45	12.91	12.91	9.915e+35	1.09e-06
13730	triHPacyl.mpttpmpmpd	6.947e+44	12.15	12.15	9.781e+35	1.07e-06
13731	triHPacyl.mmpmtmpmmpd	1.676e+44	11.31	11.31	9.654e+35	1.06e-06
13732	triHPacyl.mtptnmtmmd	3.090e+44	11.69	11.69	9.469e+35	1.04e-06
13733	triHPacyl.mmptmtmpmmd	8.201e+43	10.90	10.90	9.415e+35	1.03e-06
13734	triHPacyl.ptmpmmtmmd	2.270e+44	11.51	11.51	9.349e+35	1.03e-06
13735	triHPacyl.ttttptppmd	2.386e+45	12.91	12.91	9.343e+35	1.03e-06
13736	triHPacyl.mtttmtmpmd	2.358e+44	11.54	11.54	9.284e+35	1.02e-06
13737	triHPacyl.tptmpmmpmd	1.606e+44	11.31	11.31	9.251e+35	1.02e-06
13738	triHPacyl.mtmmtmpppd	5.937e+44	12.09	12.09	9.246e+35	1.02e-06
13739	triHPacyl.pttmmtmmpmd	2.213e+44	11.50	11.50	9.232e+35	1.01e-06
13740	triHPacyl.tpptmtmpd	5.159e+44	12.02	12.02	9.091e+35	9.99e-07
13741	triHPacyl.mmmtnmtmpd	4.959e+44	12.00	12.00	9.055e+35	9.95e-07
13742	triHPacyl.tpptpnmmpd	1.101e+44	11.10	11.10	9.008e+35	9.9e-07
13743	triHPacyl.mmpmtmpmmpd	9.849e+43	11.04	11.04	9.004e+35	9.89e-07
13744	triHPacyl.mmttmtmpmmd	3.105e+44	11.73	11.73	8.907e+35	9.79e-07
13745	triHPacyl.mpmmmmpppd	2.574e+44	11.62	11.62	8.873e+35	9.75e-07
13746	triHPacyl.pmpptmtmpd	6.386e+43	10.79	10.79	8.827e+35	9.7e-07
13747	triHPacyl.ptttmmtmmd	8.764e+44	12.35	12.35	8.774e+35	9.64e-07
13748	triHPacyl.ttttptpppd	1.009e+45	12.44	12.44	8.715e+35	9.58e-07
13749	triHPacyl.mmttmtmmd	1.362e+45	12.63	12.63	8.616e+35	9.47e-07
13750	triHPacyl.mpmmtmpmmd	4.930e+43	10.65	10.65	8.613e+35	9.46e-07
13751	triHPacyl.mmtprnmmpd	1.962e+44	11.47	11.47	8.600e+35	9.45e-07
13752	triHPacyl.mtptmtmmd	3.540e+44	11.83	11.83	8.586e+35	9.43e-07
13753	triHPacyl.ptmpnmppmd	1.709e+44	11.39	11.39	8.577e+35	9.42e-07
13754	triHPacyl.pmpptmtmpd	8.109e+43	10.95	10.95	8.559e+35	9.41e-07
13755	triHPacyl.mptmnmmpmd	1.002e+45	12.46	12.46	8.406e+35	9.24e-07
13756	triHPacyl.ptttmmtmpd	3.008e+44	11.74	11.74	8.379e+35	9.21e-07
13757	triHPacyl.mpmmmmpmd	4.346e+43	10.60	10.60	8.304e+35	9.12e-07
13758	triHPacyl.mttmpmtmmd	8.074e+43	10.97	10.97	8.240e+35	9.05e-07
13759	triHPacyl.mmpmtpppd	9.072e+43	11.05	11.05	8.123e+35	8.93e-07
13760	triHPacyl.mptmpppmd	9.165e+43	11.06	11.06	8.035e+35	8.83e-07
13761	triHPacyl.mpttmnmmpd	3.433e+44	11.85	11.85	7.999e+35	8.79e-07
13762	triHPacyl.mmpmtmtmpd	2.540e+44	11.68	11.68	7.924e+35	8.71e-07
13763	triHPacyl.tppmpmtmpd	3.703e+44	11.92	11.92	7.731e+35	8.49e-07
13764	triHPacyl.mmpmpmpmd	3.946e+43	10.58	10.58	7.708e+35	8.47e-07
13765	triHPacyl.mppmtmmtmd	7.209e+44	12.32	12.32	7.700e+35	8.46e-07
13766	triHPacyl.mmmmpnmmpd	3.156e+43	10.45	10.45	7.696e+35	8.46e-07
13767	triHPacyl.mtptmtmpd	8.220e+44	12.40	12.40	7.597e+35	8.35e-07
13768	triHPacyl.mppmtptmpd	8.131e+44	12.40	12.40	7.491e+35	8.23e-07
13769	triHPacyl.pppptpppd	1.280e+44	11.32	11.32	7.305e+35	8.03e-07
13770	triHPacyl.mpmmppppd	7.847e+43	11.03	11.03	7.224e+35	7.94e-07
13771	triHPacyl.tmttmtmmd	7.859e+44	12.41	12.41	7.210e+35	7.92e-07
13772	triHPacyl.ttptpnmppd	2.270e+44	11.67	11.67	7.108e+35	7.81e-07
13773	triHPacyl.mptmpmtmmd	2.920e+44	11.82	11.82	7.104e+35	7.81e-07
13774	triHPacyl.mpppppppd	9.734e+43	11.17	11.17	7.044e+35	7.74e-07
13775	triHPacyl.tpttpptmpd	1.741e+45	12.90	12.90	6.919e+35	7.6e-07
13776	triHPacyl.mpmtpmpmd	9.478e+43	11.17	11.17	6.915e+35	7.6e-07
13777	triHPacyl.tptmpmtmmd	1.217e+45	12.70	12.70	6.854e+35	7.53e-07
13778	triHPacyl.ttmtpptppd	6.833e+44	12.36	12.36	6.780e+35	7.45e-07
13779	triHPacyl.pmmmpmtmpd	1.294e+43	10.01	10.01	6.638e+35	7.29e-07
13780	triHPacyl.mpttppmmpd	2.283e+44	11.72	11.72	6.604e+35	7.26e-07
13781	triHPacyl.mtttmtppd	2.247e+44	11.71	11.71	6.599e+35	7.25e-07
13782	triHPacyl.mttmnmmpd	3.075e+44	11.91	11.91	6.471e+35	7.11e-07
13783	triHPacyl.mptmmpppd	2.316e+44	11.74	11.74	6.469e+35	7.11e-07
13784	triHPacyl.mppmmtmpd	3.415e+43	10.60	10.60	6.463e+35	7.1e-07
13785	triHPacyl.ptptmtmpd	5.852e+43	10.92	10.92	6.444e+35	7.08e-07
13786	triHPacyl.mpttmpppd	2.407e+44	11.78	11.78	6.279e+35	6.9e-07
13787	triHPacyl.mpttmpppd	2.930e+44	11.90	11.90	6.229e+35	6.84e-07
13788	triHPacyl.mmpmtmmpd	6.475e+43	11.01	11.01	6.220e+35	6.83e-07
13789	triHPacyl.tmmpptmpd	7.522e+43	11.10	11.10	6.183e+35	6.79e-07
13790	triHPacyl.mtmttpppd	5.445e+44	12.29	12.29	6.116e+35	6.72e-07
13791	triHPacyl.mpttmmpmd	4.699e+44	12.21	12.21	6.008e+35	6.6e-07
13792	triHPacyl.mmmprnmppd	5.094e+43	10.88	10.88	5.993e+35	6.58e-07
13793	triHPacyl.mmttmtmpd	1.838e+44	11.66	11.66	5.877e+35	6.46e-07
13794	triHPacyl.mpttmnmppd	2.782e+44	11.91	11.91	5.825e+35	6.4e-07
13795	triHPacyl.tmmpmtppd	1.207e+44	11.42	11.42	5.813e+35	6.39e-07
13796	triHPacyl.mtptmnmmd	2.311e+44	11.80	11.80	5.812e+35	6.39e-07
13797	triHPacyl.mtptmtppd	6.862e+43	11.09	11.09	5.723e+35	6.29e-07
13798	triHPacyl.pttmmtmpmd	4.672e+44	12.23	12.23	5.716e+35	6.28e-07
13799	triHPacyl.mmpmtmmpmd	6.408e+43	11.05	11.05	5.681e+35	6.24e-07

13800	triHPacyl.tmptpttmd	2.970e+45	13.34	13.34	5.653e+35	6.21e-07
13801	triHPacyl.mmmtmppmpd	1.846e+44	11.69	11.69	5.622e+35	6.18e-07
13802	triHPacyl.mmpmtptppd	2.541e+44	11.88	11.88	5.612e+35	6.17e-07
13803	triHPacyl.mttprnmpppd	7.257e+44	12.53	12.53	5.418e+35	5.95e-07
13804	triHPacyl.tpmmpptppmd	1.599e+44	11.63	11.63	5.362e+35	5.89e-07
13805	triHPacyl.tmptptpppd	8.715e+44	12.66	12.66	5.210e+35	5.72e-07
13806	triHPacyl.ttttptmpmd	1.827e+44	11.74	11.74	5.134e+35	5.64e-07
13807	triHPacyl.pmpptptppmd	3.875e+44	12.19	12.19	5.098e+35	5.6e-07
13808	triHPacyl.ttttprnmmd	1.427e+44	11.60	11.60	5.069e+35	5.57e-07
13809	triHPacyl.tmpmpmmpmd	2.877e+43	10.65	10.65	5.049e+35	5.55e-07
13810	triHPacyl.mmmppptpppd	6.465e+43	11.13	11.13	5.036e+35	5.53e-07
13811	triHPacyl.mppmtmmpd	1.887e+44	11.78	11.78	4.926e+35	5.41e-07
13812	triHPacyl.tmmppmtmpd	8.238e+43	11.30	11.30	4.856e+35	5.34e-07
13813	triHPacyl.mttmnmpppd	1.740e+44	11.78	11.78	4.561e+35	5.01e-07
13814	triHPacyl.mppmtmmpmd	1.584e+44	11.73	11.73	4.538e+35	4.99e-07
13815	triHPacyl.mmpmpmmpmd	5.499e+43	11.10	11.10	4.500e+35	4.94e-07
13816	triHPacyl.mmpmpmtmpd	2.987e+43	10.75	10.75	4.377e+35	4.81e-07
13817	triHPacyl.tmptptppmd	4.115e+44	12.32	12.32	4.368e+35	4.8e-07
13818	triHPacyl.mptmmpmpmd	2.289e+44	11.98	11.98	4.291e+35	4.72e-07
13819	triHPacyl.mmpmtmmpd	4.972e+43	11.07	11.07	4.278e+35	4.7e-07
13820	triHPacyl.mpttmmpmd	3.296e+44	12.21	12.21	4.211e+35	4.63e-07
13821	triHPacyl.mmmtmpppd	3.193e+44	12.19	12.19	4.208e+35	4.62e-07
13822	triHPacyl.tpmmpmpppd	8.352e+43	11.39	11.39	4.199e+35	4.61e-07
13823	triHPacyl.mprnmtpmmd	1.890e+44	11.89	11.89	4.108e+35	4.51e-07
13824	triHPacyl.mpttmppmd	2.425e+44	12.04	12.04	4.084e+35	4.49e-07
13825	triHPacyl.mmtmpttmd	2.977e+44	12.17	12.17	4.079e+35	4.48e-07
13826	triHPacyl.mmttmmtmpd	1.430e+45	13.11	13.11	4.034e+35	4.43e-07
13827	triHPacyl.mtttptmpd	2.110e+44	11.97	11.97	4.009e+35	4.41e-07
13828	triHPacyl.tpmtptmpd	9.585e+44	12.88	12.88	3.997e+35	4.39e-07
13829	triHPacyl.mmpmnmmpmd	2.183e+43	10.62	10.62	3.993e+35	4.39e-07
13830	triHPacyl.mppmtpppd	1.114e+44	11.61	11.61	3.893e+35	4.28e-07
13831	triHPacyl.tttmmpppd	1.961e+44	11.95	11.95	3.855e+35	4.24e-07
13832	triHPacyl.mtttmtpppd	6.565e+44	12.68	12.68	3.825e+35	4.2e-07
13833	triHPacyl.tmpmptmpd	1.152e+44	11.65	11.65	3.732e+35	4.1e-07
13834	triHPacyl.ttttptppd	1.685e+44	11.90	11.90	3.631e+35	3.99e-07
13835	triHPacyl.ttptptppd	8.719e+44	12.88	12.88	3.600e+35	3.96e-07
13836	triHPacyl.mmtmtmmpmd	2.815e+44	12.22	12.22	3.551e+35	3.9e-07
13837	triHPacyl.ptmpttmd	7.077e+43	11.40	11.40	3.488e+35	3.83e-07
13838	triHPacyl.tpmtppppd	4.092e+44	12.45	12.45	3.481e+35	3.83e-07
13839	triHPacyl.ttptmtpmd	3.033e+44	12.28	12.28	3.455e+35	3.8e-07
13840	triHPacyl.mtpmmtmpd	2.229e+44	12.10	12.10	3.400e+35	3.74e-07
13841	triHPacyl.tppmmpmpmd	1.967e+44	12.04	12.04	3.348e+35	3.68e-07
13842	triHPacyl.tmpppptmpd	1.025e+44	11.65	11.65	3.335e+35	3.66e-07
13843	triHPacyl.mpmtppppd	3.503e+43	11.01	11.01	3.317e+35	3.64e-07
13844	triHPacyl.mppmmtmpmd	2.427e+43	10.81	10.81	3.226e+35	3.55e-07
13845	triHPacyl.tpttpttmd	1.699e+45	13.35	13.35	3.191e+35	3.51e-07
13846	triHPacyl.ptmptmmd	1.606e+44	11.95	11.95	3.185e+35	3.5e-07
13847	triHPacyl.mpmmtmmpd	1.285e+44	11.82	11.82	3.142e+35	3.45e-07
13848	triHPacyl.tmptptmpd	6.568e+43	11.44	11.44	3.068e+35	3.37e-07
13849	triHPacyl.mppmtmmpmd	1.957e+44	12.10	12.10	3.017e+35	3.31e-07
13850	triHPacyl.mpmmtmmpmd	4.101e+43	11.18	11.18	2.931e+35	3.22e-07
13851	triHPacyl.ttptmmpmd	1.910e+44	12.10	12.10	2.931e+35	3.22e-07
13852	triHPacyl.mpmmtmmpmd	3.961e+43	11.16	11.16	2.918e+35	3.21e-07
13853	triHPacyl.mtttpttmd	1.576e+44	12.00	12.00	2.867e+35	3.15e-07
13854	triHPacyl.tpppmmpmd	3.934e+43	11.18	11.18	2.829e+35	3.11e-07
13855	triHPacyl.tmptptmpmd	1.199e+44	11.85	11.85	2.818e+35	3.1e-07
13856	triHPacyl.mppmmtmmd	1.836e+44	12.10	12.10	2.800e+35	3.08e-07
13857	triHPacyl.mmpmmtmpd	5.404e+44	12.75	12.75	2.783e+35	3.06e-07
13858	triHPacyl.tpmtppppd	5.334e+44	12.75	12.75	2.747e+35	3.02e-07
13859	triHPacyl.tmptpttmd	1.541e+45	13.40	13.40	2.669e+35	2.93e-07
13860	triHPacyl.tpmtpttmd	1.476e+45	13.37	13.37	2.666e+35	2.93e-07
13861	triHPacyl.mmtmmpmpmd	1.354e+44	11.96	11.96	2.631e+35	2.89e-07
13862	triHPacyl.mtmttppmd	4.142e+44	12.63	12.63	2.590e+35	2.85e-07
13863	triHPacyl.mmmtmmpmd	7.275e+44	12.98	12.98	2.565e+35	2.82e-07
13864	triHPacyl.tpmptpppd	1.791e+44	12.17	12.17	2.434e+35	2.67e-07
13865	triHPacyl.mpttmmpmd	3.097e+44	12.50	12.50	2.432e+35	2.67e-07
13866	triHPacyl.mmpmptppmd	3.045e+43	11.17	11.17	2.210e+35	2.43e-07
13867	triHPacyl.mmpmtmmpd	9.558e+43	11.86	11.86	2.195e+35	2.41e-07
13868	triHPacyl.mpttmmpmd	3.348e+44	12.61	12.61	2.176e+35	2.39e-07
13869	triHPacyl.pmpppmpmd	2.229e+43	11.00	11.00	2.164e+35	2.38e-07
13870	triHPacyl.mpmmtmmpmd	6.624e+43	11.66	11.66	2.136e+35	2.35e-07
13871	triHPacyl.mpttptppd	9.215e+44	13.23	13.23	2.122e+35	2.33e-07

13872	triHPacyl.ptttmppmpd	1.037e+44	11.93	11.93	2.115e+35	2.32e-07
13873	triHPacyl.mmttmmtmmd	2.066e+45	13.73	13.73	2.073e+35	2.28e-07
13874	triHPacyl.mppmntmmd	2.168e+43	11.03	11.03	1.991e+35	2.19e-07
13875	triHPacyl.pmntmttmd	1.014e+44	11.97	11.97	1.946e+35	2.14e-07
13876	triHPacyl.mmttmmpmpd	2.443e+44	12.50	12.50	1.929e+35	2.12e-07
13877	triHPacyl.mtppnmppd	7.304e+43	11.78	11.78	1.928e+35	2.12e-07
13878	triHPacyl.tpmtpppd	3.743e+44	12.75	12.75	1.927e+35	2.12e-07
13879	triHPacyl.mmpmmpppd	1.558e+44	12.24	12.24	1.903e+35	2.09e-07
13880	triHPacyl.ttmppttmmd	1.640e+44	12.28	12.28	1.870e+35	2.06e-07
13881	triHPacyl.mmpmtmmpmd	8.707e+43	11.90	11.90	1.868e+35	2.05e-07
13882	triHPacyl.mtpmmmmmd	5.224e+43	11.60	11.60	1.862e+35	2.05e-07
13883	triHPacyl.mpppmtppd	5.402e+43	11.63	11.63	1.825e+35	2.01e-07
13884	triHPacyl.ttttppmmmpd	1.748e+44	12.33	12.33	1.822e+35	2e-07
13885	triHPacyl.mtmtmmpppd	6.343e+44	13.10	13.10	1.821e+35	2e-07
13886	triHPacyl.mppmmtpmd	3.673e+43	11.42	11.42	1.760e+35	1.93e-07
13887	triHPacyl.ttpppmtmd	3.069e+44	12.69	12.69	1.745e+35	1.92e-07
13888	triHPacyl.mppmtmmpmd	1.698e+44	12.35	12.35	1.700e+35	1.87e-07
13889	triHPacyl.tmptptppmd	8.954e+44	13.36	13.36	1.646e+35	1.81e-07
13890	triHPacyl.mptmpmmpmd	1.558e+44	12.35	12.35	1.579e+35	1.73e-07
13891	triHPacyl.mpmmtmmtmd	1.116e+44	12.17	12.17	1.532e+35	1.68e-07
13892	triHPacyl.mtmtmmpmpd	8.499e+44	13.38	13.38	1.527e+35	1.68e-07
13893	triHPacyl.tmmpmmpppd	8.643e+43	12.03	12.03	1.491e+35	1.64e-07
13894	triHPacyl.ptmtpmtmd	2.669e+44	12.72	12.72	1.448e+35	1.59e-07
13895	triHPacyl.pmtppttmd	3.386e+44	12.88	12.88	1.395e+35	1.53e-07
13896	triHPacyl.mtttmtppmd	7.065e+44	13.33	13.33	1.385e+35	1.52e-07
13897	triHPacyl.pmpptpppd	2.313e+44	12.67	12.67	1.356e+35	1.49e-07
13898	triHPacyl.mmpmtmmpmd	6.255e+43	11.90	11.90	1.334e+35	1.47e-07
13899	triHPacyl.tmpmpttmd	1.485e+44	12.43	12.43	1.318e+35	1.45e-07
13900	triHPacyl.ttpmptpmd	8.883e+43	12.13	12.13	1.294e+35	1.42e-07
13901	triHPacyl.tmpppmtmd	8.001e+44	13.46	13.46	1.256e+35	1.38e-07
13902	triHPacyl.mppmmppmd	1.702e+44	12.54	12.54	1.246e+35	1.37e-07
13903	triHPacyl.tmppptpmd	9.281e+44	13.55	13.55	1.240e+35	1.36e-07
13904	triHPacyl.mtttmtmmd	1.912e+44	12.62	12.62	1.234e+35	1.36e-07
13905	triHPacyl.mptmmmpmd	1.596e+44	12.51	12.51	1.230e+35	1.35e-07
13906	triHPacyl.pmpmtmmpd	1.525e+43	11.12	11.12	1.210e+35	1.33e-07
13907	triHPacyl.mmpmmpppd	1.172e+44	12.34	12.34	1.195e+35	1.31e-07
13908	triHPacyl.pmpmmpmmd	5.415e+44	13.26	13.26	1.193e+35	1.31e-07
13909	triHPacyl.tmpmmpppd	5.878e+43	11.95	11.95	1.164e+35	1.28e-07
13910	triHPacyl.ttptptppmd	6.277e+44	13.39	13.39	1.111e+35	1.22e-07
13911	triHPacyl.mtttmmpppd	9.233e+44	13.62	13.62	1.098e+35	1.21e-07
13912	triHPacyl.mpmmtmmtmd	7.353e+43	12.14	12.14	1.048e+35	1.15e-07
13913	triHPacyl.tmpmmpppd	3.553e+43	11.71	11.71	1.045e+35	1.15e-07
13914	triHPacyl.mmtmpmtmd	4.448e+44	13.23	13.23	1.020e+35	1.12e-07
13915	triHPacyl.mmtmmtmmd	1.331e+44	12.53	12.53	9.954e+34	1.09e-07
13916	triHPacyl.ttttppppd	1.066e+45	13.77	13.77	9.936e+34	1.09e-07
13917	triHPacyl.tmpmptmmd	7.904e+43	12.22	12.22	9.834e+34	1.08e-07
13918	triHPacyl.mppmmmpmmd	3.100e+44	13.05	13.05	9.699e+34	1.07e-07
13919	triHPacyl.ttmtmmpppd	6.285e+44	13.47	13.47	9.596e+34	1.05e-07
13920	triHPacyl.mpmmtmtpmd	1.750e+44	12.72	12.72	9.462e+34	1.04e-07
13921	triHPacyl.ttmpptpmd	1.442e+44	12.63	12.63	9.118e+34	1e-07
13922	triHPacyl.ttpppmpppd	1.177e+44	12.53	12.53	8.719e+34	9.58e-08
13923	triHPacyl.mpppnmppd	3.281e+43	11.78	11.78	8.633e+34	9.49e-08
13924	triHPacyl.mppmmmtmmd	2.489e+44	12.99	12.99	8.620e+34	9.47e-08
13925	triHPacyl.mppmmtmmd	1.795e+43	11.42	11.42	8.601e+34	9.45e-08
13926	triHPacyl.mptmmtmmd	4.443e+44	13.34	13.34	8.503e+34	9.34e-08
13927	triHPacyl.mtpmmmtmmd	2.495e+44	13.00	13.00	8.416e+34	9.25e-08
13928	triHPacyl.ttmppmmmd	9.901e+43	12.48	12.48	8.033e+34	8.83e-08
13929	triHPacyl.ttmtmmpppd	7.128e+44	13.66	13.66	7.929e+34	8.71e-08
13930	triHPacyl.mppmmmpmmd	1.627e+44	12.79	12.79	7.796e+34	8.57e-08
13931	triHPacyl.ttppppmmd	4.749e+43	12.11	12.11	7.155e+34	7.86e-08
13932	triHPacyl.tmmpmmpmd	9.769e+43	12.55	12.55	7.068e+34	7.77e-08
13933	triHPacyl.mmttmmpmmd	2.821e+44	13.18	13.18	7.047e+34	7.74e-08
13934	triHPacyl.mppmmpmtpmd	1.387e+44	12.78	12.78	6.818e+34	7.49e-08
13935	triHPacyl.ttptmmtmmd	2.342e+44	13.12	13.12	6.464e+34	7.1e-08
13936	triHPacyl.mppmmmtmmd	5.475e+44	13.64	13.64	6.299e+34	6.92e-08
13937	triHPacyl.mtmtmmtmmd	9.343e+43	12.64	12.64	5.800e+34	6.37e-08
13938	triHPacyl.tppppmmpd	8.513e+43	12.59	12.59	5.741e+34	6.31e-08
13939	triHPacyl.mppmmmmmd	2.818e+43	11.94	11.94	5.684e+34	6.25e-08
13940	triHPacyl.tmptpmpmd	1.987e+45	14.59	14.59	4.696e+34	5.16e-08
13941	triHPacyl.mpmmtmtpmd	2.658e+44	13.39	13.39	4.667e+34	5.13e-08
13942	triHPacyl.mmpmtmmpmd	1.472e+44	13.05	13.05	4.597e+34	5.05e-08
13943	triHPacyl.tmpmptmmd	1.426e+44	13.04	13.04	4.538e+34	4.99e-08

13944	triHPacyl.mtttmmppmd	1.018e+45	14.25	14.25	4.233e+34	4.65e-08
13945	triHPacyl.tmptmpmpmd	6.653e+43	12.67	12.67	3.903e+34	4.29e-08
13946	triHPacyl.ttttppppmd	1.095e+45	14.35	14.35	3.880e+34	4.26e-08
13947	triHPacyl.tmpmptppmd	2.449e+44	13.46	13.46	3.826e+34	4.2e-08
13948	triHPacyl.pmpmmmmmpd	2.163e+43	12.02	12.02	3.821e+34	4.2e-08
13949	triHPacyl.tmppppmpmd	1.756e+44	13.27	13.27	3.754e+34	4.13e-08
13950	triHPacyl.pmppttmd	1.613e+44	13.24	13.24	3.679e+34	4.04e-08
13951	triHPacyl.tmtptmpmd	1.764e+45	14.67	14.67	3.643e+34	4e-08
13952	triHPacyl.mppmmmtmmd	3.489e+44	13.70	13.70	3.642e+34	4e-08
13953	triHPacyl.pmpmtmmd	3.150e+44	13.64	13.64	3.640e+34	4e-08
13954	triHPacyl.ttpmpmtmd	2.540e+44	13.52	13.52	3.591e+34	3.95e-08
13955	triHPacyl.mtppmmpppd	3.783e+44	13.77	13.77	3.506e+34	3.85e-08
13956	triHPacyl.mmpmtpmpd	9.894e+43	12.97	12.97	3.502e+34	3.85e-08
13957	triHPacyl.mmpmpmpmd	4.751e+43	12.59	12.59	3.212e+34	3.53e-08
13958	triHPacyl.tmtptppmd	1.217e+44	13.17	13.17	3.103e+34	3.41e-08
13959	triHPacyl.mppmtpmpd	9.504e+43	13.10	13.10	2.736e+34	3.01e-08
13960	triHPacyl.mppmtpmpd	4.121e+44	13.98	13.98	2.716e+34	2.98e-08
13961	triHPacyl.tmppmtmpd	1.314e+45	14.71	14.71	2.517e+34	2.77e-08
13962	triHPacyl.mtmtttmmd	1.780e+45	14.91	14.91	2.452e+34	2.69e-08
13963	triHPacyl.tmtptmmd	1.578e+45	14.87	14.87	2.328e+34	2.56e-08
13964	triHPacyl.mppmmmmmpd	3.982e+44	14.08	14.08	2.190e+34	2.41e-08
13965	triHPacyl.mmtmmmpmd	1.421e+44	13.48	13.48	2.164e+34	2.38e-08
13966	triHPacyl.pmppppppd	1.613e+44	13.56	13.56	2.142e+34	2.35e-08
13967	triHPacyl.ttmppmtmmd	4.659e+44	14.22	14.22	2.050e+34	2.25e-08
13968	triHPacyl.tmtptmpmd	1.576e+44	13.60	13.60	1.965e+34	2.16e-08
13969	triHPacyl.mppmmmpmd	1.534e+44	13.59	13.59	1.920e+34	2.11e-08
13970	triHPacyl.mptmmpmpd	5.125e+44	14.31	14.31	1.917e+34	2.11e-08
13971	triHPacyl.ttmppmmmpd	4.478e+43	12.89	12.89	1.815e+34	1.99e-08
13972	triHPacyl.pttmmppmmd	6.557e+43	13.14	13.14	1.769e+34	1.94e-08
13973	triHPacyl.mppmmmtmpd	7.483e+44	14.60	14.60	1.728e+34	1.9e-08
13974	triHPacyl.mppmmmpmmd	2.158e+43	12.50	12.50	1.680e+34	1.85e-08
13975	triHPacyl.tmpmpmtmmd	2.089e+44	13.89	13.89	1.585e+34	1.74e-08
13976	triHPacyl.tmppppppd	8.317e+44	14.87	14.87	1.218e+34	1.34e-08
13977	triHPacyl.mtmptppmd	6.576e+43	13.40	13.40	1.136e+34	1.25e-08
13978	triHPacyl.mppmmpppd	7.013e+43	13.47	13.47	1.077e+34	1.18e-08
13979	triHPacyl.mppppmmppd	1.272e+44	13.83	13.83	1.063e+34	1.17e-08
13980	triHPacyl.ttmppppmd	3.433e+44	14.45	14.45	1.022e+34	1.12e-08
13981	triHPacyl.mpmtppppd	1.654e+44	14.02	14.02	1.010e+34	1.11e-08
13982	triHPacyl.mppmmppmd	1.023e+44	13.76	13.76	9.701e+33	1.07e-08
13983	triHPacyl.mpmmttppd	5.832e+44	14.87	14.87	8.583e+33	9.43e-09
13984	triHPacyl.mpmtppppd	1.829e+44	14.25	14.25	7.630e+33	8.38e-09
13985	triHPacyl.mpmmtmmpd	2.574e+44	14.51	14.51	6.957e+33	7.64e-09
13986	triHPacyl.tmpppptmpd	6.167e+44	15.03	15.03	6.946e+33	7.63e-09
13987	triHPacyl.mmpmmtmpd	1.018e+44	13.99	13.99	6.544e+33	7.19e-09
13988	triHPacyl.mmpmtmmd	3.160e+45	16.11	16.11	5.765e+33	6.33e-09
13989	triHPacyl.mpmmtmmpd	4.924e+44	15.07	15.07	5.216e+33	5.73e-09
13990	triHPacyl.tmpmpppmd	3.843e+44	14.95	14.95	4.979e+33	5.47e-09
13991	triHPacyl.tmpmpmpmd	8.238e+43	14.08	14.08	4.539e+33	4.99e-09
13992	triHPacyl.pmpppmtmpd	9.372e+43	14.20	14.20	4.244e+33	4.66e-09
13993	triHPacyl.mtmppppmd	3.489e+44	15.20	15.20	2.955e+33	3.25e-09
13994	triHPacyl.mmpmmtmpd	3.045e+44	15.27	15.27	2.293e+33	2.52e-09
13995	triHPacyl.mpmmtmmmpd	3.531e+44	15.59	15.59	1.563e+33	1.72e-09
13996	triHPacyl.mppmmmtmpd	1.122e+44	15.06	15.06	1.190e+33	1.31e-09
13997	triHPacyl.mppmmtmpd	4.701e+44	16.47	16.47	4.683e+32	5.15e-10
13998	Total				9.101e+43	100

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CO elimination from (2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)

Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.triHPacyl.COelim.tmtmmmmmpd	1.681e+44	0.73	0.73	4.963e+43	6.85
TS.triHPacyl.COelim.tmtmmtmmpd	1.042e+44	0.65	0.65	3.526e+43	4.87
TS.triHPacyl.COelim.pppmtpmpd	3.494e+43	0.00	0.00	3.494e+43	4.82
TS.triHPacyl.COelim.ppppptmpd	1.136e+44	0.72	0.72	3.373e+43	4.66
TS.triHPacyl.COelim.tmtmpmmmpd	6.169e+44	1.74	1.74	3.359e+43	4.64

14016	TS.triHPacyl.COelim.pptmptmmpd	8.751e+43	0.86	0.86	2.058e+43	2.84
14017	TS.triHPacyl.COelim.pppppptpmd	1.567e+44	1.37	1.37	1.586e+43	2.19
14018	TS.triHPacyl.COelim.pppppptppd	2.109e+44	1.62	1.62	1.399e+43	1.93
14019	TS.triHPacyl.COelim.pppmptppd	4.172e+43	0.65	0.65	1.397e+43	1.93
14020	TS.triHPacyl.COelim.mmtmpmnmmpd	1.128e+44	1.28	1.28	1.326e+43	1.83
14021	TS.triHPacyl.COelim.pppmmmpmmd	1.300e+44	1.42	1.42	1.205e+43	1.66
14022	TS.triHPacyl.COelim.pppmptmmpd	1.020e+44	1.30	1.30	1.155e+43	1.59
14023	TS.triHPacyl.COelim.pptmptmmpd	1.555e+44	1.60	1.60	1.066e+43	1.47
14024	TS.triHPacyl.COelim.tmtpmmtmmd	1.673e+44	1.83	1.83	7.731e+42	1.07
14025	TS.triHPacyl.COelim.tmtpmmtmmd	1.717e+44	1.87	1.87	7.450e+42	1.03
14026	TS.triHPacyl.COelim.tmtpmmtmmd	2.234e+44	2.05	2.05	7.155e+42	0.988
14027	TS.triHPacyl.COelim.pppppptppmd	2.397e+43	0.73	0.73	7.033e+42	0.971
14028	TS.triHPacyl.COelim.pppppppmmd	3.973e+44	2.45	2.45	6.574e+42	0.908
14029	TS.triHPacyl.COelim.tmtmptmmpd	2.837e+44	2.26	2.26	6.456e+42	0.891
14030	TS.triHPacyl.COelim.tmmmmtppd	7.948e+43	1.50	1.50	6.402e+42	0.884
14031	TS.triHPacyl.COelim.pptpmtmmd	1.379e+44	1.83	1.83	6.402e+42	0.884
14032	TS.triHPacyl.COelim.tppmmmpmmd	7.176e+43	1.45	1.45	6.301e+42	0.87
14033	TS.triHPacyl.COelim.tppmmmtmmd	3.990e+43	1.12	1.12	6.074e+42	0.839
14034	TS.triHPacyl.COelim.pppmptmmpd	7.432e+43	1.50	1.50	6.051e+42	0.835
14035	TS.triHPacyl.COelim.mmtmptmmpd	1.724e+44	2.00	2.00	6.031e+42	0.833
14036	TS.triHPacyl.COelim.pppppptppd	3.540e+44	2.44	2.44	5.949e+42	0.821
14037	TS.triHPacyl.COelim.tmtmmmmmmmd	3.033e+44	2.36	2.36	5.805e+42	0.802
14038	TS.triHPacyl.COelim.pmtmmmmmpd	1.042e+44	1.73	1.73	5.694e+42	0.786
14039	TS.triHPacyl.COelim.pptpmtmmd	1.048e+44	1.75	1.75	5.597e+42	0.773
14040	TS.triHPacyl.COelim.tmtpmmtmmd	1.288e+44	1.88	1.88	5.496e+42	0.759
14041	TS.triHPacyl.COelim.tppmmmmppd	3.511e+43	1.12	1.12	5.390e+42	0.744
14042	TS.triHPacyl.COelim.tmmmmmmmpd	9.926e+43	1.80	1.80	4.843e+42	0.669
14043	TS.triHPacyl.COelim.pppmmmtmmd	1.175e+45	3.28	3.28	4.769e+42	0.659
14044	TS.triHPacyl.COelim.pptmptmmd	1.301e+44	1.99	1.99	4.646e+42	0.641
14045	TS.triHPacyl.COelim.pptmptmmd	3.081e+44	2.53	2.53	4.443e+42	0.614
14046	TS.triHPacyl.COelim.tmtmmtmmd	1.735e+44	2.19	2.19	4.432e+42	0.612
14047	TS.triHPacyl.COelim.tptmmtmmd	3.743e+44	2.65	2.65	4.384e+42	0.605
14048	TS.triHPacyl.COelim.pppmmptmmd	1.638e+44	2.16	2.16	4.366e+42	0.603
14049	TS.triHPacyl.COelim.tmtppmmmmmd	1.024e+45	3.26	3.26	4.337e+42	0.599
14050	TS.triHPacyl.COelim.tppmmmtmmd	2.273e+43	1.00	1.00	4.268e+42	0.589
14051	TS.triHPacyl.COelim.pppppptmmd	4.141e+44	2.73	2.73	4.236e+42	0.585
14052	TS.triHPacyl.COelim.mppppmmpmd	4.387e+43	1.41	1.41	4.128e+42	0.57
14053	TS.triHPacyl.COelim.mmtppmtmmd	3.408e+44	2.64	2.64	4.076e+42	0.563
14054	TS.triHPacyl.COelim.mmtmpmnmmpd	1.866e+44	2.30	2.30	3.924e+42	0.542
14055	TS.triHPacyl.COelim.ptpppmtmmd	2.067e+43	1.06	1.06	3.519e+42	0.486
14056	TS.triHPacyl.COelim.pptpmtmmd	3.588e+44	2.79	2.79	3.331e+42	0.46
14057	TS.triHPacyl.COelim.pmtmptmmpd	8.758e+43	1.96	1.96	3.271e+42	0.452
14058	TS.triHPacyl.COelim.pptppptmmd	2.111e+44	2.49	2.49	3.248e+42	0.448
14059	TS.triHPacyl.COelim.mmtppmmmmmd	1.319e+44	2.21	2.21	3.233e+42	0.446
14060	TS.triHPacyl.COelim.tmmmmmtmmd	1.531e+44	2.30	2.30	3.213e+42	0.444
14061	TS.triHPacyl.COelim.tppmmmtmmd	1.557e+44	2.33	2.33	3.121e+42	0.431
14062	TS.triHPacyl.COelim.tpppmtmmd	1.873e+44	2.44	2.44	3.104e+42	0.429
14063	TS.triHPacyl.COelim.pppmmmpmmd	9.833e+43	2.06	2.06	3.094e+42	0.427
14064	TS.triHPacyl.COelim.pppmmmtmmd	1.111e+44	2.15	2.15	3.026e+42	0.418
14065	TS.triHPacyl.COelim.tmmmmmmmpd	1.772e+44	2.43	2.43	3.000e+42	0.414
14066	TS.triHPacyl.COelim.pppmptmmd	3.177e+44	2.80	2.80	2.893e+42	0.399
14067	TS.triHPacyl.COelim.ppppmtmmd	2.043e+44	2.55	2.55	2.818e+42	0.389
14068	TS.triHPacyl.COelim.ppppmtmmd	4.605e+43	1.67	1.67	2.805e+42	0.387
14069	TS.triHPacyl.COelim.tppmmmtmmd	2.819e+44	2.76	2.76	2.754e+42	0.38
14070	TS.triHPacyl.COelim.ptpppmtmmd	1.527e+43	1.03	1.03	2.701e+42	0.373
14071	TS.triHPacyl.COelim.tmtpmmtmmd	5.096e+44	3.14	3.14	2.644e+42	0.365
14072	TS.triHPacyl.COelim.pptmptmmd	2.464e+44	2.74	2.74	2.471e+42	0.341
14073	TS.triHPacyl.COelim.pppmptppd	1.449e+44	2.43	2.43	2.452e+42	0.339
14074	TS.triHPacyl.COelim.tmtmptmmd	7.371e+44	3.43	3.43	2.336e+42	0.323
14075	TS.triHPacyl.COelim.pppmptmmd	4.467e+43	1.77	1.77	2.300e+42	0.318
14076	TS.triHPacyl.COelim.ppppppmpmd	3.513e+43	1.63	1.63	2.271e+42	0.314
14077	TS.triHPacyl.COelim.mpppppmpmd	5.981e+43	1.95	1.95	2.258e+42	0.312
14078	TS.triHPacyl.COelim.pppmptppd	3.477e+44	3.01	3.01	2.231e+42	0.308
14079	TS.triHPacyl.COelim.pptpmtmmd	2.271e+44	2.76	2.76	2.199e+42	0.304
14080	TS.triHPacyl.COelim.tmtppmtmmd	6.407e+44	3.41	3.41	2.097e+42	0.289
14081	TS.triHPacyl.COelim.pmtmptmmd	1.004e+44	2.31	2.31	2.083e+42	0.288
14082	TS.triHPacyl.COelim.ppppmtmmd	3.597e+43	1.72	1.72	2.021e+42	0.279
14083	TS.triHPacyl.COelim.tptmmtmmd	5.976e+44	3.39	3.39	2.019e+42	0.279
14084	TS.triHPacyl.COelim.tmtmptppd	3.568e+44	3.09	3.09	2.007e+42	0.277
14085	TS.triHPacyl.COelim.pptmptmmd	2.174e+44	2.80	2.80	1.991e+42	0.275
14086	TS.triHPacyl.COelim.pptmptmmd	3.705e+44	3.12	3.12	1.982e+42	0.274
14087	TS.triHPacyl.COelim.pppmmmmmpd	1.081e+44	2.40	2.40	1.944e+42	0.268

14088	TS.triHPacyl.COelim.ppmmtpppd	9.096e+43	2.30	2.30	1.931e+42	0.267
14089	TS.triHPacyl.COelim.tmtmmmtppmd	4.823e+44	3.30	3.30	1.891e+42	0.261
14090	TS.triHPacyl.COelim.pmtmmmmmmmd	1.550e+44	2.64	2.64	1.861e+42	0.257
14091	TS.triHPacyl.COelim.ptppppmmmd	1.161e+44	2.47	2.47	1.848e+42	0.255
14092	TS.triHPacyl.COelim.ttpmttppmd	2.057e+43	1.44	1.44	1.840e+42	0.254
14093	TS.triHPacyl.COelim.pppmmppmmd	6.822e+43	2.16	2.16	1.824e+42	0.252
14094	TS.triHPacyl.COelim.pppppptppmd	9.349e+43	2.35	2.35	1.815e+42	0.251
14095	TS.triHPacyl.COelim.pmpppmpmmd	1.906e+43	1.41	1.41	1.800e+42	0.248
14096	TS.triHPacyl.COelim.pptmpptppmd	4.727e+44	3.33	3.33	1.761e+42	0.243
14097	TS.triHPacyl.COelim.tmtmmtppmd	3.531e+44	3.16	3.16	1.748e+42	0.241
14098	TS.triHPacyl.COelim.tmmmmmtppmd	1.761e+44	2.78	2.78	1.668e+42	0.23
14099	TS.triHPacyl.COelim.tppmttppd	5.560e+44	3.47	3.47	1.656e+42	0.229
14100	TS.triHPacyl.COelim.pppmptppd	5.336e+44	3.46	3.46	1.617e+42	0.223
14101	TS.triHPacyl.COelim.ptppmmtpmd	2.478e+43	1.64	1.64	1.588e+42	0.219
14102	TS.triHPacyl.COelim.pptpptommd	2.569e+44	3.04	3.04	1.577e+42	0.218
14103	TS.triHPacyl.COelim.tptmmmmmpmd	2.429e+44	3.02	3.02	1.534e+42	0.212
14104	TS.triHPacyl.COelim.pmtmmtnmpd	1.120e+44	2.56	2.56	1.527e+42	0.211
14105	TS.triHPacyl.COelim.tmtmmtppd	3.278e+44	3.20	3.20	1.518e+42	0.21
14106	TS.triHPacyl.COelim.tmtmmmmppd	3.287e+44	3.21	3.21	1.508e+42	0.208
14107	TS.triHPacyl.COelim.pptmppmmmd	2.003e+44	2.93	2.93	1.475e+42	0.204
14108	TS.triHPacyl.COelim.tmpmmtmmpd	1.209e+44	2.66	2.66	1.401e+42	0.193
14109	TS.triHPacyl.COelim.pptmpptppd	1.017e+45	3.94	3.94	1.371e+42	0.189
14110	TS.triHPacyl.COelim.tmpmtnmmmd	9.668e+43	2.55	2.55	1.342e+42	0.185
14111	TS.triHPacyl.COelim.pmpmtpmmd	7.910e+43	2.44	2.44	1.324e+42	0.183
14112	TS.triHPacyl.COelim.ptmmmtppmd	2.384e+44	3.10	3.10	1.321e+42	0.182
14113	TS.triHPacyl.COelim.tpmmmtpmmd	8.741e+43	2.50	2.50	1.310e+42	0.181
14114	TS.triHPacyl.COelim.pppmptppmd	3.412e+44	3.33	3.33	1.290e+42	0.178
14115	TS.triHPacyl.COelim.pppppptmmd	3.662e+44	3.37	3.37	1.286e+42	0.178
14116	TS.triHPacyl.COelim.tmtppppmmmd	5.976e+44	3.67	3.67	1.264e+42	0.175
14117	TS.triHPacyl.COelim.tmpmmmmmmmd	1.141e+44	2.69	2.69	1.262e+42	0.174
14118	TS.triHPacyl.COelim.tmmmmmmppmd	3.285e+44	3.32	3.32	1.258e+42	0.174
14119	TS.triHPacyl.COelim.tpmppmmmpmd	8.046e+43	2.48	2.48	1.256e+42	0.173
14120	TS.triHPacyl.COelim.mmtmptmmd	2.005e+44	3.03	3.03	1.239e+42	0.171
14121	TS.triHPacyl.COelim.pmtpmmmmmmd	1.050e+44	2.66	2.66	1.216e+42	0.168
14122	TS.triHPacyl.COelim.pppmmtmmd	2.140e+44	3.10	3.10	1.189e+42	0.164
14123	TS.triHPacyl.COelim.tmtpmmmmpd	6.895e+44	3.79	3.79	1.188e+42	0.164
14124	TS.triHPacyl.COelim.mmpmpmmmpd	2.355e+44	3.17	3.17	1.162e+42	0.16
14125	TS.triHPacyl.COelim.tmpmtpmmd	9.516e+43	2.64	2.64	1.141e+42	0.158
14126	TS.triHPacyl.COelim.tppppmmpmd	1.635e+44	2.99	2.99	1.090e+42	0.151
14127	TS.triHPacyl.COelim.pptppptppd	4.344e+44	3.57	3.57	1.089e+42	0.15
14128	TS.triHPacyl.COelim.pmtmptppmd	2.147e+45	4.52	4.52	1.089e+42	0.15
14129	TS.triHPacyl.COelim.mmpmptmmpd	9.954e+43	2.70	2.70	1.074e+42	0.148
14130	TS.triHPacyl.COelim.tmtmtpmmd	4.573e+44	3.61	3.61	1.073e+42	0.148
14131	TS.triHPacyl.COelim.tptmmtppmd	4.454e+44	3.60	3.60	1.065e+42	0.147
14132	TS.triHPacyl.COelim.mppppmmmmmd	3.313e+43	2.05	2.05	1.065e+42	0.147
14133	TS.triHPacyl.COelim.pppppptppd	2.830e+44	3.35	3.35	1.034e+42	0.143
14134	TS.triHPacyl.COelim.pppmptmmpd	1.845e+44	3.11	3.11	1.003e+42	0.139
14135	TS.triHPacyl.COelim.pppppppmmd	9.741e+43	2.73	2.73	9.947e+41	0.137
14136	TS.triHPacyl.COelim.tmtppptppd	6.061e+44	3.84	3.84	9.688e+41	0.134
14137	TS.triHPacyl.COelim.tmpmmmmmpd	1.899e+44	3.15	3.15	9.670e+41	0.134
14138	TS.triHPacyl.COelim.pppppppmmd	1.889e+44	3.15	3.15	9.549e+41	0.132
14139	TS.triHPacyl.COelim.tptmmmpmmd	1.534e+44	3.04	3.04	9.435e+41	0.13
14140	TS.triHPacyl.COelim.ptppmmmpmd	3.807e+43	2.21	2.21	9.365e+41	0.129
14141	TS.triHPacyl.COelim.pptmptppd	5.133e+43	2.39	2.39	9.359e+41	0.129
14142	TS.triHPacyl.COelim.mppppmtpd	1.294e+44	2.94	2.94	9.333e+41	0.129
14143	TS.triHPacyl.COelim.pppppppppd	1.818e+44	3.16	3.16	9.052e+41	0.125
14144	TS.triHPacyl.COelim.pppmptmmd	5.142e+43	2.41	2.41	9.003e+41	0.124
14145	TS.triHPacyl.COelim.tmtmptppd	1.290e+45	4.36	4.36	8.632e+41	0.119
14146	TS.triHPacyl.COelim.pppppptppd	2.343e+43	1.97	1.97	8.580e+41	0.118
14147	TS.triHPacyl.COelim.ppppptommd	1.860e+44	3.25	3.25	7.953e+41	0.11
14148	TS.triHPacyl.COelim.mppppptppd	3.485e+44	3.65	3.65	7.654e+41	0.106
14149	TS.triHPacyl.COelim.tmtmtpmmd	1.119e+45	4.35	4.35	7.587e+41	0.105
14150	TS.triHPacyl.COelim.pptppmmmpd	3.096e+44	3.60	3.60	7.380e+41	0.102
14151	TS.triHPacyl.COelim.tmtmptppd	1.172e+45	4.41	4.41	7.242e+41	0.1
14152	TS.triHPacyl.COelim.tmtmptmmd	4.630e+44	3.85	3.85	7.230e+41	0.0998
14153	TS.triHPacyl.COelim.tmmmmtppd	1.901e+44	3.32	3.32	7.198e+41	0.0994
14154	TS.triHPacyl.COelim.tppmmmmppd	3.199e+43	2.26	2.26	7.178e+41	0.0991
14155	TS.triHPacyl.COelim.tmtmtpmmd	1.404e+45	4.52	4.52	7.104e+41	0.0981
14156	TS.triHPacyl.COelim.tptmtnmmmd	2.745e+44	3.57	3.57	6.891e+41	0.0951
14157	TS.triHPacyl.COelim.pmtppmmd	6.487e+43	2.72	2.72	6.763e+41	0.0934
14158	TS.triHPacyl.COelim.mmtppmmmpd	2.894e+44	3.61	3.61	6.734e+41	0.093
14159	TS.triHPacyl.COelim.pppmptppmd	1.096e+44	3.05	3.05	6.603e+41	0.0912

14160	TS.triHPacyl.COelim.pppppppmpd	4.677e+43	2.55	2.55	6.523e+41	0.0901
14161	TS.triHPacyl.COelim.ppttpttpmd	5.384e+44	4.01	4.01	6.458e+41	0.0892
14162	TS.triHPacyl.COelim.tptmmtmmmd	3.902e+44	3.82	3.82	6.432e+41	0.0888
14163	TS.triHPacyl.COelim.pmpptpmpd	7.947e+43	2.88	2.88	6.392e+41	0.0883
14164	TS.triHPacyl.COelim.tptmmtppmd	6.348e+44	4.12	4.12	6.303e+41	0.087
14165	TS.triHPacyl.COelim.tmtppmmmpd	2.376e+45	4.91	4.91	6.287e+41	0.0868
14166	TS.triHPacyl.COelim.tmmmmmpmpd	2.568e+44	3.59	3.59	6.265e+41	0.0865
14167	TS.triHPacyl.COelim.tpppmmtppd	3.808e+44	3.82	3.82	6.255e+41	0.0864
14168	TS.triHPacyl.COelim.tmtpmtmpmd	3.031e+44	3.69	3.69	6.207e+41	0.0857
14169	TS.triHPacyl.COelim.ptmmpptmpd	1.858e+44	3.41	3.41	6.081e+41	0.084
14170	TS.triHPacyl.COelim.pppmpptppd	3.644e+44	3.83	3.83	5.935e+41	0.0819
14171	TS.triHPacyl.COelim.tmmmtmmmd	3.533e+44	3.81	3.81	5.930e+41	0.0819
14172	TS.triHPacyl.COelim.mppppptpmd	9.397e+43	3.03	3.03	5.856e+41	0.0809
14173	TS.triHPacyl.COelim.tppmmmpmd	7.025e+43	2.86	2.86	5.809e+41	0.0802
14174	TS.triHPacyl.COelim.tmtppptpmd	2.272e+45	4.94	4.94	5.756e+41	0.0795
14175	TS.triHPacyl.COelim.tmmmmmtppd	1.892e+44	3.47	3.47	5.639e+41	0.0779
14176	TS.triHPacyl.COelim.tppppptpmd	3.091e+44	3.76	3.76	5.638e+41	0.0779
14177	TS.triHPacyl.COelim.pmmmpmtppd	5.716e+43	2.75	2.75	5.638e+41	0.0778
14178	TS.triHPacyl.COelim.tmmmmmpmpd	2.595e+44	3.67	3.67	5.497e+41	0.0759
14179	TS.triHPacyl.COelim.pptppppmpd	5.480e+44	4.13	4.13	5.386e+41	0.0744
14180	TS.triHPacyl.COelim.ptmmmmmpmd	2.248e+44	3.60	3.60	5.377e+41	0.0742
14181	TS.triHPacyl.COelim.tppmpmpmpd	4.458e+44	4.01	4.01	5.370e+41	0.0741
14182	TS.triHPacyl.COelim.tmmmtmpmd	3.276e+44	3.83	3.83	5.316e+41	0.0734
14183	TS.triHPacyl.COelim.tptmmttppd	7.379e+44	4.32	4.32	5.218e+41	0.072
14184	TS.triHPacyl.COelim.pmmmpmtmpd	1.671e+44	3.44	3.44	5.209e+41	0.0719
14185	TS.triHPacyl.COelim.pmpmmmmmpd	1.604e+44	3.42	3.42	5.152e+41	0.0711
14186	TS.triHPacyl.COelim.mmtppptmpd	4.814e+44	4.08	4.08	5.096e+41	0.0704
14187	TS.triHPacyl.COelim.tpppmtmpmd	7.515e+43	2.98	2.98	5.093e+41	0.0703
14188	TS.triHPacyl.COelim.tmtppmmmpd	2.817e+44	3.77	3.77	5.053e+41	0.0698
14189	TS.triHPacyl.COelim.tptpmttppd	9.643e+44	4.50	4.50	5.049e+41	0.0697
14190	TS.triHPacyl.COelim.pppmmmpmpd	1.015e+45	4.54	4.54	5.021e+41	0.0693
14191	TS.triHPacyl.COelim.tpppmtmpmd	4.701e+43	2.71	2.71	4.983e+41	0.0688
14192	TS.triHPacyl.COelim.pppppppmpd	1.907e+44	3.58	3.58	4.733e+41	0.0653
14193	TS.triHPacyl.COelim.pptmpmpmpd	4.010e+43	2.65	2.65	4.688e+41	0.0647
14194	TS.triHPacyl.COelim.pmtppptpmd	1.249e+44	3.33	3.33	4.646e+41	0.0641
14195	TS.triHPacyl.COelim.ppppmtmpd	1.804e+44	3.56	3.56	4.625e+41	0.0639
14196	TS.triHPacyl.COelim.pppppptmpd	1.575e+44	3.49	3.49	4.534e+41	0.0626
14197	TS.triHPacyl.COelim.pmpppptpmd	2.846e+43	2.47	2.47	4.522e+41	0.0624
14198	TS.triHPacyl.COelim.tmmmtttmpd	1.694e+44	3.54	3.54	4.464e+41	0.0616
14199	TS.triHPacyl.COelim.pmtmptmmmd	1.432e+44	3.45	3.45	4.422e+41	0.0611
14200	TS.triHPacyl.COelim.mppppptmmmd	3.654e+43	2.64	2.64	4.356e+41	0.0601
14201	TS.triHPacyl.COelim.pmpmmmtmmd	1.221e+44	3.37	3.37	4.259e+41	0.0588
14202	TS.triHPacyl.COelim.tmmmmmtmpd	2.005e+44	3.68	3.68	4.180e+41	0.0577
14203	TS.triHPacyl.COelim.pptpptpppd	4.702e+44	4.19	4.19	4.174e+41	0.0576
14204	TS.triHPacyl.COelim.tptmmmmppd	4.938e+43	2.85	2.85	4.159e+41	0.0574
14205	TS.triHPacyl.COelim.ptppmptpmd	2.396e+43	2.43	2.43	4.070e+41	0.0562
14206	TS.triHPacyl.COelim.pppmpmpppd	9.338e+43	3.25	3.25	3.994e+41	0.0552
14207	TS.triHPacyl.COelim.mmpmtmmmd	2.172e+44	3.77	3.77	3.866e+41	0.0534
14208	TS.triHPacyl.COelim.tpppmtmmmd	3.237e+44	4.01	4.01	3.855e+41	0.0532
14209	TS.triHPacyl.COelim.pmtppmmmpd	1.977e+44	3.73	3.73	3.820e+41	0.0527
14210	TS.triHPacyl.COelim.pmpmmmtppd	1.215e+44	3.44	3.44	3.794e+41	0.0524
14211	TS.triHPacyl.COelim.pppmpmpmpd	7.923e+43	3.20	3.20	3.714e+41	0.0513
14212	TS.triHPacyl.COelim.pptpptpmpd	1.502e+45	4.95	4.95	3.710e+41	0.0512
14213	TS.triHPacyl.COelim.pptmptpppd	1.288e+44	3.50	3.50	3.638e+41	0.0502
14214	TS.triHPacyl.COelim.tmttmttppd	6.072e+44	4.43	4.43	3.583e+41	0.0495
14215	TS.triHPacyl.COelim.tppmmmpmpd	4.097e+43	2.85	2.85	3.424e+41	0.0473
14216	TS.triHPacyl.COelim.mmpptppmpd	1.591e+44	3.67	3.67	3.351e+41	0.0463
14217	TS.triHPacyl.COelim.tmmmpmmmpd	4.093e+44	4.24	4.24	3.349e+41	0.0462
14218	TS.triHPacyl.COelim.tmttmttppd	5.387e+44	4.40	4.40	3.336e+41	0.0461
14219	TS.triHPacyl.COelim.tmmmmtpppd	1.734e+44	3.73	3.73	3.303e+41	0.0456
14220	TS.triHPacyl.COelim.pptppptmmd	2.878e+44	4.04	4.04	3.266e+41	0.0451
14221	TS.triHPacyl.COelim.tppmptmpmd	1.225e+44	3.53	3.53	3.262e+41	0.045
14222	TS.triHPacyl.COelim.pmtppmtppd	1.490e+44	3.65	3.65	3.262e+41	0.045
14223	TS.triHPacyl.COelim.pppmmtmpd	4.981e+44	4.37	4.37	3.247e+41	0.0448
14224	TS.triHPacyl.COelim.pptpptppmd	8.898e+44	4.72	4.72	3.245e+41	0.0448
14225	TS.triHPacyl.COelim.pppmptmpd	1.631e+44	3.72	3.72	3.200e+41	0.0442
14226	TS.triHPacyl.COelim.pppppptppd	2.958e+44	4.07	4.07	3.181e+41	0.0439
14227	TS.triHPacyl.COelim.pmtmppppmd	6.338e+44	4.54	4.54	3.099e+41	0.0428
14228	TS.triHPacyl.COelim.mppmpmmppd	9.388e+43	3.41	3.41	3.098e+41	0.0428
14229	TS.triHPacyl.COelim.mppmmmmmmmd	9.708e+43	3.43	3.43	3.098e+41	0.0428
14230	TS.triHPacyl.COelim.ppttptmmd	2.980e+44	4.10	4.10	3.086e+41	0.0426
14231	TS.triHPacyl.COelim.tppmptmpmd	2.883e+43	2.71	2.71	3.057e+41	0.0422

14232	TS.triHPacyl.COelim.pppmmmmmd	2.273e+44	3.95	3.95	3.012e+41	0.0416
14233	TS.triHPacyl.COelim.pttpptpmmd	7.606e+43	3.30	3.30	2.987e+41	0.0412
14234	TS.triHPacyl.COelim.tptpmtmmpd	6.978e+44	4.63	4.63	2.953e+41	0.0408
14235	TS.triHPacyl.COelim.pppmmpppmd	1.498e+44	3.71	3.71	2.951e+41	0.0407
14236	TS.triHPacyl.COelim.ppppptompd	9.262e+44	4.80	4.80	2.939e+41	0.0406
14237	TS.triHPacyl.COelim.tmmmmmmmd	3.786e+44	4.27	4.27	2.915e+41	0.0402
14238	TS.triHPacyl.COelim.tmmmmpppd	1.238e+44	3.61	3.61	2.908e+41	0.0401
14239	TS.triHPacyl.COelim.pppmttmmd	1.091e+44	3.54	3.54	2.869e+41	0.0396
14240	TS.triHPacyl.COelim.tpmmttmmd	3.168e+44	4.19	4.19	2.825e+41	0.039
14241	TS.triHPacyl.COelim.tmpmmppmd	3.624e+43	2.90	2.90	2.810e+41	0.0388
14242	TS.triHPacyl.COelim.tmtptpppd	1.322e+45	5.05	5.05	2.764e+41	0.0382
14243	TS.triHPacyl.COelim.tppmmmtmd	4.730e+44	4.45	4.45	2.731e+41	0.0377
14244	TS.triHPacyl.COelim.ppmmttmmd	3.483e+44	4.27	4.27	2.717e+41	0.0375
14245	TS.triHPacyl.COelim.ppmmtmmpmd	6.353e+44	4.62	4.62	2.717e+41	0.0375
14246	TS.triHPacyl.COelim.tptmmmtmpd	8.828e+44	4.82	4.82	2.707e+41	0.0374
14247	TS.triHPacyl.COelim.tptmmttmmd	1.842e+44	3.89	3.89	2.693e+41	0.0372
14248	TS.triHPacyl.COelim.pptpmmpmpd	3.923e+44	4.34	4.34	2.692e+41	0.0372
14249	TS.triHPacyl.COelim.pppppptmmd	3.600e+44	4.30	4.30	2.661e+41	0.0367
14250	TS.triHPacyl.COelim.tmpmpmmmpd	2.684e+44	4.12	4.12	2.660e+41	0.0367
14251	TS.triHPacyl.COelim.pppmmpppmd	1.014e+44	3.54	3.54	2.654e+41	0.0366
14252	TS.triHPacyl.COelim.tmmmmppmd	4.031e+44	4.38	4.38	2.590e+41	0.0358
14253	TS.triHPacyl.COelim.tmtppptppd	9.823e+44	4.91	4.91	2.588e+41	0.0357
14254	TS.triHPacyl.COelim.pmmmpmmppd	5.068e+43	3.15	3.15	2.582e+41	0.0356
14255	TS.triHPacyl.COelim.mmpmpmtppd	3.712e+44	4.34	4.34	2.572e+41	0.0355
14256	TS.triHPacyl.COelim.tmpmmmmmpd	2.054e+44	3.99	3.99	2.566e+41	0.0354
14257	TS.triHPacyl.COelim.pmmmmppmmmd	3.595e+44	4.32	4.32	2.555e+41	0.0353
14258	TS.triHPacyl.COelim.tmtpttmmd	2.663e+44	4.15	4.15	2.544e+41	0.0351
14259	TS.triHPacyl.COelim.tptpmttmmd	1.200e+44	3.67	3.67	2.543e+41	0.0351
14260	TS.triHPacyl.COelim.tptmmtmmpd	7.525e+43	3.40	3.40	2.522e+41	0.0348
14261	TS.triHPacyl.COelim.pptpmmpmmd	3.088e+44	4.25	4.25	2.475e+41	0.0342
14262	TS.triHPacyl.COelim.tmtpmmtmmd	2.675e+44	4.17	4.17	2.456e+41	0.0339
14263	TS.triHPacyl.COelim.pppmmpppmd	3.214e+44	4.28	4.28	2.452e+41	0.0339
14264	TS.triHPacyl.COelim.tptmptmmpd	3.328e+44	4.31	4.31	2.428e+41	0.0335
14265	TS.triHPacyl.COelim.pmtppmmmmmd	6.869e+43	3.37	3.37	2.427e+41	0.0335
14266	TS.triHPacyl.COelim.tptmmmtpmmd	7.251e+44	4.78	4.78	2.391e+41	0.033
14267	TS.triHPacyl.COelim.tpmppppmmd	2.251e+44	4.08	4.08	2.386e+41	0.0329
14268	TS.triHPacyl.COelim.tppmtmmpmd	2.580e+44	4.17	4.17	2.382e+41	0.0329
14269	TS.triHPacyl.COelim.tptpmmmmmmd	1.803e+44	3.95	3.95	2.377e+41	0.0328
14270	TS.triHPacyl.COelim.pptmptppmd	1.614e+45	5.26	5.26	2.376e+41	0.0328
14271	TS.triHPacyl.COelim.tptmppmmpd	7.436e+44	4.80	4.80	2.364e+41	0.0326
14272	TS.triHPacyl.COelim.tpmpttmmd	2.675e+44	4.20	4.20	2.340e+41	0.0323
14273	TS.triHPacyl.COelim.tmmptmmpd	5.704e+44	4.65	4.65	2.319e+41	0.032
14274	TS.triHPacyl.COelim.pmtppptppd	3.592e+44	4.38	4.38	2.314e+41	0.032
14275	TS.triHPacyl.COelim.tmtmmmmmpd	2.542e+45	5.55	5.55	2.294e+41	0.0317
14276	TS.triHPacyl.COelim.pppmmmpmpmd	4.006e+44	4.46	4.46	2.272e+41	0.0314
14277	TS.triHPacyl.COelim.ppmmtmmtmmd	1.686e+45	5.31	5.31	2.265e+41	0.0313
14278	TS.triHPacyl.COelim.ptmmpmmmpd	2.566e+44	4.21	4.21	2.198e+41	0.0303
14279	TS.triHPacyl.COelim.tmtmmmmmmmd	1.311e+45	5.19	5.19	2.180e+41	0.0301
14280	TS.triHPacyl.COelim.pppmptppmd	1.226e+44	3.78	3.78	2.179e+41	0.0301
14281	TS.triHPacyl.COelim.tpmmmmtmmd	3.718e+44	4.44	4.44	2.162e+41	0.0298
14282	TS.triHPacyl.COelim.tmtpppmmpd	1.690e+45	5.35	5.35	2.155e+41	0.0297
14283	TS.triHPacyl.COelim.tmtmmmtmpd	4.038e+44	4.50	4.50	2.143e+41	0.0296
14284	TS.triHPacyl.COelim.tmmmtmmpmd	1.249e+44	3.80	3.80	2.142e+41	0.0296
14285	TS.triHPacyl.COelim.ptppmpmmd	4.332e+43	3.17	3.17	2.115e+41	0.0292
14286	TS.triHPacyl.COelim.mmpmpmpmpd	6.601e+43	3.44	3.44	2.061e+41	0.0285
14287	TS.triHPacyl.COelim.tptmmpmmd	3.069e+44	4.36	4.36	2.049e+41	0.0283
14288	TS.triHPacyl.COelim.tptpmtmmpd	8.093e+44	4.94	4.94	2.035e+41	0.0281
14289	TS.triHPacyl.COelim.pptmpppppd	2.396e+44	4.22	4.22	2.030e+41	0.028
14290	TS.triHPacyl.COelim.pptppppmpd	9.400e+44	5.03	5.03	2.028e+41	0.028
14291	TS.triHPacyl.COelim.ppttpptpmd	6.638e+44	4.83	4.83	2.022e+41	0.0279
14292	TS.triHPacyl.COelim.tpmmtpppd	1.201e+44	3.81	3.81	2.014e+41	0.0278
14293	TS.triHPacyl.COelim.tpmmttppd	3.918e+44	4.52	4.52	1.990e+41	0.0275
14294	TS.triHPacyl.COelim.pptpptompd	5.088e+44	4.69	4.69	1.940e+41	0.0268
14295	TS.triHPacyl.COelim.ppmmtmmpd	9.675e+44	5.09	5.09	1.899e+41	0.0262
14296	TS.triHPacyl.COelim.pptpppppmd	1.795e+45	5.46	5.46	1.896e+41	0.0262
14297	TS.triHPacyl.COelim.pptpptompd	6.307e+44	4.84	4.84	1.892e+41	0.0261
14298	TS.triHPacyl.COelim.tmmptmmpmd	2.917e+44	4.38	4.38	1.869e+41	0.0258
14299	TS.triHPacyl.COelim.ptmptmmpd	6.989e+43	3.53	3.53	1.863e+41	0.0257
14300	TS.triHPacyl.COelim.pmtmmmmppd	1.880e+44	4.13	4.13	1.857e+41	0.0256
14301	TS.triHPacyl.COelim.tppmtppmd	2.571e+44	4.32	4.32	1.826e+41	0.0252
14302	TS.triHPacyl.COelim.tptmmmmmmmd	2.958e+44	4.41	4.41	1.813e+41	0.025
14303	TS.triHPacyl.COelim.tmmmtpmmd	2.402e+44	4.29	4.29	1.797e+41	0.0248

14304	TS.triHPacyl.COelim.pttpptpmd	5.822e+43	3.45	3.45	1.796e+41	0.0248
14305	TS.triHPacyl.COelim.pmtmptmppd	1.513e+44	4.02	4.02	1.783e+41	0.0246
14306	TS.triHPacyl.COelim.tptpnmnmmd	5.265e+44	4.77	4.77	1.773e+41	0.0245
14307	TS.triHPacyl.COelim.tmtmtmnmmd	8.316e+44	5.04	5.04	1.766e+41	0.0244
14308	TS.triHPacyl.COelim.ppmtmmpmmd	4.558e+44	4.69	4.69	1.755e+41	0.0242
14309	TS.triHPacyl.COelim.ppptpmpmd	5.033e+44	4.75	4.75	1.748e+41	0.0241
14310	TS.triHPacyl.COelim.mmppppmtmd	2.951e+44	4.43	4.43	1.743e+41	0.0241
14311	TS.triHPacyl.COelim.tpmmmmtmpd	4.787e+44	4.72	4.72	1.743e+41	0.0241
14312	TS.triHPacyl.COelim.ppptpppmd	6.090e+44	4.87	4.87	1.734e+41	0.0239
14313	TS.triHPacyl.COelim.pmpmtmmpd	1.879e+44	4.17	4.17	1.729e+41	0.0239
14314	TS.triHPacyl.COelim.tmpppmtmpd	7.559e+44	5.00	5.00	1.728e+41	0.0239
14315	TS.triHPacyl.COelim.pptpppppd	7.706e+44	5.02	5.02	1.701e+41	0.0235
14316	TS.triHPacyl.COelim.tptpnmnmmd	7.309e+44	4.99	4.99	1.688e+41	0.0233
14317	TS.triHPacyl.COelim.tmpmtmmpd	1.213e+44	3.93	3.93	1.674e+41	0.0231
14318	TS.triHPacyl.COelim.pppmpmnmmd	4.433e+44	4.70	4.70	1.668e+41	0.0231
14319	TS.triHPacyl.COelim.pmtpnmmpmd	1.011e+45	5.20	5.20	1.648e+41	0.0228
14320	TS.triHPacyl.COelim.pmmmtmpmd	1.094e+45	5.25	5.25	1.642e+41	0.0227
14321	TS.triHPacyl.COelim.tttmmmpmd	1.290e+44	3.98	3.98	1.640e+41	0.0226
14322	TS.triHPacyl.COelim.ppppppmpd	4.672e+44	4.75	4.75	1.632e+41	0.0225
14323	TS.triHPacyl.COelim.tmtmtmmpd	1.152e+45	5.29	5.29	1.617e+41	0.0223
14324	TS.triHPacyl.COelim.ptpmpptpd	1.990e+43	2.87	2.87	1.608e+41	0.0222
14325	TS.triHPacyl.COelim.tttmmmmmpd	5.864e+43	3.52	3.52	1.594e+41	0.0222
14326	TS.triHPacyl.COelim.tpmmpmtppd	6.315e+43	3.57	3.57	1.588e+41	0.0219
14327	TS.triHPacyl.COelim.pmtmtmmd	3.373e+44	4.57	4.57	1.578e+41	0.0218
14328	TS.triHPacyl.COelim.pmpmpmpmd	2.022e+44	4.27	4.27	1.572e+41	0.0217
14329	TS.triHPacyl.COelim.tmtmtmmpd	3.317e+44	4.56	4.56	1.571e+41	0.0217
14330	TS.triHPacyl.COelim.pmtmmtmppd	4.137e+44	4.70	4.70	1.559e+41	0.0215
14331	TS.triHPacyl.COelim.pmtppmtppd	4.276e+44	4.72	4.72	1.551e+41	0.0214
14332	TS.triHPacyl.COelim.tttmmmmppd	8.555e+43	3.77	3.77	1.544e+41	0.0213
14333	TS.triHPacyl.COelim.tpmptmnmmd	3.095e+44	4.54	4.54	1.521e+41	0.0211
14334	TS.triHPacyl.COelim.pmpmpppmd	4.759e+43	3.43	3.43	1.511e+41	0.0209
14335	TS.triHPacyl.COelim.tmpmnmmpmd	3.698e+44	4.65	4.65	1.509e+41	0.0208
14336	TS.triHPacyl.COelim.tmtmmmpmd	3.933e+44	4.69	4.69	1.507e+41	0.0208
14337	TS.triHPacyl.COelim.pmtmpptpmd	5.421e+44	4.88	4.88	1.503e+41	0.0207
14338	TS.triHPacyl.COelim.tmpmtmmpd	4.994e+44	4.83	4.83	1.502e+41	0.0207
14339	TS.triHPacyl.COelim.pppmptpmd	1.765e+44	4.22	4.22	1.487e+41	0.0205
14340	TS.triHPacyl.COelim.tttpnmtpmd	7.362e+43	3.70	3.70	1.477e+41	0.0204
14341	TS.triHPacyl.COelim.tmtmtmmpd	8.670e+44	5.18	5.18	1.468e+41	0.0203
14342	TS.triHPacyl.COelim.pttpptmmd	6.147e+43	3.60	3.60	1.461e+41	0.0202
14343	TS.triHPacyl.COelim.tmmpmtmnmmd	4.496e+44	4.79	4.79	1.458e+41	0.0201
14344	TS.triHPacyl.COelim.pttmtmmpd	5.554e+43	3.56	3.56	1.428e+41	0.0197
14345	TS.triHPacyl.COelim.ttpnmmtmmd	8.449e+43	3.81	3.81	1.423e+41	0.0196
14346	TS.triHPacyl.COelim.pptpmtmpmd	6.466e+43	3.66	3.66	1.390e+41	0.0192
14347	TS.triHPacyl.COelim.ppppmtmmd	7.571e+44	5.13	5.13	1.383e+41	0.0191
14348	TS.triHPacyl.COelim.pmmptmmpd	1.352e+44	4.11	4.11	1.380e+41	0.0191
14349	TS.triHPacyl.COelim.ptppptmmd	6.828e+43	3.70	3.70	1.379e+41	0.0191
14350	TS.triHPacyl.COelim.tttpmtpmd	6.117e+43	3.64	3.64	1.369e+41	0.0189
14351	TS.triHPacyl.COelim.mpmmpmpmpd	7.034e+43	3.72	3.72	1.364e+41	0.0188
14352	TS.triHPacyl.COelim.pmpmmpmpd	1.330e+44	4.11	4.11	1.353e+41	0.0187
14353	TS.triHPacyl.COelim.pmpmmpmnmmd	1.117e+44	4.01	4.01	1.350e+41	0.0186
14354	TS.triHPacyl.COelim.ptppptpmd	5.135e+43	3.55	3.55	1.332e+41	0.0184
14355	TS.triHPacyl.COelim.pptpmpmnmmd	4.974e+44	4.90	4.90	1.330e+41	0.0184
14356	TS.triHPacyl.COelim.pttpptpmd	4.771e+43	3.51	3.51	1.325e+41	0.0183
14357	TS.triHPacyl.COelim.pmtpmtmpmd	9.570e+44	5.30	5.30	1.313e+41	0.0181
14358	TS.triHPacyl.COelim.tmtpnmpppd	1.003e+45	5.33	5.33	1.309e+41	0.0181
14359	TS.triHPacyl.COelim.tmtmtpmpd	4.598e+44	4.87	4.87	1.308e+41	0.0181
14360	TS.triHPacyl.COelim.pptpmtppd	1.720e+44	4.28	4.28	1.308e+41	0.0181
14361	TS.triHPacyl.COelim.ptpppmtmd	9.892e+43	3.95	3.95	1.304e+41	0.0181
14362	TS.triHPacyl.COelim.pppmpppmmd	4.023e+44	4.80	4.80	1.293e+41	0.0178
14363	TS.triHPacyl.COelim.pmtmmpmnmmd	1.216e+44	4.08	4.08	1.291e+41	0.0178
14364	TS.triHPacyl.COelim.tpmptmtpmd	2.582e+44	4.53	4.53	1.290e+41	0.0178
14365	TS.triHPacyl.COelim.ppptpppmpd	8.190e+44	5.22	5.22	1.287e+41	0.0178
14366	TS.triHPacyl.COelim.tmttpmtpmd	1.927e+45	5.73	5.73	1.280e+41	0.0177
14367	TS.triHPacyl.COelim.ptmmpmtmpmd	1.298e+44	4.13	4.13	1.272e+41	0.0176
14368	TS.triHPacyl.COelim.tmpmtmmpd	2.175e+44	4.44	4.44	1.268e+41	0.0175
14369	TS.triHPacyl.COelim.pmtpnmmpd	5.852e+44	5.03	5.03	1.264e+41	0.0175
14370	TS.triHPacyl.COelim.tpppmtmpmd	6.208e+43	3.70	3.70	1.262e+41	0.0174
14371	TS.triHPacyl.COelim.tttmtmmpd	8.588e+43	3.89	3.89	1.259e+41	0.0174
14372	TS.triHPacyl.COelim.mtmmpmmpmd	1.584e+44	4.26	4.26	1.246e+41	0.0172
14373	TS.triHPacyl.COelim.tmtmtmtpd	5.869e+44	5.05	5.05	1.236e+41	0.0171
14374	TS.triHPacyl.COelim.pmpmpmnmmd	3.550e+43	3.38	3.38	1.232e+41	0.0171
14375	TS.triHPacyl.COelim.mtpppmpmmd	6.974e+43	3.79	3.79	1.217e+41	0.0168

14376	TS.triHPacyl.COelim.ppmpppmmmd	2.888e+44	4.63	4.63	1.214e+41	0.0168
14377	TS.triHPacyl.COelim.pmmppppmpmd	1.275e+44	4.15	4.15	1.214e+41	0.0168
14378	TS.triHPacyl.COelim.tttmmtmpmd	1.049e+44	4.03	4.03	1.211e+41	0.0167
14379	TS.triHPacyl.COelim.tttmmtmmpd	4.532e+43	3.54	3.54	1.198e+41	0.0165
14380	TS.triHPacyl.COelim.tmpmpppmmpd	2.628e+44	4.59	4.59	1.195e+41	0.0165
14381	TS.triHPacyl.COelim.ppmppptpmd	2.884e+44	4.65	4.65	1.183e+41	0.0163
14382	TS.triHPacyl.COelim.pmtmpmpmpd	1.372e+44	4.22	4.22	1.155e+41	0.0159
14383	TS.triHPacyl.COelim.mmpmpptmpd	2.865e+44	4.68	4.68	1.122e+41	0.0155
14384	TS.triHPacyl.COelim.tpppmmpmpd	1.827e+44	4.41	4.41	1.118e+41	0.0154
14385	TS.triHPacyl.COelim.pppmpptmmd	2.265e+44	4.55	4.55	1.107e+41	0.0153
14386	TS.triHPacyl.COelim.tttmtmpmd	1.413e+45	5.64	5.64	1.095e+41	0.0151
14387	TS.triHPacyl.COelim.ppptptmmpd	3.314e+44	4.78	4.78	1.093e+41	0.0151
14388	TS.triHPacyl.COelim.tppmmmmmd	1.968e+43	3.10	3.10	1.080e+41	0.0149
14389	TS.triHPacyl.COelim.tppppmtppd	4.406e+44	4.97	4.97	1.055e+41	0.0146
14390	TS.triHPacyl.COelim.pptmmppppd	2.230e+44	4.56	4.56	1.055e+41	0.0146
14391	TS.triHPacyl.COelim.pmpmttppd	7.587e+43	3.92	3.92	1.054e+41	0.0146
14392	TS.triHPacyl.COelim.pppttppmd	1.270e+45	5.61	5.61	1.036e+41	0.0143
14393	TS.triHPacyl.COelim.tmmmttmmd	3.280e+44	4.81	4.81	1.027e+41	0.0142
14394	TS.triHPacyl.COelim.tppmtmmd	7.896e+43	3.96	3.96	1.025e+41	0.0141
14395	TS.triHPacyl.COelim.pmpmtmmmd	1.717e+44	4.43	4.43	1.022e+41	0.0141
14396	TS.triHPacyl.COelim.tppppmpmd	3.335e+44	4.82	4.82	1.022e+41	0.0141
14397	TS.triHPacyl.COelim.tpmmpmpmpd	1.208e+44	4.23	4.23	1.005e+41	0.0139
14398	TS.triHPacyl.COelim.tmptmmmpd	2.727e+44	4.72	4.72	9.913e+40	0.0137
14399	TS.triHPacyl.COelim.mmpmpmpmpd	2.289e+43	3.26	3.26	9.614e+40	0.0133
14400	TS.triHPacyl.COelim.mmpmpmtmpd	2.602e+44	4.71	4.71	9.571e+40	0.0132
14401	TS.triHPacyl.COelim.tmpppmmmpd	3.959e+44	4.97	4.97	9.542e+40	0.0132
14402	TS.triHPacyl.COelim.076e+44	4.076e+44	5.00	5.00	9.311e+40	0.0129
14403	TS.triHPacyl.COelim.ppptttmpd	1.494e+45	5.78	5.78	9.158e+40	0.0126
14404	TS.triHPacyl.COelim.tmmmmmtmmd	5.051e+44	5.14	5.14	9.122e+40	0.0126
14405	TS.triHPacyl.COelim.pmmmpmmmpd	1.526e+44	4.43	4.43	9.075e+40	0.0125
14406	TS.triHPacyl.COelim.tppppmtmmd	7.802e+44	5.40	5.40	9.064e+40	0.0125
14407	TS.triHPacyl.COelim.tpmmppppd	1.118e+44	4.25	4.25	9.024e+40	0.0125
14408	TS.triHPacyl.COelim.mtmmpmpmpd	2.141e+44	4.64	4.64	8.945e+40	0.0124
14409	TS.triHPacyl.COelim.tmmmmmtmpd	6.531e+44	5.30	5.30	8.933e+40	0.0123
14410	TS.triHPacyl.COelim.tpmmtmpmd	1.113e+44	4.25	4.25	8.911e+40	0.0123
14411	TS.triHPacyl.COelim.tpmpppppd	6.424e+43	3.92	3.92	8.907e+40	0.0123
14412	TS.triHPacyl.COelim.tppppmpmd	5.504e+44	5.21	5.21	8.794e+40	0.0121
14413	TS.triHPacyl.COelim.pmpptmmpd	6.936e+43	3.99	3.99	8.579e+40	0.0118
14414	TS.triHPacyl.COelim.mmpmpptmpd	2.494e+43	3.39	3.39	8.490e+40	0.0117
14415	TS.triHPacyl.COelim.pmpptmmpd	1.686e+44	4.54	4.54	8.310e+40	0.0115
14416	TS.triHPacyl.COelim.pmtpmmtppd	3.787e+44	5.03	5.03	8.223e+40	0.0114
14417	TS.triHPacyl.COelim.tttpmmmmd	5.032e+43	3.83	3.83	8.204e+40	0.0113
14418	TS.triHPacyl.COelim.tmpppmmmd	4.650e+44	5.15	5.15	8.193e+40	0.0113
14419	TS.triHPacyl.COelim.tttpmmmppd	2.967e+44	4.89	4.89	8.127e+40	0.0112
14420	TS.triHPacyl.COelim.tttptmmpd	4.509e+43	3.77	3.77	8.025e+40	0.0111
14421	TS.triHPacyl.COelim.pmpmmmmmd	3.262e+43	3.58	3.58	7.984e+40	0.0111
14422	TS.triHPacyl.COelim.tptppmtppd	3.284e+45	6.33	6.33	7.971e+40	0.0111
14423	TS.triHPacyl.COelim.pppppptmpd	9.568e+44	5.60	5.60	7.938e+40	0.0111
14424	TS.triHPacyl.COelim.pptptmmpd	4.786e+44	5.19	5.19	7.935e+40	0.0111
14425	TS.triHPacyl.COelim.mppmmmtmpd	3.662e+44	5.04	5.04	7.777e+40	0.0107
14426	TS.triHPacyl.COelim.pmtppmpmpd	3.634e+44	5.04	5.04	7.737e+40	0.0107
14427	TS.triHPacyl.COelim.tpmmpmmmd	6.182e+44	5.36	5.36	7.648e+40	0.0106
14428	TS.triHPacyl.COelim.tttptmmpd	3.823e+44	5.08	5.08	7.640e+40	0.0105
14429	TS.triHPacyl.COelim.ppptpmpd	7.261e+44	5.47	5.47	7.564e+40	0.0104
14430	TS.triHPacyl.COelim.mmmmpmmmpd	8.534e+43	4.19	4.19	7.561e+40	0.0104
14431	TS.triHPacyl.COelim.tppmtmmpd	1.387e+44	4.48	4.48	7.548e+40	0.0104
14432	TS.triHPacyl.COelim.tpmmpptmpd	5.187e+44	5.27	5.27	7.540e+40	0.0104
14433	TS.triHPacyl.COelim.ppptpmpd	3.778e+44	5.08	5.08	7.516e+40	0.0104
14434	TS.triHPacyl.COelim.pmtppmtppd	3.472e+44	5.03	5.03	7.513e+40	0.0104
14435	TS.triHPacyl.COelim.mttppmmppd	4.693e+44	5.21	5.21	7.462e+40	0.0103
14436	TS.triHPacyl.COelim.tmmmmmpd	8.236e+44	5.55	5.55	7.446e+40	0.0103
14437	TS.triHPacyl.COelim.pmtptmmpd	2.055e+44	4.73	4.73	7.382e+40	0.0102
14438	TS.triHPacyl.COelim.tpmmmmpmd	2.323e+44	4.80	4.80	7.349e+40	0.0101
14439	TS.triHPacyl.COelim.tpmmmptppd	4.621e+44	5.22	5.22	7.298e+40	0.0101
14440	TS.triHPacyl.COelim.mmpmtmmpd	1.524e+44	4.58	4.58	7.072e+40	0.00976
14441	TS.triHPacyl.COelim.tmmmpmpppd	8.516e+44	5.60	5.60	7.065e+40	0.00975
14442	TS.triHPacyl.COelim.tppppppmpd	3.793e+44	5.11	5.11	7.025e+40	0.0097
14443	TS.triHPacyl.COelim.pttmppmpd	8.469e+43	4.23	4.23	7.013e+40	0.00968
14444	TS.triHPacyl.COelim.ppptptmpd	3.170e+44	5.02	5.02	6.947e+40	0.00959
14445	TS.triHPacyl.COelim.tppmmmpmd	1.753e+44	4.67	4.67	6.923e+40	0.00956
14446	TS.triHPacyl.COelim.tptmtmpd	1.248e+45	5.84	5.84	6.892e+40	0.00952
14447	TS.triHPacyl.COelim.ppmppppmpd	1.477e+44	4.57	4.57	6.891e+40	0.00951

14448	TS.triHPacyl.COelim.pppmpptpmd	3.429e+44	5.08	5.08	6.829e+40	0.00943
14449	TS.triHPacyl.COelim.tmtppmpppd	4.040e+45	6.56	6.56	6.775e+40	0.00935
14450	TS.triHPacyl.COelim.tmmpmtmppd	1.669e+44	4.66	4.66	6.720e+40	0.00928
14451	TS.triHPacyl.COelim.tmttmmpppd	1.143e+45	5.81	5.81	6.656e+40	0.00919
14452	TS.triHPacyl.COelim.tptpnmppmd	4.418e+44	5.25	5.25	6.579e+40	0.00908
14453	TS.triHPacyl.COelim.tpptmtppd	2.017e+45	6.16	6.16	6.563e+40	0.00906
14454	TS.triHPacyl.COelim.mptmmmmmpd	4.922e+44	5.32	5.32	6.515e+40	0.00899
14455	TS.triHPacyl.COelim.pmmmpmtmmmd	2.336e+44	4.88	4.88	6.482e+40	0.00895
14456	TS.triHPacyl.COelim.mmttpmmmmmd	4.253e+44	5.24	5.24	6.441e+40	0.00889
14457	TS.triHPacyl.COelim.mmtppmmtpmd	5.910e+44	5.44	5.44	6.400e+40	0.00884
14458	TS.triHPacyl.COelim.pptpmmpppd	5.748e+44	5.44	5.44	6.309e+40	0.00871
14459	TS.triHPacyl.COelim.pppmptmmmd	7.684e+43	4.25	4.25	6.146e+40	0.00849
14460	TS.triHPacyl.COelim.ttmmpmtmpmd	5.813e+44	5.46	5.46	6.142e+40	0.00848
14461	TS.triHPacyl.COelim.ptptptmmmd	2.114e+44	4.86	4.86	6.116e+40	0.00844
14462	TS.triHPacyl.COelim.pmtptmtpd	4.330e+44	5.29	5.29	6.088e+40	0.00841
14463	TS.triHPacyl.COelim.pmtppppmpd	3.714e+44	5.20	5.20	6.050e+40	0.00835
14464	TS.triHPacyl.COelim.tptppmmmmmd	3.930e+44	5.24	5.24	6.033e+40	0.00833
14465	TS.triHPacyl.COelim.ttpmmmtppd	3.136e+43	3.73	3.73	6.011e+40	0.0083
14466	TS.triHPacyl.COelim.tptmppmmmd	1.946e+45	6.20	6.20	5.968e+40	0.00824
14467	TS.triHPacyl.COelim.pttmptmtpd	7.429e+43	4.25	4.25	5.956e+40	0.00822
14468	TS.triHPacyl.COelim.tppppptppd	5.529e+44	5.45	5.45	5.947e+40	0.00821
14469	TS.triHPacyl.COelim.ppmtppmppd	1.442e+44	4.67	4.67	5.727e+40	0.00791
14470	TS.triHPacyl.COelim.tmppmmtpd	3.280e+44	5.17	5.17	5.604e+40	0.00774
14471	TS.triHPacyl.COelim.mmtptmtpmd	1.361e+45	6.02	6.02	5.564e+40	0.00768
14472	TS.triHPacyl.COelim.mmpptmmmmmd	4.601e+44	5.38	5.38	5.562e+40	0.00768
14473	TS.triHPacyl.COelim.ptppmmmpmd	5.209e+43	4.08	4.08	5.549e+40	0.00766
14474	TS.triHPacyl.COelim.pttmmpmtpd	5.718e+43	4.14	4.14	5.546e+40	0.00766
14475	TS.triHPacyl.COelim.tpmmpmtpmd	1.894e+44	4.85	4.85	5.521e+40	0.00762
14476	TS.triHPacyl.COelim.ppptptppmd	3.956e+44	5.29	5.29	5.514e+40	0.00761
14477	TS.triHPacyl.COelim.tmttmmmmmd	3.035e+45	6.51	6.51	5.497e+40	0.00759
14478	TS.triHPacyl.COelim.tmpppppmmpd	8.609e+44	5.76	5.76	5.473e+40	0.00756
14479	TS.triHPacyl.COelim.tmmtmmmmmd	1.442e+44	4.70	4.70	5.459e+40	0.00754
14480	TS.triHPacyl.COelim.pttpmtmtpd	2.007e+44	4.90	4.90	5.450e+40	0.00753
14481	TS.triHPacyl.COelim.mtppppptpmd	2.836e+43	3.73	3.73	5.450e+40	0.00752
14482	TS.triHPacyl.COelim.mmpmpmmmmmd	8.933e+43	4.42	4.42	5.449e+40	0.00752
14483	TS.triHPacyl.COelim.pmptmmmmmd	1.170e+44	4.58	4.58	5.409e+40	0.00747
14484	TS.triHPacyl.COelim.pptpmppppd	2.360e+44	5.00	5.00	5.396e+40	0.00745
14485	TS.triHPacyl.COelim.ttpmmmmmpd	2.080e+43	3.55	3.55	5.382e+40	0.00743
14486	TS.triHPacyl.COelim.pmpppptmtpd	4.893e+43	4.06	4.06	5.351e+40	0.00739
14487	TS.triHPacyl.COelim.ptpmpptppd	1.691e+43	3.44	3.44	5.315e+40	0.00734
14488	TS.triHPacyl.COelim.tmttmtmpmd	2.149e+45	6.32	6.32	5.307e+40	0.00733
14489	TS.triHPacyl.COelim.mmtppmtpmd	3.900e+44	5.31	5.31	5.263e+40	0.00727
14490	TS.triHPacyl.COelim.mppmptmtpd	7.195e+43	4.31	4.31	5.252e+40	0.00725
14491	TS.triHPacyl.COelim.ptppmmmmmd	1.807e+43	3.48	3.48	5.244e+40	0.00724
14492	TS.triHPacyl.COelim.pmtmptmtpd	8.579e+43	4.42	4.42	5.197e+40	0.00718
14493	TS.triHPacyl.COelim.pttpmmtpmd	1.370e+44	4.70	4.70	5.141e+40	0.0071
14494	TS.triHPacyl.COelim.mppmpppppd	7.052e+43	4.31	4.31	5.122e+40	0.00707
14495	TS.triHPacyl.COelim.tpmmpmtpd	4.817e+44	5.45	5.45	5.119e+40	0.00707
14496	TS.triHPacyl.COelim.tmtmmppppd	3.586e+44	5.28	5.28	5.109e+40	0.00705
14497	TS.triHPacyl.COelim.ttpmmtmmd	5.914e+43	4.21	4.21	5.045e+40	0.00697
14498	TS.triHPacyl.COelim.tpppmtmtpd	3.875e+44	5.33	5.33	5.045e+40	0.00697
14499	TS.triHPacyl.COelim.pmmmmmmmpd	7.010e+43	4.32	4.32	5.025e+40	0.00694
14500	TS.triHPacyl.COelim.tmtmmmmmpmd	2.211e+45	6.38	6.38	4.985e+40	0.00688
14501	TS.triHPacyl.COelim.mmpmpmtpmd	1.203e+44	4.64	4.64	4.973e+40	0.00687
14502	TS.triHPacyl.COelim.ppttpptppd	6.988e+44	5.70	5.70	4.959e+40	0.00685
14503	TS.triHPacyl.COelim.mmpmpptppd	1.647e+44	4.83	4.83	4.949e+40	0.00683
14504	TS.triHPacyl.COelim.ptmtpmtpmd	2.805e+44	5.15	5.15	4.942e+40	0.00682
14505	TS.triHPacyl.COelim.mmmmpmtpmd	8.237e+43	4.42	4.42	4.925e+40	0.0068
14506	TS.triHPacyl.COelim.ppttpmtpd	1.623e+45	6.21	6.21	4.885e+40	0.00674
14507	TS.triHPacyl.COelim.ttpmmmpmd	1.527e+45	6.17	6.17	4.856e+40	0.00671
14508	TS.triHPacyl.COelim.pppppppppd	3.363e+44	5.28	5.28	4.775e+40	0.00659
14509	TS.triHPacyl.COelim.pttpmtmtpd	5.147e+43	4.17	4.17	4.740e+40	0.00655
14510	TS.triHPacyl.COelim.mmpppmtpmd	4.427e+43	4.08	4.08	4.684e+40	0.00647
14511	TS.triHPacyl.COelim.ptmmtmtpd	2.325e+44	5.07	5.07	4.677e+40	0.00646
14512	TS.triHPacyl.COelim.mtptmtpmd	2.849e+44	5.20	5.20	4.648e+40	0.00642
14513	TS.triHPacyl.COelim.tpppmtmtpd	1.420e+44	4.79	4.79	4.579e+40	0.00632
14514	TS.triHPacyl.COelim.pttpmtpmd	4.098e+43	4.06	4.06	4.547e+40	0.00628
14515	TS.triHPacyl.COelim.mtmtmtpmd	1.086e+44	4.64	4.64	4.495e+40	0.00621
14516	TS.triHPacyl.COelim.tmmmmmtmmd	5.608e+44	5.62	5.62	4.492e+40	0.0062
14517	TS.triHPacyl.COelim.mptmmmpmmpd	3.092e+44	5.27	5.27	4.490e+40	0.0062
14518	TS.triHPacyl.COelim.pppmpptmmd	8.217e+44	5.85	5.85	4.469e+40	0.00617
14519	TS.triHPacyl.COelim.tmppmtpmd	2.376e+44	5.12	5.12	4.463e+40	0.00616

14520	TS.triHPacyl.COelim.mppmmtmpmd	8.314e+43	4.49	4.49	4.457e+40	0.00615
14521	TS.triHPacyl.COelim.tppmmpmpmd	2.582e+44	5.17	5.17	4.457e+40	0.00615
14522	TS.triHPacyl.COelim.mppmptpmd	2.188e+44	5.07	5.07	4.449e+40	0.00614
14523	TS.triHPacyl.COelim.pmttmnmmd	2.220e+45	6.45	6.45	4.444e+40	0.00614
14524	TS.triHPacyl.COelim.tppmpppmd	8.667e+43	4.52	4.52	4.443e+40	0.00614
14525	TS.triHPacyl.COelim.mppmmtmpmd	1.653e+44	4.90	4.90	4.419e+40	0.0061
14526	TS.triHPacyl.COelim.tptmnmppd	1.685e+44	4.92	4.92	4.392e+40	0.00606
14527	TS.triHPacyl.COelim.pptmpmpmd	2.949e+44	5.25	5.25	4.383e+40	0.00605
14528	TS.triHPacyl.COelim.mtppmmpmd	2.651e+44	5.20	5.20	4.353e+40	0.00601
14529	TS.triHPacyl.COelim.mppmptpmd	1.530e+44	4.87	4.87	4.338e+40	0.00599
14530	TS.triHPacyl.COelim.tpppmmpmd	9.328e+43	4.58	4.58	4.332e+40	0.00598
14531	TS.triHPacyl.COelim.ppptpmtmd	1.630e+45	6.29	6.29	4.297e+40	0.00593
14532	TS.triHPacyl.COelim.tttptmpmd	1.481e+44	4.86	4.86	4.293e+40	0.00593
14533	TS.triHPacyl.COelim.mmtptmmd	5.639e+44	5.66	5.66	4.263e+40	0.00589
14534	TS.triHPacyl.COelim.tppmpmpmd	1.045e+44	4.66	4.66	4.240e+40	0.00585
14535	TS.triHPacyl.COelim.tptmmpmd	4.415e+44	5.52	5.52	4.222e+40	0.00583
14536	TS.triHPacyl.COelim.mppmmpmpmd	5.517e+43	4.28	4.28	4.204e+40	0.00581
14537	TS.triHPacyl.COelim.pptpmtmpmd	3.736e+44	5.42	5.42	4.197e+40	0.0058
14538	TS.triHPacyl.COelim.mppmmpmpd	7.379e+43	4.46	4.46	4.184e+40	0.00578
14539	TS.triHPacyl.COelim.pptpmpmd	1.726e+45	6.34	6.34	4.183e+40	0.00578
14540	TS.triHPacyl.COelim.mppmmpmpd	1.418e+44	4.85	4.85	4.156e+40	0.00574
14541	TS.triHPacyl.COelim.pptpmpmpd	3.277e+44	5.35	5.35	4.132e+40	0.0057
14542	TS.triHPacyl.COelim.tmpmmpmpd	4.050e+44	5.48	5.48	4.095e+40	0.00565
14543	TS.triHPacyl.COelim.tmpmmpmpd	1.824e+44	5.01	5.01	4.068e+40	0.00562
14544	TS.triHPacyl.COelim.pptpmpmd	1.698e+45	6.35	6.35	4.034e+40	0.00557
14545	TS.triHPacyl.COelim.tmtptppmd	9.630e+44	6.01	6.01	4.023e+40	0.00555
14546	TS.triHPacyl.COelim.pppmptppd	1.047e+44	4.69	4.69	4.020e+40	0.00555
14547	TS.triHPacyl.COelim.pmtppmpmd	2.596e+44	5.23	5.23	4.016e+40	0.00555
14548	TS.triHPacyl.COelim.tmtmtpppd	3.483e+44	5.41	5.41	3.987e+40	0.00551
14549	TS.triHPacyl.COelim.tptmtmmd	8.200e+44	5.92	5.92	3.985e+40	0.0055
14550	TS.triHPacyl.COelim.tttmmpmpd	1.504e+44	4.91	4.91	3.985e+40	0.0055
14551	TS.triHPacyl.COelim.tptpmpmd	1.519e+45	6.29	6.29	3.962e+40	0.00547
14552	TS.triHPacyl.COelim.tppmtmpmd	1.851e+45	6.41	6.41	3.949e+40	0.00545
14553	TS.triHPacyl.COelim.tptmtmpmd	1.334e+45	6.23	6.23	3.862e+40	0.00533
14554	TS.triHPacyl.COelim.pptppmpd	9.710e+44	6.04	6.04	3.838e+40	0.0053
14555	TS.triHPacyl.COelim.tptmpmpmd	1.219e+45	6.18	6.18	3.831e+40	0.00529
14556	TS.triHPacyl.COelim.ttmmtmmd	4.166e+44	5.55	5.55	3.802e+40	0.00525
14557	TS.triHPacyl.COelim.pptmpmpmd	1.527e+45	6.32	6.32	3.771e+40	0.00521
14558	TS.triHPacyl.COelim.mtppmpppd	1.035e+44	4.72	4.72	3.757e+40	0.00519
14559	TS.triHPacyl.COelim.pmtppmpd	9.095e+43	4.65	4.65	3.745e+40	0.00517
14560	TS.triHPacyl.COelim.pmpmptppd	1.797e+44	5.05	5.05	3.743e+40	0.00517
14561	TS.triHPacyl.COelim.tmpmptppd	1.663e+44	5.01	5.01	3.741e+40	0.00517
14562	TS.triHPacyl.COelim.mmtppmpd	7.363e+44	5.90	5.90	3.736e+40	0.00516
14563	TS.triHPacyl.COelim.tmmmpptppd	6.296e+44	5.80	5.80	3.732e+40	0.00515
14564	TS.triHPacyl.COelim.tppmpmpmd	5.846e+43	4.39	4.39	3.731e+40	0.00515
14565	TS.triHPacyl.COelim.pptmpmpd	3.340e+44	5.43	5.43	3.710e+40	0.00512
14566	TS.triHPacyl.COelim.pptmpppd	1.306e+44	4.87	4.87	3.706e+40	0.00512
14567	TS.triHPacyl.COelim.mppmppppd	5.493e+43	4.35	4.35	3.705e+40	0.00512
14568	TS.triHPacyl.COelim.tptmtpmmd	5.515e+44	5.73	5.73	3.698e+40	0.00511
14569	TS.triHPacyl.COelim.tmtmmpmpd	2.010e+45	6.51	6.51	3.667e+40	0.00506
14570	TS.triHPacyl.COelim.pptmmpmpd	1.129e+45	6.17	6.17	3.637e+40	0.00502
14571	TS.triHPacyl.COelim.tptmmpmpd	1.730e+44	5.05	5.05	3.631e+40	0.00501
14572	TS.triHPacyl.COelim.tppmmpmpd	5.312e+43	4.36	4.36	3.553e+40	0.00491
14573	TS.triHPacyl.COelim.tmtmmpmpd	6.448e+44	5.85	5.85	3.538e+40	0.00489
14574	TS.triHPacyl.COelim.pptppmpd	1.392e+45	6.31	6.31	3.523e+40	0.00486
14575	TS.triHPacyl.COelim.pppmpmpd	1.581e+43	3.64	3.64	3.515e+40	0.00485
14576	TS.triHPacyl.COelim.pppmptppd	2.182e+44	5.21	5.21	3.509e+40	0.00485
14577	TS.triHPacyl.COelim.tppmtmmpd	3.289e+44	5.45	5.45	3.506e+40	0.00484
14578	TS.triHPacyl.COelim.mptmmpmpd	1.195e+45	6.22	6.22	3.489e+40	0.00482
14579	TS.triHPacyl.COelim.tttptmpmd	1.323e+44	4.91	4.91	3.484e+40	0.00481
14580	TS.triHPacyl.COelim.tmmmpmpd	4.509e+44	5.66	5.66	3.399e+40	0.00469
14581	TS.triHPacyl.COelim.tmpmmpmpd	5.967e+44	5.83	5.83	3.389e+40	0.00468
14582	TS.triHPacyl.COelim.pmpmpppd	3.855e+43	4.20	4.20	3.374e+40	0.00466
14583	TS.triHPacyl.COelim.pptpmpmd	5.503e+44	5.79	5.79	3.360e+40	0.00464
14584	TS.triHPacyl.COelim.tmtppmpd	1.317e+45	6.31	6.31	3.337e+40	0.00461
14585	TS.triHPacyl.COelim.tttmmtmmd	1.233e+44	4.90	4.90	3.321e+40	0.00459
14586	TS.triHPacyl.COelim.pptmmpmpd	1.836e+44	5.14	5.14	3.307e+40	0.00457
14587	TS.triHPacyl.COelim.pptmppppd	8.803e+44	6.08	6.08	3.300e+40	0.00456
14588	TS.triHPacyl.COelim.pptmpmpmd	1.993e+45	6.57	6.57	3.287e+40	0.00454
14589	TS.triHPacyl.COelim.pmpmptppd	3.693e+43	4.19	4.19	3.285e+40	0.00454
14590	TS.triHPacyl.COelim.pmtmmpmpd	2.554e+44	5.34	5.34	3.285e+40	0.00454
14591	TS.triHPacyl.COelim.tptmtpppd	8.453e+44	6.05	6.05	3.284e+40	0.00453

14592	TS.triHPacyl.COelim.tmmpttppmd	4.305e+44	5.65	5.65	3.277e+40	0.00452
14593	TS.triHPacyl.COelim.tmmmtmmpmd	5.863e+44	5.84	5.84	3.259e+40	0.0045
14594	TS.triHPacyl.COelim.tppmmmpmd	4.371e+43	4.30	4.30	3.214e+40	0.00444
14595	TS.triHPacyl.COelim.pttmppptmpd	1.112e+44	4.87	4.87	3.172e+40	0.00438
14596	TS.triHPacyl.COelim.tppppptmpmd	3.660e+44	5.58	5.58	3.170e+40	0.00438
14597	TS.triHPacyl.COelim.ptmtmtmpmd	2.749e+44	5.41	5.41	3.164e+40	0.00437
14598	TS.triHPacyl.COelim.pmmmpptpppd	1.992e+44	5.22	5.22	3.144e+40	0.00434
14599	TS.triHPacyl.COelim.pmtpmmpppd	1.193e+45	6.30	6.30	3.095e+40	0.00427
14600	TS.triHPacyl.COelim.pmttpttppmd	5.750e+44	5.87	5.87	3.066e+40	0.00423
14601	TS.triHPacyl.COelim.pmptmmmpmd	1.097e+45	6.25	6.25	3.060e+40	0.00423
14602	TS.triHPacyl.COelim.ptppmmppmd	5.035e+43	4.42	4.42	3.048e+40	0.00421
14603	TS.triHPacyl.COelim.tptpmtmpmd	7.222e+43	4.63	4.63	3.042e+40	0.0042
14604	TS.triHPacyl.COelim.pmmmpptmpd	3.140e+43	4.14	4.14	3.038e+40	0.0042
14605	TS.triHPacyl.COelim.tppmmmtmpmd	2.986e+44	5.48	5.48	3.036e+40	0.00419
14606	TS.triHPacyl.COelim.mmmmmmpmd	5.567e+44	5.86	5.86	3.021e+40	0.00417
14607	TS.triHPacyl.COelim.tptpmtppd	2.329e+44	5.34	5.34	3.019e+40	0.00417
14608	TS.triHPacyl.COelim.tmmmttppmd	1.539e+45	6.46	6.46	3.006e+40	0.00415
14609	TS.triHPacyl.COelim.pmmmpmpmd	1.536e+44	5.09	5.09	2.989e+40	0.00413
14610	TS.triHPacyl.COelim.tptmmtpppd	2.368e+44	5.35	5.35	2.986e+40	0.00412
14611	TS.triHPacyl.COelim.pmptmmtppmd	6.621e+44	5.97	5.97	2.982e+40	0.00412
14612	TS.triHPacyl.COelim.pmpmmppmd	1.226e+44	4.96	4.96	2.977e+40	0.00411
14613	TS.triHPacyl.COelim.pttpttppd	1.273e+44	4.99	4.99	2.936e+40	0.00405
14614	TS.triHPacyl.COelim.tppppptmpd	4.219e+44	5.71	5.71	2.932e+40	0.00405
14615	TS.triHPacyl.COelim.tmmppptmpd	3.021e+44	5.51	5.51	2.916e+40	0.00403
14616	TS.triHPacyl.COelim.mmtmpmtppd	6.961e+44	6.01	6.01	2.890e+40	0.00399
14617	TS.triHPacyl.COelim.mttpttppd	2.635e+44	5.44	5.44	2.887e+40	0.00399
14618	TS.triHPacyl.COelim.ppmmtmmpmd	8.027e+44	6.10	6.10	2.887e+40	0.00399
14619	TS.triHPacyl.COelim.tptmppppd	2.559e+45	6.79	6.79	2.879e+40	0.00397
14620	TS.triHPacyl.COelim.mpmmpmmpmd	1.665e+44	5.17	5.17	2.873e+40	0.00397
14621	TS.triHPacyl.COelim.tptmtpmpd	9.420e+44	6.20	6.20	2.845e+40	0.00393
14622	TS.triHPacyl.COelim.mmpmmmpmd	4.889e+43	4.44	4.44	2.830e+40	0.00391
14623	TS.triHPacyl.COelim.mmtmmpmmpmd	1.074e+45	6.30	6.30	2.771e+40	0.00383
14624	TS.triHPacyl.COelim.tmmmtmmpmd	9.121e+44	6.20	6.20	2.771e+40	0.00383
14625	TS.triHPacyl.COelim.tmmpttmmmd	4.505e+44	5.78	5.78	2.761e+40	0.00381
14626	TS.triHPacyl.COelim.pmptmmmpmd	1.731e+44	5.22	5.22	2.741e+40	0.00379
14627	TS.triHPacyl.COelim.pmtpppppd	1.084e+45	6.31	6.31	2.739e+40	0.00378
14628	TS.triHPacyl.COelim.ppptppmpmd	4.346e+44	5.77	5.77	2.735e+40	0.00378
14629	TS.triHPacyl.COelim.ptppptppd	5.708e+43	4.56	4.56	2.732e+40	0.00377
14630	TS.triHPacyl.COelim.tmmtpmpmd	1.117e+44	4.96	4.96	2.731e+40	0.00377
14631	TS.triHPacyl.COelim.tppmmtppmd	7.886e+44	6.13	6.13	2.709e+40	0.00374
14632	TS.triHPacyl.COelim.tmttppmmpmd	2.714e+45	6.87	6.87	2.700e+40	0.00373
14633	TS.triHPacyl.COelim.pttmppmpd	5.380e+43	4.53	4.53	2.699e+40	0.00373
14634	TS.triHPacyl.COelim.mtppppmpmd	3.550e+43	4.28	4.28	2.699e+40	0.00373
14635	TS.triHPacyl.COelim.tmtmmpmpd	5.809e+44	5.95	5.95	2.687e+40	0.00371
14636	TS.triHPacyl.COelim.tpmmpptppd	7.882e+44	6.14	6.14	2.672e+40	0.00369
14637	TS.triHPacyl.COelim.tptmmmmmpmd	8.366e+44	6.17	6.17	2.665e+40	0.00368
14638	TS.triHPacyl.COelim.tpmmpmtppd	2.693e+44	5.50	5.50	2.650e+40	0.00366
14639	TS.triHPacyl.COelim.pttpmmtppd	3.691e+44	5.69	5.69	2.650e+40	0.00366
14640	TS.triHPacyl.COelim.tttmmpmmpmd	9.286e+43	4.87	4.87	2.642e+40	0.00365
14641	TS.triHPacyl.COelim.ppttptmmpd	2.054e+44	5.34	5.34	2.627e+40	0.00363
14642	TS.triHPacyl.COelim.ppttptppd	4.161e+44	5.77	5.77	2.616e+40	0.00361
14643	TS.triHPacyl.COelim.pttppptppd	1.186e+44	5.02	5.02	2.602e+40	0.00359
14644	TS.triHPacyl.COelim.mttmmpmmpd	1.003e+44	4.92	4.92	2.598e+40	0.00359
14645	TS.triHPacyl.COelim.tttpttmmmd	9.582e+43	4.90	4.90	2.565e+40	0.00354
14646	TS.triHPacyl.COelim.pmptpmmpd	4.975e+43	4.52	4.52	2.548e+40	0.00352
14647	TS.triHPacyl.COelim.mmpptmtpd	3.480e+44	5.68	5.68	2.529e+40	0.00349
14648	TS.triHPacyl.COelim.ppptpppppd	7.936e+44	6.17	6.17	2.526e+40	0.00349
14649	TS.triHPacyl.COelim.ptmtpttmmmd	3.846e+44	5.75	5.75	2.503e+40	0.00346
14650	TS.triHPacyl.COelim.tmmmtmmpmd	5.500e+44	5.96	5.96	2.494e+40	0.00344
14651	TS.triHPacyl.COelim.pmmpttmpd	1.932e+44	5.34	5.34	2.482e+40	0.00343
14652	TS.triHPacyl.COelim.ppptptmmpd	2.056e+44	5.38	5.38	2.476e+40	0.00342
14653	TS.triHPacyl.COelim.tpmmpptppd	4.079e+44	5.79	5.79	2.461e+40	0.0034
14654	TS.triHPacyl.COelim.tppmmmtppd	1.551e+45	6.59	6.59	2.443e+40	0.00337
14655	TS.triHPacyl.COelim.mmtmmpmmpd	5.469e+44	5.98	5.98	2.399e+40	0.00331
14656	TS.triHPacyl.COelim.pmtppmmpd	1.918e+44	5.36	5.36	2.392e+40	0.0033
14657	TS.triHPacyl.COelim.tmpmmtppd	7.490e+43	4.80	4.80	2.379e+40	0.00328
14658	TS.triHPacyl.COelim.ttmmppmpmd	3.301e+44	5.69	5.69	2.377e+40	0.00328
14659	TS.triHPacyl.COelim.mpmmpmmpmd	6.040e+43	4.68	4.68	2.370e+40	0.00327
14660	TS.triHPacyl.COelim.pmtpmmpmmd	1.008e+44	5.00	5.00	2.309e+40	0.00319
14661	TS.triHPacyl.COelim.pmmmpmtppd	2.251e+44	5.48	5.48	2.306e+40	0.00318
14662	TS.triHPacyl.COelim.tttmtpmpd	2.133e+44	5.45	5.45	2.295e+40	0.00317
14663	TS.triHPacyl.COelim.ppttpppppd	1.134e+45	6.44	6.44	2.294e+40	0.00317

14664	TS.triHPacyl.COelim.pmpppppmpmd	6.744e+43	4.76	4.76	2.293e+40	0.00317
14665	TS.triHPacyl.COelim.ttmtmmmpd	4.888e+44	5.94	5.94	2.293e+40	0.00317
14666	TS.triHPacyl.COelim.pttmpttpmd	1.485e+44	5.24	5.24	2.275e+40	0.00314
14667	TS.triHPacyl.COelim.pttmmtmpmd	6.915e+43	4.78	4.78	2.269e+40	0.00313
14668	TS.triHPacyl.COelim.tmtptmpd	1.444e+45	6.59	6.59	2.268e+40	0.00313
14669	TS.triHPacyl.COelim.mppppmpmd	1.111e+44	5.07	5.07	2.261e+40	0.00312
14670	TS.triHPacyl.COelim.mtppppmpmd	3.777e+43	4.43	4.43	2.253e+40	0.00311
14671	TS.triHPacyl.COelim.ppptpmpd	1.313e+45	6.54	6.54	2.245e+40	0.0031
14672	TS.triHPacyl.COelim.mppmptmpmd	3.225e+43	4.33	4.33	2.243e+40	0.0031
14673	TS.triHPacyl.COelim.tpmtmmmpmd	3.234e+44	5.71	5.71	2.223e+40	0.00307
14674	TS.triHPacyl.COelim.tpptmtpd	1.245e+45	6.52	6.52	2.217e+40	0.00306
14675	TS.triHPacyl.COelim.tmmppmmmpmd	1.229e+44	5.14	5.14	2.212e+40	0.00305
14676	TS.triHPacyl.COelim.tptmttppd	1.412e+45	6.60	6.60	2.209e+40	0.00305
14677	TS.triHPacyl.COelim.pptppppmd	1.288e+45	6.54	6.54	2.202e+40	0.00304
14678	TS.triHPacyl.COelim.ptmtpppmpd	3.852e+44	5.83	5.83	2.198e+40	0.00304
14679	TS.triHPacyl.COelim.pmmppmtpd	1.104e+44	5.08	5.08	2.198e+40	0.00303
14680	TS.triHPacyl.COelim.pmtmmmpmd	7.052e+44	6.19	6.19	2.194e+40	0.00303
14681	TS.triHPacyl.COelim.tptmmpppd	1.246e+44	5.15	5.15	2.192e+40	0.00303
14682	TS.triHPacyl.COelim.pttpmpmpd	5.478e+43	4.68	4.68	2.149e+40	0.00297
14683	TS.triHPacyl.COelim.ptpmmmmpmd	5.747e+43	4.71	4.71	2.141e+40	0.00296
14684	TS.triHPacyl.COelim.pttmmmmmpd	5.404e+43	4.67	4.67	2.137e+40	0.00295
14685	TS.triHPacyl.COelim.pppppppmd	9.688e+43	5.03	5.03	2.103e+40	0.0029
14686	TS.triHPacyl.COelim.mmmppmmmpd	2.286e+44	5.54	5.54	2.102e+40	0.0029
14687	TS.triHPacyl.COelim.tpmtmtpd	3.056e+44	5.71	5.71	2.099e+40	0.0029
14688	TS.triHPacyl.COelim.tmtpppppd	2.491e+45	6.97	6.97	2.094e+40	0.00289
14689	TS.triHPacyl.COelim.mtppppmpd	2.892e+43	4.32	4.32	2.076e+40	0.00287
14690	TS.triHPacyl.COelim.tpmtmmpd	5.810e+44	6.11	6.11	2.063e+40	0.00285
14691	TS.triHPacyl.COelim.tmtmmpppd	1.246e+45	6.56	6.56	2.062e+40	0.00285
14692	TS.triHPacyl.COelim.mmpmpmpd	2.967e+44	5.71	5.71	2.043e+40	0.00282
14693	TS.triHPacyl.COelim.ppmtppppd	1.771e+44	5.41	5.41	2.038e+40	0.00281
14694	TS.triHPacyl.COelim.tpmppppmd	1.728e+44	5.39	5.39	2.037e+40	0.00281
14695	TS.triHPacyl.COelim.pmptmtpd	7.221e+44	6.25	6.25	2.030e+40	0.0028
14696	TS.triHPacyl.COelim.mptpmtpmd	5.409e+44	6.08	6.08	2.028e+40	0.0028
14697	TS.triHPacyl.COelim.tppmtmmd	2.218e+44	5.55	5.55	2.009e+40	0.00277
14698	TS.triHPacyl.COelim.tptpmtmpd	1.182e+45	6.55	6.55	2.005e+40	0.00277
14699	TS.triHPacyl.COelim.mpppmpmpd	4.519e+44	5.98	5.98	2.004e+40	0.00277
14700	TS.triHPacyl.COelim.tmpmtmmmd	2.586e+44	5.64	5.64	2.003e+40	0.00277
14701	TS.triHPacyl.COelim.pmpmpppmd	2.402e+44	5.61	5.61	1.982e+40	0.00274
14702	TS.triHPacyl.COelim.mmtmmmpmd	4.329e+44	5.96	5.96	1.973e+40	0.00272
14703	TS.triHPacyl.COelim.tmpmpmpd	7.339e+43	4.91	4.91	1.950e+40	0.00269
14704	TS.triHPacyl.COelim.ptmtmpmpd	2.634e+44	5.68	5.68	1.933e+40	0.00267
14705	TS.triHPacyl.COelim.ppppmmmpd	1.022e+44	5.11	5.11	1.927e+40	0.00266
14706	TS.triHPacyl.COelim.mpppmtppd	5.243e+44	6.09	6.09	1.925e+40	0.00266
14707	TS.triHPacyl.COelim.pmtmmmpd	9.649e+44	6.46	6.46	1.914e+40	0.00264
14708	TS.triHPacyl.COelim.pptmpmpmd	1.106e+45	6.55	6.55	1.887e+40	0.00261
14709	TS.triHPacyl.COelim.ppmmmmmmd	8.422e+44	6.38	6.38	1.885e+40	0.0026
14710	TS.triHPacyl.COelim.ptpmpmpd	4.851e+43	4.69	4.69	1.864e+40	0.00257
14711	TS.triHPacyl.COelim.mmmmmmtmpd	7.115e+43	4.92	4.92	1.861e+40	0.00257
14712	TS.triHPacyl.COelim.tmtptppd	2.444e+45	7.03	7.03	1.860e+40	0.00257
14713	TS.triHPacyl.COelim.pptmpmpd	4.651e+44	6.04	6.04	1.842e+40	0.00254
14714	TS.triHPacyl.COelim.mpppmtmmd	1.251e+45	6.64	6.64	1.831e+40	0.00253
14715	TS.triHPacyl.COelim.pmmppmpd	1.553e+44	5.40	5.40	1.816e+40	0.00251
14716	TS.triHPacyl.COelim.ptptmmmpd	1.291e+44	5.29	5.29	1.805e+40	0.00249
14717	TS.triHPacyl.COelim.ttmtmtpd	4.031e+44	5.98	5.98	1.788e+40	0.00247
14718	TS.triHPacyl.COelim.tmttmtppd	1.097e+45	6.57	6.57	1.786e+40	0.00247
14719	TS.triHPacyl.COelim.mppmmmtppd	3.684e+43	4.55	4.55	1.782e+40	0.00246
14720	TS.triHPacyl.COelim.mtppmmmpmd	1.494e+44	5.41	5.41	1.711e+40	0.00236
14721	TS.triHPacyl.COelim.tmpptmpmd	4.817e+44	6.11	6.11	1.709e+40	0.00236
14722	TS.triHPacyl.COelim.pmtmmtmpmd	1.493e+44	5.41	5.41	1.699e+40	0.00235
14723	TS.triHPacyl.COelim.tmtmpmpd	1.265e+45	6.69	6.69	1.684e+40	0.00232
14724	TS.triHPacyl.COelim.ptppmmmpd	2.849e+43	4.44	4.44	1.661e+40	0.00229
14725	TS.triHPacyl.COelim.pmmmmmtppd	5.433e+43	4.82	4.82	1.661e+40	0.00229
14726	TS.triHPacyl.COelim.pmmmpmtpd	2.887e+44	5.82	5.82	1.658e+40	0.00229
14727	TS.triHPacyl.COelim.pmmmmmmmpd	7.491e+43	5.02	5.02	1.657e+40	0.00229
14728	TS.triHPacyl.COelim.tmmppmpmd	4.129e+44	6.04	6.04	1.655e+40	0.00229
14729	TS.triHPacyl.COelim.mmtmmtmpmd	3.697e+44	5.97	5.97	1.653e+40	0.00228
14730	TS.triHPacyl.COelim.tmtmmppd	1.543e+45	6.82	6.82	1.649e+40	0.00228
14731	TS.triHPacyl.COelim.tttmmtmpd	1.759e+44	5.53	5.53	1.648e+40	0.00227
14732	TS.triHPacyl.COelim.tppmpmpmd	9.192e+43	5.14	5.14	1.647e+40	0.00227
14733	TS.triHPacyl.COelim.pmptmmpd	1.227e+44	5.32	5.32	1.638e+40	0.00226
14734	TS.triHPacyl.COelim.tttmmmtmpd	2.141e+44	5.65	5.65	1.636e+40	0.00226
14735	TS.triHPacyl.COelim.tppmtmmmd	1.918e+43	4.21	4.21	1.634e+40	0.00226

14736	TS.triHPacyl.COelim.mppmmmpmnd	2.780e+44	5.81	5.81	1.632e+40	0.00225
14737	TS.triHPacyl.COelim.pmtppppppd	9.343e+44	6.53	6.53	1.625e+40	0.00224
14738	TS.triHPacyl.COelim.pptpmtmpd	1.371e+45	6.77	6.77	1.616e+40	0.00223
14739	TS.triHPacyl.COelim.tttpmttppd	1.449e+44	5.43	5.43	1.596e+40	0.0022
14740	TS.triHPacyl.COelim.mmpmptpppd	2.824e+44	5.84	5.84	1.566e+40	0.00216
14741	TS.triHPacyl.COelim.tttpmmtppd	1.605e+44	5.51	5.51	1.564e+40	0.00216
14742	TS.triHPacyl.COelim.pmtmptmpd	5.465e+44	6.24	6.24	1.563e+40	0.00216
14743	TS.triHPacyl.COelim.tnmpmtmmpd	2.040e+44	5.65	5.65	1.552e+40	0.00214
14744	TS.triHPacyl.COelim.mppmptmnd	4.201e+44	6.09	6.09	1.549e+40	0.00214
14745	TS.triHPacyl.COelim.pttmppmnd	3.368e+44	5.96	5.96	1.542e+40	0.00213
14746	TS.triHPacyl.COelim.ptpppptppd	6.782e+43	5.00	5.00	1.539e+40	0.00213
14747	TS.triHPacyl.COelim.ppmtmmmpd	6.635e+44	6.36	6.36	1.537e+40	0.00212
14748	TS.triHPacyl.COelim.pmmppmnd	2.004e+44	5.65	5.65	1.533e+40	0.00212
14749	TS.triHPacyl.COelim.mmtpmmtppd	9.828e+44	6.60	6.60	1.517e+40	0.00209
14750	TS.triHPacyl.COelim.ppmtmmpd	4.422e+44	6.13	6.13	1.515e+40	0.00209
14751	TS.triHPacyl.COelim.pttptmnd	1.868e+44	5.62	5.62	1.512e+40	0.00209
14752	TS.triHPacyl.COelim.pppmmpppd	9.845e+43	5.24	5.24	1.504e+40	0.00208
14753	TS.triHPacyl.COelim.tptmmpmpd	5.586e+44	6.28	6.28	1.492e+40	0.00206
14754	TS.triHPacyl.COelim.mptmptmpd	3.689e+44	6.03	6.03	1.491e+40	0.00206
14755	TS.triHPacyl.COelim.pptppppmd	5.770e+44	6.30	6.30	1.488e+40	0.00205
14756	TS.triHPacyl.COelim.pmttptmpd	4.825e+44	6.20	6.20	1.477e+40	0.00204
14757	TS.triHPacyl.COelim.ppmtmmpppd	3.653e+44	6.04	6.04	1.464e+40	0.00202
14758	TS.triHPacyl.COelim.mmtmmpmpd	3.557e+44	6.03	6.03	1.450e+40	0.00202
14759	TS.triHPacyl.COelim.tmpmmtppd	2.249e+44	5.75	5.75	1.446e+40	0.002
14760	TS.triHPacyl.COelim.mppppmnd	3.468e+43	4.65	4.65	1.432e+40	0.00198
14761	TS.triHPacyl.COelim.tmtmtppmd	1.408e+45	6.86	6.86	1.427e+40	0.00197
14762	TS.triHPacyl.COelim.tpmmpmmpd	1.052e+44	5.31	5.31	1.424e+40	0.00197
14763	TS.triHPacyl.COelim.mmtmmmtmpd	9.833e+44	6.64	6.64	1.422e+40	0.00196
14764	TS.triHPacyl.COelim.mppmptmnd	8.480e+44	6.56	6.56	1.418e+40	0.00196
14765	TS.triHPacyl.COelim.pmmppppmpd	3.267e+43	4.63	4.63	1.391e+40	0.00192
14766	TS.triHPacyl.COelim.mmttmmmpd	7.924e+44	6.53	6.53	1.382e+40	0.00191
14767	TS.triHPacyl.COelim.ttmmtmtpd	1.409e+45	6.88	6.88	1.380e+40	0.00191
14768	TS.triHPacyl.COelim.mtmmpmnd	2.533e+45	7.23	7.23	1.376e+40	0.0019
14769	TS.triHPacyl.COelim.pptppppmd	3.266e+44	6.02	6.02	1.354e+40	0.00187
14770	TS.triHPacyl.COelim.tptpppppd	7.996e+44	6.55	6.55	1.346e+40	0.00186
14771	TS.triHPacyl.COelim.ttpmmtmpd	1.105e+44	5.37	5.37	1.342e+40	0.00185
14772	TS.triHPacyl.COelim.pppppppmd	3.386e+44	6.05	6.05	1.336e+40	0.00184
14773	TS.triHPacyl.COelim.pppmptmnd	1.668e+44	5.62	5.62	1.334e+40	0.00184
14774	TS.triHPacyl.COelim.tmtmttppd	9.779e+44	6.68	6.68	1.332e+40	0.00184
14775	TS.triHPacyl.COelim.pmtmmpmpd	3.320e+44	6.04	6.04	1.321e+40	0.00182
14776	TS.triHPacyl.COelim.pttppptmpd	1.080e+44	5.37	5.37	1.314e+40	0.00181
14777	TS.triHPacyl.COelim.pmmmpmtmpd	2.440e+44	5.86	5.86	1.313e+40	0.00181
14778	TS.triHPacyl.COelim.pttmmtpmd	2.871e+44	5.96	5.96	1.306e+40	0.0018
14779	TS.triHPacyl.COelim.tnmpmtmnd	5.677e+44	6.37	6.37	1.304e+40	0.0018
14780	TS.triHPacyl.COelim.ppmmpmnd	5.199e+44	6.32	6.32	1.303e+40	0.0018
14781	TS.triHPacyl.COelim.pmtmmpmpd	3.708e+44	6.12	6.12	1.286e+40	0.00178
14782	TS.triHPacyl.COelim.pmmptmnd	3.907e+44	6.15	6.15	1.286e+40	0.00178
14783	TS.triHPacyl.COelim.tnmpmtppd	4.665e+44	6.26	6.26	1.275e+40	0.00176
14784	TS.triHPacyl.COelim.tttppmmpd	1.450e+44	5.57	5.57	1.273e+40	0.00176
14785	TS.triHPacyl.COelim.pttppmmpd	3.854e+44	6.16	6.16	1.265e+40	0.00175
14786	TS.triHPacyl.COelim.tppmmpmnd	2.297e+45	7.23	7.23	1.237e+40	0.00171
14787	TS.triHPacyl.COelim.tttmmmmnd	8.290e+43	5.25	5.25	1.234e+40	0.0017
14788	TS.triHPacyl.COelim.tppmmmpd	3.442e+44	6.10	6.10	1.232e+40	0.0017
14789	TS.triHPacyl.COelim.mmtptppd	5.773e+44	6.42	6.42	1.220e+40	0.00169
14790	TS.triHPacyl.COelim.tttmmpmnd	7.297e+45	7.94	7.94	1.209e+40	0.00167
14791	TS.triHPacyl.COelim.pttmtmnd	7.034e+43	5.17	5.17	1.205e+40	0.00166
14792	TS.triHPacyl.COelim.tmmptppd	3.870e+44	6.19	6.19	1.199e+40	0.00165
14793	TS.triHPacyl.COelim.ttmmtmmpd	4.026e+44	6.22	6.22	1.188e+40	0.00164
14794	TS.triHPacyl.COelim.tttmmtmnd	6.343e+43	5.12	5.12	1.187e+40	0.00164
14795	TS.triHPacyl.COelim.pmttptppd	4.704e+44	6.32	6.32	1.179e+40	0.00163
14796	TS.triHPacyl.COelim.pptmptmpd	2.203e+44	5.87	5.87	1.174e+40	0.00162
14797	TS.triHPacyl.COelim.mmmmtmmpd	3.101e+44	6.07	6.07	1.166e+40	0.00161
14798	TS.triHPacyl.COelim.ptmptmpd	7.205e+44	6.58	6.58	1.158e+40	0.0016
14799	TS.triHPacyl.COelim.pppmmmpd	9.047e+43	5.35	5.35	1.141e+40	0.00158
14800	TS.triHPacyl.COelim.pmmptmnd	2.108e+44	5.86	5.86	1.139e+40	0.00157
14801	TS.triHPacyl.COelim.ttpmtpd	8.828e+43	5.34	5.34	1.135e+40	0.00157
14802	TS.triHPacyl.COelim.tppmtmpd	1.630e+45	7.08	7.08	1.131e+40	0.00156
14803	TS.triHPacyl.COelim.ttmmtmmpd	1.017e+45	6.80	6.80	1.126e+40	0.00156
14804	TS.triHPacyl.COelim.tmtptmnd	1.301e+45	6.95	6.95	1.123e+40	0.00155
14805	TS.triHPacyl.COelim.ppttptmpd	2.169e+44	5.88	5.88	1.120e+40	0.00155
14806	TS.triHPacyl.COelim.tppmmtmnd	4.960e+44	6.39	6.39	1.107e+40	0.00153
14807	TS.triHPacyl.COelim.tppmmtmpd	6.051e+44	6.51	6.51	1.104e+40	0.00152

14808	TS.triHPacyl.COelim.ttpmtpmpmd	4.082e+43	4.90	4.90	1.100e+40	0.00152
14809	TS.triHPacyl.COelim.mmpppmpmd	5.449e+43	5.07	5.07	1.095e+40	0.00151
14810	TS.triHPacyl.COelim.ppmtmppmpmd	1.894e+44	5.82	5.82	1.087e+40	0.0015
14811	TS.triHPacyl.COelim.tttmmtmpmd	1.377e+44	5.64	5.64	1.079e+40	0.00149
14812	TS.triHPacyl.COelim.pmtmmppmpmd	2.813e+44	6.07	6.07	1.073e+40	0.00148
14813	TS.triHPacyl.COelim.tmpmmmpmpmd	6.083e+43	5.15	5.15	1.072e+40	0.00148
14814	TS.triHPacyl.COelim.tppppmpmd	9.095e+43	5.40	5.40	1.067e+40	0.00147
14815	TS.triHPacyl.COelim.ttmmpmpmd	9.557e+44	6.80	6.80	1.065e+40	0.00147
14816	TS.triHPacyl.COelim.pmttptmpmd	4.071e+44	6.29	6.29	1.061e+40	0.00146
14817	TS.triHPacyl.COelim.pmttppmpmd	2.772e+45	7.44	7.44	1.061e+40	0.00146
14818	TS.triHPacyl.COelim.mmppppmpmd	5.290e+43	5.08	5.08	1.054e+40	0.00146
14819	TS.triHPacyl.COelim.ptmtptmpmd	2.564e+44	6.02	6.02	1.050e+40	0.00145
14820	TS.triHPacyl.COelim.pttpptmpmd	5.206e+43	5.08	5.08	1.045e+40	0.00144
14821	TS.triHPacyl.COelim.ppmtmpmmmd	4.029e+44	6.30	6.30	1.041e+40	0.00144
14822	TS.triHPacyl.COelim.mmtmmtmpmd	6.809e+44	6.61	6.61	1.040e+40	0.00144
14823	TS.triHPacyl.COelim.ttmmtmpmd	5.879e+43	5.15	5.15	1.037e+40	0.00143
14824	TS.triHPacyl.COelim.tmpmmtpmd	2.565e+44	6.03	6.03	1.035e+40	0.00143
14825	TS.triHPacyl.COelim.pmpptmpmd	4.791e+43	5.04	5.04	1.021e+40	0.00141
14826	TS.triHPacyl.COelim.tttptmpmd	8.520e+44	6.76	6.76	1.015e+40	0.0014
14827	TS.triHPacyl.COelim.tptmpmpmd	3.674e+44	6.26	6.26	1.008e+40	0.00139
14828	TS.triHPacyl.COelim.tpmmpmpmd	3.605e+44	6.25	6.25	1.006e+40	0.00139
14829	TS.triHPacyl.COelim.ttmppmpmd	4.553e+44	6.39	6.39	1.006e+40	0.00139
14830	TS.triHPacyl.COelim.pmtppmpmd	2.191e+44	5.96	5.96	9.980e+39	0.00138
14831	TS.triHPacyl.COelim.mpmmpmpmd	2.603e+43	4.69	4.69	9.912e+39	0.00137
14832	TS.triHPacyl.COelim.tpptmtmpmd	7.382e+44	6.69	6.69	9.909e+39	0.00137
14833	TS.triHPacyl.COelim.ttmmtmpmd	9.967e+44	6.87	6.87	9.844e+39	0.00136
14834	TS.triHPacyl.COelim.tppppmpmd	1.031e+44	5.52	5.52	9.824e+39	0.00136
14835	TS.triHPacyl.COelim.ttpmmtpmd	2.202e+43	4.61	4.61	9.689e+39	0.00134
14836	TS.triHPacyl.COelim.pttmtmpmd	3.836e+43	4.95	4.95	9.566e+39	0.00132
14837	TS.triHPacyl.COelim.pttptmpmd	7.402e+43	5.34	5.34	9.526e+39	0.00132
14838	TS.triHPacyl.COelim.mmmppmpmd	7.784e+43	5.37	5.37	9.510e+39	0.00131
14839	TS.triHPacyl.COelim.ttmmtmpmd	5.798e+44	6.57	6.57	9.508e+39	0.00131
14840	TS.triHPacyl.COelim.tttmmmpmd	2.678e+44	6.11	6.11	9.454e+39	0.00131
14841	TS.triHPacyl.COelim.mptmmmpmd	7.393e+44	6.72	6.72	9.453e+39	0.00131
14842	TS.triHPacyl.COelim.ptpmtpmpmd	2.045e+43	4.58	4.58	9.423e+39	0.0013
14843	TS.triHPacyl.COelim.pttmmmpmd	3.200e+44	6.22	6.22	9.395e+39	0.0013
14844	TS.triHPacyl.COelim.pmtmmmpmd	7.021e+44	6.69	6.69	9.331e+39	0.00129
14845	TS.triHPacyl.COelim.pmpmtmpmd	5.276e+44	6.53	6.53	9.290e+39	0.00128
14846	TS.triHPacyl.COelim.tptmmpmpmd	9.827e+44	6.90	6.90	9.276e+39	0.00128
14847	TS.triHPacyl.COelim.tpppmpmd	5.320e+44	6.53	6.53	9.268e+39	0.00128
14848	TS.triHPacyl.COelim.tpmmpmpmd	3.749e+44	6.32	6.32	9.258e+39	0.00128
14849	TS.triHPacyl.COelim.mtpmpmpmd	3.153e+43	4.85	4.85	9.232e+39	0.00127
14850	TS.triHPacyl.COelim.tppmtpmpmd	4.704e+44	6.46	6.46	9.230e+39	0.00127
14851	TS.triHPacyl.COelim.pttppmpmd	4.944e+43	5.12	5.12	9.205e+39	0.00127
14852	TS.triHPacyl.COelim.mmpppmpmd	6.705e+43	5.30	5.30	9.163e+39	0.00127
14853	TS.triHPacyl.COelim.ttmmtmpmd	4.868e+44	6.49	6.49	9.126e+39	0.00126
14854	TS.triHPacyl.COelim.tmmppmpmd	1.585e+45	7.20	7.20	9.069e+39	0.00125
14855	TS.triHPacyl.COelim.tttmmtmpmd	1.508e+44	5.79	5.79	9.064e+39	0.00125
14856	TS.triHPacyl.COelim.tmpmtmpmd	4.049e+44	6.38	6.38	9.061e+39	0.00125
14857	TS.triHPacyl.COelim.ttpppmpmd	1.723e+44	5.88	5.88	9.006e+39	0.00124
14858	TS.triHPacyl.COelim.pptptmpmd	1.314e+44	5.72	5.72	9.005e+39	0.00124
14859	TS.triHPacyl.COelim.ppmtpmpmd	5.207e+44	6.54	6.54	8.942e+39	0.00123
14860	TS.triHPacyl.COelim.tmtmtmpmd	2.059e+45	7.36	7.36	8.939e+39	0.00123
14861	TS.triHPacyl.COelim.mmtptmpmd	1.105e+45	6.99	6.99	8.911e+39	0.00123
14862	TS.triHPacyl.COelim.tmpmtmpmd	2.923e+44	6.20	6.20	8.887e+39	0.00123
14863	TS.triHPacyl.COelim.ptpmpmpmd	1.286e+43	4.34	4.34	8.868e+39	0.00122
14864	TS.triHPacyl.COelim.tmpmpmpmd	1.222e+44	5.69	5.69	8.818e+39	0.00122
14865	TS.triHPacyl.COelim.ptpmmpmpmd	1.823e+43	4.56	4.56	8.745e+39	0.00121
14866	TS.triHPacyl.COelim.ttmmtmpmd	6.725e+44	6.71	6.71	8.724e+39	0.0012
14867	TS.triHPacyl.COelim.pttmmmpmd	8.770e+43	5.49	5.49	8.719e+39	0.0012
14868	TS.triHPacyl.COelim.tmpmpmpmd	3.122e+44	6.25	6.25	8.718e+39	0.0012
14869	TS.triHPacyl.COelim.pmtppmpmd	4.699e+44	6.50	6.50	8.689e+39	0.0012
14870	TS.triHPacyl.COelim.ptppmpmpmd	1.834e+43	4.57	4.57	8.554e+39	0.00118
14871	TS.triHPacyl.COelim.pmtptmpmd	3.307e+44	6.30	6.30	8.539e+39	0.00118
14872	TS.triHPacyl.COelim.tpppmpmd	1.891e+45	7.34	7.34	8.483e+39	0.00117
14873	TS.triHPacyl.COelim.pmtmtmpmd	8.397e+44	6.86	6.86	8.460e+39	0.00117
14874	TS.triHPacyl.COelim.pmpmpmpmd	3.674e+44	6.37	6.37	8.411e+39	0.00116
14875	TS.triHPacyl.COelim.tppmtpmpmd	7.530e+44	6.81	6.81	8.269e+39	0.00114
14876	TS.triHPacyl.COelim.mtmppmpmd	1.222e+44	5.72	5.72	8.258e+39	0.00114
14877	TS.triHPacyl.COelim.mmtptmpmd	5.115e+44	6.58	6.58	8.248e+39	0.00114
14878	TS.triHPacyl.COelim.pmtmtmpmd	4.601e+44	6.53	6.53	8.103e+39	0.00112
14879	TS.triHPacyl.COelim.tptmmmpmd	1.860e+44	5.99	5.99	8.082e+39	0.00112

14880	TS.triHPacyl.COelim.tpmmpmmpmd	1.422e+44	5.83	5.83	8.059e+39	0.00111
14881	TS.triHPacyl.COelim.ttmtptmmpd	3.215e+45	7.69	7.69	8.027e+39	0.00111
14882	TS.triHPacyl.COelim.pttpptmmpd	9.818e+43	5.61	5.61	8.016e+39	0.00111
14883	TS.triHPacyl.COelim.pppmmpmmpmd	7.388e+44	6.82	6.82	7.956e+39	0.0011
14884	TS.triHPacyl.COelim.pttpptmmpd	2.678e+44	6.22	6.22	7.909e+39	0.00109
14885	TS.triHPacyl.COelim.ptmpmtmpmd	7.045e+43	5.42	5.42	7.903e+39	0.00109
14886	TS.triHPacyl.COelim.pmtptmtpd	5.317e+44	6.63	6.63	7.850e+39	0.00108
14887	TS.triHPacyl.COelim.ptmpmtmpmd	1.677e+44	5.94	5.94	7.833e+39	0.00108
14888	TS.triHPacyl.COelim.tmmtmmtppd	1.013e+45	7.02	7.02	7.804e+39	0.00108
14889	TS.triHPacyl.COelim.tpttmmpmmd	6.201e+44	6.73	6.73	7.746e+39	0.00107
14890	TS.triHPacyl.COelim.pppmptmmd	1.180e+45	7.11	7.11	7.746e+39	0.00107
14891	TS.triHPacyl.COelim.tptmmtmpmd	2.014e+45	7.43	7.43	7.731e+39	0.00107
14892	TS.triHPacyl.COelim.mmmppmnmmd	6.222e+43	5.36	5.36	7.707e+39	0.00106
14893	TS.triHPacyl.COelim.mpmtptmtpd	1.511e+45	7.28	7.28	7.557e+39	0.00104
14894	TS.triHPacyl.COelim.tttppmmpd	6.413e+44	6.77	6.77	7.543e+39	0.00104
14895	TS.triHPacyl.COelim.tpmmpppppd	2.838e+44	6.29	6.29	7.419e+39	0.00102
14896	TS.triHPacyl.COelim.mmtptmmpd	1.014e+45	7.05	7.05	7.413e+39	0.00102
14897	TS.triHPacyl.COelim.tppmmpmmd	1.875e+44	6.05	6.05	7.371e+39	0.00102
14898	TS.triHPacyl.COelim.mtmppppmd	5.641e+43	5.33	5.33	7.366e+39	0.00102
14899	TS.triHPacyl.COelim.tmtptmtpd	9.101e+44	6.99	6.99	7.366e+39	0.00102
14900	TS.triHPacyl.COelim.pmpmtmtpd	3.987e+44	6.50	6.50	7.363e+39	0.00102
14901	TS.triHPacyl.COelim.mppmmtmmd	8.723e+44	6.97	6.97	7.358e+39	0.00102
14902	TS.triHPacyl.COelim.tmmtmmtmpd	1.048e+45	7.08	7.08	7.351e+39	0.00101
14903	TS.triHPacyl.COelim.tpppmtmpd	2.022e+45	7.47	7.47	7.295e+39	0.00101
14904	TS.triHPacyl.COelim.pmmtptmmpd	1.856e+44	6.05	6.05	7.278e+39	0.001
14905	TS.triHPacyl.COelim.tmmtmmtmpd	6.850e+44	6.83	6.83	7.241e+39	0.001
14906	TS.triHPacyl.COelim.tpmmpmmpd	1.243e+44	5.81	5.81	7.238e+39	0.000999
14907	TS.triHPacyl.COelim.ptptmtpmd	6.243e+44	6.78	6.78	7.231e+39	0.000998
14908	TS.triHPacyl.COelim.tmttmmpmd	1.554e+45	7.32	7.32	7.227e+39	0.000998
14909	TS.triHPacyl.COelim.ppttpmmpd	2.583e+44	6.25	6.25	7.219e+39	0.000997
14910	TS.triHPacyl.COelim.pptppmtpd	2.280e+45	7.55	7.55	7.212e+39	0.000996
14911	TS.triHPacyl.COelim.ptttmtpmd	2.555e+44	6.25	6.25	7.211e+39	0.000996
14912	TS.triHPacyl.COelim.pmppmmpmmd	1.499e+44	5.93	5.93	7.134e+39	0.000985
14913	TS.triHPacyl.COelim.pmtptmtpd	1.438e+44	5.91	5.91	7.103e+39	0.000981
14914	TS.triHPacyl.COelim.tptmtpmtpd	6.162e+44	6.78	6.78	7.093e+39	0.000979
14915	TS.triHPacyl.COelim.pppmmpmmpd	2.455e+44	6.23	6.23	7.081e+39	0.000978
14916	TS.triHPacyl.COelim.ptmtpmmpd	2.132e+44	6.16	6.16	6.954e+39	0.00096
14917	TS.triHPacyl.COelim.mptpmmpmmd	2.902e+44	6.35	6.35	6.915e+39	0.000955
14918	TS.triHPacyl.COelim.tptmmtmmd	1.544e+45	7.34	7.34	6.909e+39	0.000954
14919	TS.triHPacyl.COelim.mmpmmpmmpd	2.245e+44	6.20	6.20	6.874e+39	0.000949
14920	TS.triHPacyl.COelim.tptmmpmmd	5.689e+44	6.75	6.75	6.861e+39	0.000947
14921	TS.triHPacyl.COelim.tppmmtmmd	3.117e+44	6.40	6.40	6.818e+39	0.000941
14922	TS.triHPacyl.COelim.ptttmtpmd	3.261e+44	6.43	6.43	6.800e+39	0.000939
14923	TS.triHPacyl.COelim.mttppmmpmmd	1.066e+44	5.76	5.76	6.789e+39	0.000937
14924	TS.triHPacyl.COelim.pmtmmtpmd	2.144e+44	6.18	6.18	6.747e+39	0.000932
14925	TS.triHPacyl.COelim.pmtptmmpd	9.956e+43	5.73	5.73	6.716e+39	0.000927
14926	TS.triHPacyl.COelim.mtppmmpmmd	3.740e+43	5.15	5.15	6.647e+39	0.000918
14927	TS.triHPacyl.COelim.ptmmpmmpd	5.401e+43	5.37	5.37	6.594e+39	0.00091
14928	TS.triHPacyl.COelim.tmptmmtppd	5.402e+44	6.75	6.75	6.580e+39	0.000908
14929	TS.triHPacyl.COelim.ptmtpmmpd	3.375e+44	6.47	6.47	6.543e+39	0.000903
14930	TS.triHPacyl.COelim.tptmtpmtpd	1.755e+45	7.46	7.46	6.507e+39	0.000898
14931	TS.triHPacyl.COelim.mtmppppmmd	2.414e+43	4.90	4.90	6.458e+39	0.000892
14932	TS.triHPacyl.COelim.tmmmpmmtmmd	4.551e+44	6.66	6.66	6.453e+39	0.000891
14933	TS.triHPacyl.COelim.tpmppmtpmd	2.583e+44	6.32	6.32	6.430e+39	0.000888
14934	TS.triHPacyl.COelim.pmpppmtpmd	1.202e+44	5.86	5.86	6.421e+39	0.000887
14935	TS.triHPacyl.COelim.ptmmtmtpmd	1.063e+45	7.17	7.17	6.387e+39	0.000882
14936	TS.triHPacyl.COelim.tttmmpmmpd	1.316e+45	7.29	7.29	6.385e+39	0.000882
14937	TS.triHPacyl.COelim.pmpmtpmmd	8.505e+43	5.66	5.66	6.374e+39	0.00088
14938	TS.triHPacyl.COelim.ptppmtpmd	4.936e+43	5.34	5.34	6.336e+39	0.000875
14939	TS.triHPacyl.COelim.ptmmpmtpd	5.053e+43	5.36	5.36	6.331e+39	0.000874
14940	TS.triHPacyl.COelim.mppmmpmmpd	5.902e+43	5.45	5.45	6.309e+39	0.000871
14941	TS.triHPacyl.COelim.tttmtpmtpd	2.648e+44	6.35	6.35	6.290e+39	0.000869
14942	TS.triHPacyl.COelim.tptmtpmmpd	2.624e+45	7.72	7.72	6.270e+39	0.000866
14943	TS.triHPacyl.COelim.mptmmpmmpd	4.542e+44	6.68	6.68	6.229e+39	0.00086
14944	TS.triHPacyl.COelim.pmmmtmmpd	5.312e+43	5.40	5.40	6.224e+39	0.000859
14945	TS.triHPacyl.COelim.ptppmmpmd	2.560e+43	4.96	4.96	6.222e+39	0.000859
14946	TS.triHPacyl.COelim.pmtmtpmmpd	3.739e+44	6.56	6.56	6.198e+39	0.000856
14947	TS.triHPacyl.COelim.mppmmpmmpd	4.809e+45	8.09	8.09	6.191e+39	0.000855
14948	TS.triHPacyl.COelim.tppmtpmtpd	8.212e+44	7.03	7.03	6.188e+39	0.000854
14949	TS.triHPacyl.COelim.mtpmmpmmpd	3.225e+43	5.10	5.10	6.182e+39	0.000854
14950	TS.triHPacyl.COelim.tmptmtpmd	4.523e+44	6.69	6.69	6.088e+39	0.000841
14951	TS.triHPacyl.COelim.mppmtpmmpd	4.618e+43	5.33	5.33	6.086e+39	0.00084

14952	TS.triHPacyl.COelim.tpmmptppd	5.584e+44	6.81	6.81	6.081e+39	0.00084
14953	TS.triHPacyl.COelim.mmtpmmmmpd	3.070e+44	6.46	6.46	6.070e+39	0.000838
14954	TS.triHPacyl.COelim.tptmtppmd	1.298e+45	7.32	7.32	6.027e+39	0.000832
14955	TS.triHPacyl.COelim.tpmmmtpmmd	3.121e+44	6.47	6.47	6.018e+39	0.000831
14956	TS.triHPacyl.COelim.tmpmptppd	5.136e+44	6.77	6.77	5.991e+39	0.000827
14957	TS.triHPacyl.COelim.pmpptppd	8.268e+43	5.68	5.68	5.974e+39	0.000825
14958	TS.triHPacyl.COelim.tmtpmtpmd	7.998e+44	7.04	7.04	5.941e+39	0.00082
14959	TS.triHPacyl.COelim.mmpptppmd	1.330e+44	5.98	5.98	5.896e+39	0.000814
14960	TS.triHPacyl.COelim.pmmtpmmmd	1.130e+44	5.88	5.88	5.858e+39	0.000809
14961	TS.triHPacyl.COelim.tppmptppd	3.295e+44	6.52	6.52	5.852e+39	0.000808
14962	TS.triHPacyl.COelim.pmtmtmmpd	6.004e+44	6.88	6.88	5.841e+39	0.000806
14963	TS.triHPacyl.COelim.mttmmmpmd	7.959e+44	7.05	7.05	5.823e+39	0.000804
14964	TS.triHPacyl.COelim.pmtmptppd	5.008e+44	6.77	6.77	5.813e+39	0.000803
14965	TS.triHPacyl.COelim.tppppmpd	8.077e+44	7.06	7.06	5.812e+39	0.000802
14966	TS.triHPacyl.COelim.tppmmmpd	7.480e+43	5.24	5.24	5.759e+39	0.000795
14967	TS.triHPacyl.COelim.tppmmmmmd	6.278e+44	6.92	6.92	5.755e+39	0.000795
14968	TS.triHPacyl.COelim.tptpmtmmd	4.441e+45	8.08	8.08	5.748e+39	0.000794
14969	TS.triHPacyl.COelim.mtppmpmpd	2.858e+44	6.45	6.45	5.744e+39	0.000793
14970	TS.triHPacyl.COelim.mtmtpmmpd	5.460e+44	6.83	6.83	5.736e+39	0.000792
14971	TS.triHPacyl.COelim.mmpptmtpmd	3.669e+44	6.60	6.60	5.734e+39	0.000792
14972	TS.triHPacyl.COelim.tttmmtpd	2.281e+44	6.31	6.31	5.728e+39	0.000791
14973	TS.triHPacyl.COelim.tmtmtpmmd	1.271e+44	5.97	5.97	5.726e+39	0.000791
14974	TS.triHPacyl.COelim.pppmptppd	1.050e+45	7.23	7.23	5.714e+39	0.000789
14975	TS.triHPacyl.COelim.tptpmmmmd	1.676e+45	7.51	7.51	5.697e+39	0.000787
14976	TS.triHPacyl.COelim.pmpptmmmd	4.031e+43	5.29	5.29	5.652e+39	0.00078
14977	TS.triHPacyl.COelim.tmmtmmtmmd	7.630e+44	7.04	7.04	5.631e+39	0.000777
14978	TS.triHPacyl.COelim.mtpppmpd	1.693e+44	6.15	6.15	5.606e+39	0.000774
14979	TS.triHPacyl.COelim.pmptmmtmmd	4.168e+44	6.69	6.69	5.549e+39	0.000766
14980	TS.triHPacyl.COelim.tpptmtpmd	1.119e+45	7.29	7.29	5.475e+39	0.000756
14981	TS.triHPacyl.COelim.pmpmpmpmd	2.175e+43	4.94	4.94	5.465e+39	0.000755
14982	TS.triHPacyl.COelim.tmpmpmtpd	5.448e+44	6.86	6.86	5.442e+39	0.000751
14983	TS.triHPacyl.COelim.tmpppmtpd	6.295e+43	5.58	5.58	5.424e+39	0.000749
14984	TS.triHPacyl.COelim.tmtmmtmmd	8.087e+44	7.11	7.11	5.394e+39	0.000745
14985	TS.triHPacyl.COelim.tppmtpppd	1.416e+44	6.07	6.07	5.381e+39	0.000743
14986	TS.triHPacyl.COelim.mtmmmmmpd	5.472e+44	6.88	6.88	5.353e+39	0.000739
14987	TS.triHPacyl.COelim.tmtmmpmpd	1.769e+44	6.22	6.22	5.213e+39	0.00072
14988	TS.triHPacyl.COelim.mtmtmmpd	9.423e+43	5.84	5.84	5.211e+39	0.00072
14989	TS.triHPacyl.COelim.pttpttppd	2.063e+44	6.31	6.31	5.198e+39	0.000718
14990	TS.triHPacyl.COelim.pttpmmmpd	1.765e+44	6.22	6.22	5.173e+39	0.000714
14991	TS.triHPacyl.COelim.mmtpmtpmd	4.024e+45	8.09	8.09	5.170e+39	0.000714
14992	TS.triHPacyl.COelim.tpmmmmtmmd	4.301e+45	8.13	8.13	5.155e+39	0.000712
14993	TS.triHPacyl.COelim.tptmtppd	1.609e+45	7.55	7.55	5.131e+39	0.000708
14994	TS.triHPacyl.COelim.tmmmtmmd	5.200e+44	6.87	6.87	5.105e+39	0.000705
14995	TS.triHPacyl.COelim.tptmtpppd	2.104e+44	6.34	6.34	5.079e+39	0.000701
14996	TS.triHPacyl.COelim.pmmtpmmpd	6.468e+44	7.01	7.01	5.077e+39	0.000701
14997	TS.triHPacyl.COelim.pmtppppmd	9.431e+43	5.86	5.86	5.074e+39	0.000701
14998	TS.triHPacyl.COelim.tptppppmd	1.680e+45	7.58	7.58	5.036e+39	0.000695
14999	TS.triHPacyl.COelim.tptmmtmmd	1.785e+45	7.63	7.63	4.926e+39	0.00068
15000	TS.triHPacyl.COelim.tttpmmmmpd	1.215e+44	6.03	6.03	4.918e+39	0.000679
15001	TS.triHPacyl.COelim.tttmmtmmd	9.636e+43	5.90	5.90	4.891e+39	0.000675
15002	TS.triHPacyl.COelim.tttmtmmpd	2.256e+44	6.40	6.40	4.883e+39	0.000674
15003	TS.triHPacyl.COelim.pmmtmmpmd	1.176e+44	6.02	6.02	4.880e+39	0.000674
15004	TS.triHPacyl.COelim.ppptmtpd	2.936e+44	6.56	6.56	4.871e+39	0.000673
15005	TS.triHPacyl.COelim.pmtmmtmmd	4.843e+44	6.86	6.86	4.856e+39	0.00067
15006	TS.triHPacyl.COelim.pmpmtpmmd	3.574e+43	5.31	5.31	4.826e+39	0.000666
15007	TS.triHPacyl.COelim.ptpmtpmmd	1.200e+43	4.66	4.66	4.799e+39	0.000663
15008	TS.triHPacyl.COelim.ptppptppd	3.840e+43	5.36	5.36	4.794e+39	0.000662
15009	TS.triHPacyl.COelim.tttmmmmmpd	1.739e+44	6.26	6.26	4.783e+39	0.00066
15010	TS.triHPacyl.COelim.ttptmmpd	4.615e+44	6.84	6.84	4.781e+39	0.00066
15011	TS.triHPacyl.COelim.tmpmmmpd	6.063e+43	5.63	5.63	4.780e+39	0.00066
15012	TS.triHPacyl.COelim.tpmmtmmpd	4.340e+43	5.44	5.44	4.762e+39	0.000658
15013	TS.triHPacyl.COelim.mptmtpmmd	2.203e+45	7.78	7.78	4.759e+39	0.000657
15014	TS.triHPacyl.COelim.pppptppd	1.457e+44	6.17	6.17	4.668e+39	0.000645
15015	TS.triHPacyl.COelim.tpppmpd	3.193e+44	6.65	6.65	4.586e+39	0.000633
15016	TS.triHPacyl.COelim.mmtmtpmmd	1.297e+45	7.48	7.48	4.581e+39	0.000633
15017	TS.triHPacyl.COelim.pttmmmmmd	7.526e+43	5.79	5.79	4.567e+39	0.000631
15018	TS.triHPacyl.COelim.pmtppmtpd	2.240e+44	6.44	6.44	4.551e+39	0.000628
15019	TS.triHPacyl.COelim.tptmmpmd	1.943e+45	7.73	7.73	4.517e+39	0.000624
15020	TS.triHPacyl.COelim.pmpppmmmd	7.197e+43	5.77	5.77	4.511e+39	0.000623
15021	TS.triHPacyl.COelim.tpmppmtpd	2.105e+44	6.41	6.41	4.504e+39	0.000622
15022	TS.triHPacyl.COelim.mtppmmmpd	1.144e+44	6.05	6.05	4.480e+39	0.000619
15023	TS.triHPacyl.COelim.pmpmtpmmd	1.493e+45	7.58	7.58	4.477e+39	0.000618

15024	TS.triHPacyl.COelim.tmttppmpdpd	4.706e+45	8.27	8.27	4.474e+39	0.000618
15025	TS.triHPacyl.COelim.ppttpttmmd	3.136e+45	8.03	8.03	4.470e+39	0.000617
15026	TS.triHPacyl.COelim.mttmpmmmd	1.377e+44	6.16	6.16	4.465e+39	0.000617
15027	TS.triHPacyl.COelim.tpptpmtmmd	3.156e+45	8.03	8.03	4.462e+39	0.000616
15028	TS.triHPacyl.COelim.mptmmpptpmd	7.998e+44	7.21	7.21	4.452e+39	0.000615
15029	TS.triHPacyl.COelim.pmmmmmpmmd	1.098e+44	6.03	6.03	4.433e+39	0.000612
15030	TS.triHPacyl.COelim.tptpmtmpd	4.434e+45	8.24	8.24	4.392e+39	0.000606
15031	TS.triHPacyl.COelim.pppmptmmpd	4.625e+44	6.90	6.90	4.335e+39	0.000599
15032	TS.triHPacyl.COelim.tppmmmtmmd	6.255e+44	7.08	7.08	4.332e+39	0.000598
15033	TS.triHPacyl.COelim.tppppmpmpd	4.102e+44	6.83	6.83	4.316e+39	0.000596
15034	TS.triHPacyl.COelim.ptmmpptpmd	3.838e+44	6.80	6.80	4.303e+39	0.000594
15035	TS.triHPacyl.COelim.ptptpmmmpd	3.452e+44	6.73	6.73	4.297e+39	0.000593
15036	TS.triHPacyl.COelim.mtmtpttmmd	5.680e+44	7.03	7.03	4.273e+39	0.00059
15037	TS.triHPacyl.COelim.mmptpoptpmd	7.293e+44	7.18	7.18	4.269e+39	0.000589
15038	TS.triHPacyl.COelim.mtttppmmpd	2.243e+44	6.63	6.63	4.260e+39	0.000588
15039	TS.triHPacyl.COelim.tptpmmppmd	8.418e+44	7.27	7.27	4.244e+39	0.000586
15040	TS.triHPacyl.COelim.mmpptpmpmd	3.128e+43	5.31	5.31	4.243e+39	0.000586
15041	TS.triHPacyl.COelim.ppptppmmmd	3.484e+44	6.75	6.75	4.224e+39	0.000583
15042	TS.triHPacyl.COelim.tppmpptmmd	1.270e+44	6.15	6.15	4.202e+39	0.00058
15043	TS.triHPacyl.COelim.tptmtmmpd	3.978e+44	6.83	6.83	4.199e+39	0.00058
15044	TS.triHPacyl.COelim.mtptpoptmmd	2.429e+44	6.54	6.54	4.199e+39	0.00058
15045	TS.triHPacyl.COelim.mptpmmptpd	1.200e+45	7.49	7.49	4.198e+39	0.00058
15046	TS.triHPacyl.COelim.mttppmpppd	2.243e+45	7.87	7.87	4.168e+39	0.000575
15047	TS.triHPacyl.COelim.ttptmtmmd	4.685e+44	6.93	6.93	4.167e+39	0.000575
15048	TS.triHPacyl.COelim.pmtppppmpd	3.818e+44	6.81	6.81	4.160e+39	0.000574
15049	TS.triHPacyl.COelim.ttptpmpmmd	3.643e+44	6.79	6.79	4.149e+39	0.000573
15050	TS.triHPacyl.COelim.tmmpmmtmpd	3.384e+44	6.74	6.74	4.142e+39	0.000572
15051	TS.triHPacyl.COelim.mmptpmtmmd	1.006e+45	7.39	7.39	4.127e+39	0.00057
15052	TS.triHPacyl.COelim.mtppmmpd	5.878e+43	5.70	5.70	4.127e+39	0.00057
15053	TS.triHPacyl.COelim.ptmmpptppd	5.744e+44	7.06	7.06	4.125e+39	0.00057
15054	TS.triHPacyl.COelim.tmmpmmtmpd	1.759e+44	6.36	6.36	4.083e+39	0.000564
15055	TS.triHPacyl.COelim.tptppmpppd	1.150e+45	7.49	7.49	4.044e+39	0.000558
15056	TS.triHPacyl.COelim.tpttmtpppd	9.765e+44	7.39	7.39	4.029e+39	0.000556
15057	TS.triHPacyl.COelim.tmpmmtmpmd	8.705e+43	5.95	5.95	4.003e+39	0.000553
15058	TS.triHPacyl.COelim.tmmmmppmmd	1.918e+44	6.43	6.43	3.994e+39	0.000551
15059	TS.triHPacyl.COelim.ptpppppmd	4.368e+43	5.56	5.56	3.915e+39	0.000541
15060	TS.triHPacyl.COelim.tpmmptmmd	4.020e+45	8.25	8.25	3.905e+39	0.000539
15061	TS.triHPacyl.COelim.pmmpppmpmd	6.299e+43	5.78	5.78	3.875e+39	0.000535
15062	TS.triHPacyl.COelim.mptpmtmmd	4.560e+44	6.96	6.96	3.851e+39	0.000532
15063	TS.triHPacyl.COelim.ttpmmtppd	8.755e+43	5.98	5.98	3.851e+39	0.000532
15064	TS.triHPacyl.COelim.tmttppmpmd	4.781e+45	8.37	8.37	3.840e+39	0.00053
15065	TS.triHPacyl.COelim.mtmtptmpmd	5.333e+43	5.69	5.69	3.834e+39	0.000529
15066	TS.triHPacyl.COelim.tpttmtmmd	1.472e+45	7.67	7.67	3.816e+39	0.000527
15067	TS.triHPacyl.COelim.tppmmmpmd	3.011e+43	5.35	5.35	3.809e+39	0.000526
15068	TS.triHPacyl.COelim.ptmmmtmpmd	1.010e+45	7.45	7.45	3.767e+39	0.00052
15069	TS.triHPacyl.COelim.mttptpmpd	1.372e+45	7.64	7.64	3.758e+39	0.000519
15070	TS.triHPacyl.COelim.mptmmtmpd	1.700e+45	7.76	7.76	3.758e+39	0.000519
15071	TS.triHPacyl.COelim.pptmptmmd	8.522e+44	7.35	7.35	3.752e+39	0.000518
15072	TS.triHPacyl.COelim.mmtppmpppd	2.093e+45	7.89	7.89	3.750e+39	0.000518
15073	TS.triHPacyl.COelim.pppmmpmpd	3.780e+44	6.87	6.87	3.729e+39	0.000515
15074	TS.triHPacyl.COelim.tptpppppd	3.903e+45	8.26	8.26	3.722e+39	0.000514
15075	TS.triHPacyl.COelim.ptmmpmmpd	6.456e+43	5.82	5.82	3.717e+39	0.000513
15076	TS.triHPacyl.COelim.tttmtmpmd	5.453e+44	7.09	7.09	3.710e+39	0.000512
15077	TS.triHPacyl.COelim.ptmmmmmpmd	1.221e+45	7.58	7.58	3.679e+39	0.000508
15078	TS.triHPacyl.COelim.pttmptpmd	1.969e+44	6.49	6.49	3.679e+39	0.000508
15079	TS.triHPacyl.COelim.tppmtpmmd	2.010e+43	5.13	5.13	3.679e+39	0.000508
15080	TS.triHPacyl.COelim.tpmmmtmmd	1.608e+45	7.75	7.75	3.653e+39	0.000504
15081	TS.triHPacyl.COelim.ttmmtmtpd	1.475e+45	7.70	7.70	3.641e+39	0.000503
15082	TS.triHPacyl.COelim.tppmppppd	2.450e+44	6.63	6.63	3.637e+39	0.000502
15083	TS.triHPacyl.COelim.mppmppppd	1.700e+44	6.41	6.41	3.624e+39	0.0005
15084	TS.triHPacyl.COelim.tttmtmpmd	6.727e+44	7.24	7.24	3.603e+39	0.000497
15085	TS.triHPacyl.COelim.pttppmpppd	5.198e+44	7.08	7.08	3.602e+39	0.000497
15086	TS.triHPacyl.COelim.tppmtmmd	2.917e+43	5.37	5.37	3.562e+39	0.000492
15087	TS.triHPacyl.COelim.mppmpmpmd	1.136e+45	7.56	7.56	3.543e+39	0.000489
15088	TS.triHPacyl.COelim.ptmtpmpmd	2.939e+44	6.76	6.76	3.516e+39	0.000486
15089	TS.triHPacyl.COelim.tppmptmpd	4.157e+43	5.59	5.59	3.510e+39	0.000485
15090	TS.triHPacyl.COelim.mpmtpmpd	2.523e+45	8.04	8.04	3.508e+39	0.000484
15091	TS.triHPacyl.COelim.mppmmmmmd	1.369e+44	6.31	6.31	3.482e+39	0.000481
15092	TS.triHPacyl.COelim.tmpmmmmmd	3.527e+44	6.87	6.87	3.464e+39	0.000478
15093	TS.triHPacyl.COelim.tptmmmpmd	2.362e+44	6.64	6.64	3.453e+39	0.000477
15094	TS.triHPacyl.COelim.ppmtpmpd	4.016e+44	6.96	6.96	3.441e+39	0.000475
15095	TS.triHPacyl.COelim.tmmtmpmmd	7.320e+44	7.32	7.32	3.421e+39	0.000472

15096	TS.triHPacyl.COelim.mtmtptmppd	3.724e+44	6.92	6.92	3.404e+39	0.00047
15097	TS.triHPacyl.COelim.mtttptmppd	2.430e+44	6.66	6.66	3.397e+39	0.000469
15098	TS.triHPacyl.COelim.pppmtmppd	7.039e+43	5.93	5.93	3.379e+39	0.000467
15099	TS.triHPacyl.COelim.ttmpmtmppd	1.419e+44	6.35	6.35	3.372e+39	0.000466
15100	TS.triHPacyl.COelim.tppppmmpd	6.455e+43	5.88	5.88	3.358e+39	0.000464
15101	TS.triHPacyl.COelim.ttmppmmmpd	1.575e+44	6.41	6.41	3.353e+39	0.000463
15102	TS.triHPacyl.COelim.ptppmtmmd	7.853e+43	6.00	6.00	3.318e+39	0.000458
15103	TS.triHPacyl.COelim.pmmmtppmd	2.715e+43	5.38	5.38	3.293e+39	0.000455
15104	TS.triHPacyl.COelim.pmtmmppmd	7.219e+44	7.33	7.33	3.277e+39	0.000452
15105	TS.triHPacyl.COelim.mtppppmmd	7.997e+43	6.02	6.02	3.269e+39	0.000451
15106	TS.triHPacyl.COelim.tpptptmmd	1.133e+45	7.60	7.60	3.269e+39	0.000451
15107	TS.triHPacyl.COelim.ttpmtppmd	1.069e+44	6.20	6.20	3.266e+39	0.000451
15108	TS.triHPacyl.COelim.ptpmpmpd	2.766e+43	5.39	5.39	3.262e+39	0.00045
15109	TS.triHPacyl.COelim.mmtppmmmpd	1.476e+45	7.76	7.76	3.254e+39	0.000449
15110	TS.triHPacyl.COelim.mmpmmtmmd	9.948e+44	6.56	6.56	3.246e+39	0.000448
15111	TS.triHPacyl.COelim.tmpmmmpmd	9.014e+43	6.10	6.10	3.223e+39	0.000445
15112	TS.triHPacyl.COelim.tppmptmmd	3.282e+45	8.25	8.25	3.219e+39	0.000444
15113	TS.triHPacyl.COelim.mpttpmpd	1.983e+44	6.58	6.58	3.204e+39	0.000442
15114	TS.triHPacyl.COelim.tmpmtmppd	1.703e+44	6.49	6.49	3.203e+39	0.000442
15115	TS.triHPacyl.COelim.pttmtmppd	2.984e+44	6.82	6.82	3.195e+39	0.000441
15116	TS.triHPacyl.COelim.mptpmtppd	8.941e+44	7.48	7.48	3.193e+39	0.000441
15117	TS.triHPacyl.COelim.pppppmmpd	8.542e+43	6.08	6.08	3.185e+39	0.00044
15118	TS.triHPacyl.COelim.tmpmmtmmd	3.002e+44	6.83	6.83	3.172e+39	0.000438
15119	TS.triHPacyl.COelim.tppmmtmpd	7.328e+44	7.36	7.36	3.162e+39	0.000437
15120	TS.triHPacyl.COelim.pmtptmpmd	2.569e+44	6.75	6.75	3.114e+39	0.00043
15121	TS.triHPacyl.COelim.mppppmtmpd	4.527e+44	7.09	7.09	3.104e+39	0.000429
15122	TS.triHPacyl.COelim.ttmtmtmpd	5.064e+44	7.16	7.16	3.099e+39	0.000428
15123	TS.triHPacyl.COelim.tppmtppmd	6.412e+44	7.30	7.30	3.098e+39	0.000428
15124	TS.triHPacyl.COelim.pptmppmmd	1.626e+44	6.48	6.48	3.081e+39	0.000425
15125	TS.triHPacyl.COelim.tpptptpmd	2.885e+45	8.20	8.20	3.081e+39	0.000425
15126	TS.triHPacyl.COelim.tpppmtmmd	7.613e+44	7.40	7.40	3.075e+39	0.000425
15127	TS.triHPacyl.COelim.pttmtmpmd	6.306e+44	7.29	7.29	3.074e+39	0.000424
15128	TS.triHPacyl.COelim.tmpmmtmpd	3.334e+44	6.91	6.91	3.072e+39	0.000424
15129	TS.triHPacyl.COelim.pmmppptpmd	2.739e+44	6.80	6.80	3.061e+39	0.000423
15130	TS.triHPacyl.COelim.ptppmtppd	2.692e+44	6.79	6.79	3.060e+39	0.000423
15131	TS.triHPacyl.COelim.pppmptppmd	5.065e+44	7.17	7.17	3.036e+39	0.000419
15132	TS.triHPacyl.COelim.mtmtppmmpd	5.733e+44	7.25	7.25	3.013e+39	0.000416
15133	TS.triHPacyl.COelim.tpptmtppd	6.261e+44	7.30	7.30	3.006e+39	0.000415
15134	TS.triHPacyl.COelim.mppmmpmmd	1.157e+44	6.30	6.30	2.970e+39	0.00041
15135	TS.triHPacyl.COelim.ptppptmmd	1.676e+43	5.15	5.15	2.947e+39	0.000407
15136	TS.triHPacyl.COelim.pmmmpmmpd	3.500e+44	6.97	6.97	2.945e+39	0.000407
15137	TS.triHPacyl.COelim.tmtmtmpmd	8.025e+44	7.46	7.46	2.930e+39	0.000405
15138	TS.triHPacyl.COelim.ptpmtppd	4.200e+43	5.71	5.71	2.898e+39	0.0004
15139	TS.triHPacyl.COelim.mppmmmmmpd	2.908e+44	6.87	6.87	2.891e+39	0.000399
15140	TS.triHPacyl.COelim.tpptptppd	1.374e+45	7.79	7.79	2.891e+39	0.000399
15141	TS.triHPacyl.COelim.tppppptmmd	2.244e+44	6.71	6.71	2.884e+39	0.000398
15142	TS.triHPacyl.COelim.tttmtmpmd	3.795e+44	7.03	7.03	2.882e+39	0.000398
15143	TS.triHPacyl.COelim.mmtppmtmmd	9.521e+44	7.58	7.58	2.877e+39	0.000397
15144	TS.triHPacyl.COelim.tmmppmtppd	3.304e+44	6.95	6.95	2.853e+39	0.000394
15145	TS.triHPacyl.COelim.tppppmmpd	1.745e+45	7.95	7.95	2.829e+39	0.000391
15146	TS.triHPacyl.COelim.pmtppmmmd	3.004e+44	6.90	6.90	2.805e+39	0.000387
15147	TS.triHPacyl.COelim.mppppmmpd	1.866e+44	6.62	6.62	2.793e+39	0.000386
15148	TS.triHPacyl.COelim.mtmmptpmd	1.032e+44	6.28	6.28	2.768e+39	0.000382
15149	TS.triHPacyl.COelim.tttmtmpmd	2.681e+44	6.85	6.85	2.761e+39	0.000381
15150	TS.triHPacyl.COelim.tpptmpppd	2.742e+45	8.24	8.24	2.734e+39	0.000378
15151	TS.triHPacyl.COelim.pptpmtppd	3.339e+45	8.36	8.36	2.727e+39	0.000377
15152	TS.triHPacyl.COelim.tmtmmmpmmd	1.905e+45	8.03	8.03	2.703e+39	0.000373
15153	TS.triHPacyl.COelim.ttmtmmmpmd	6.807e+43	6.04	6.04	2.701e+39	0.000373
15154	TS.triHPacyl.COelim.tttmtppmd	1.671e+45	7.95	7.95	2.689e+39	0.000371
15155	TS.triHPacyl.COelim.ttptmppmd	1.875e+44	6.66	6.66	2.652e+39	0.000366
15156	TS.triHPacyl.COelim.tmmppmtmmd	4.343e+44	7.16	7.16	2.651e+39	0.000366
15157	TS.triHPacyl.COelim.mmtppmtpd	2.451e+44	6.82	6.82	2.640e+39	0.000364
15158	TS.triHPacyl.COelim.ptmmmmmpd	6.158e+44	7.37	7.37	2.632e+39	0.000363
15159	TS.triHPacyl.COelim.ptmtptpmd	1.395e+44	6.49	6.49	2.617e+39	0.000361
15160	TS.triHPacyl.COelim.pttptppd	1.845e+44	6.66	6.66	2.594e+39	0.000358
15161	TS.triHPacyl.COelim.tppppppmd	1.439e+44	6.52	6.52	2.573e+39	0.000355
15162	TS.triHPacyl.COelim.tppppmmpd	1.250e+45	7.81	7.81	2.566e+39	0.000354
15163	TS.triHPacyl.COelim.mmtppmtpmd	2.851e+44	6.93	6.93	2.559e+39	0.000353
15164	TS.triHPacyl.COelim.ptmmpmmpd	6.366e+44	7.41	7.41	2.557e+39	0.000353
15165	TS.triHPacyl.COelim.mmmppmmpd	1.397e+45	7.88	7.88	2.547e+39	0.000352
15166	TS.triHPacyl.COelim.pttppmmpd	6.169e+43	6.02	6.02	2.542e+39	0.000351
15167	TS.triHPacyl.COelim.pttptppmd	1.364e+44	6.50	6.50	2.496e+39	0.000345

15168	TS.triHPacyl.COelim.ttmppmpmd	1.122e+44	6.39	6.39	2.463e+39	0.00034
15169	TS.triHPacyl.COelim.tmttmmtmpd	1.897e+45	8.08	8.08	2.458e+39	0.000339
15170	TS.triHPacyl.COelim.tmmmpptmmd	1.150e+45	7.78	7.78	2.456e+39	0.000339
15171	TS.triHPacyl.COelim.pmptmmpmd	6.584e+44	7.45	7.45	2.454e+39	0.000339
15172	TS.triHPacyl.COelim.pmpmtmmpmd	4.072e+44	7.17	7.17	2.433e+39	0.000336
15173	TS.triHPacyl.COelim.mptpmmmmpd	9.039e+44	7.66	7.66	2.392e+39	0.00033
15174	TS.triHPacyl.COelim.mpppmpmpd	7.564e+43	6.18	6.18	2.390e+39	0.00033
15175	TS.triHPacyl.COelim.tpppmpppd	5.383e+44	7.35	7.35	2.368e+39	0.000327
15176	TS.triHPacyl.COelim.pmttptmpmd	4.355e+44	7.23	7.23	2.352e+39	0.000325
15177	TS.triHPacyl.COelim.mttmptmpmd	6.606e+43	6.11	6.11	2.341e+39	0.000323
15178	TS.triHPacyl.COelim.pttmptppd	1.338e+44	6.53	6.53	2.341e+39	0.000323
15179	TS.triHPacyl.COelim.pmtmmtmpd	5.350e+44	7.36	7.36	2.338e+39	0.000323
15180	TS.triHPacyl.COelim.pmmppmtmmd	2.133e+44	6.81	6.81	2.336e+39	0.000323
15181	TS.triHPacyl.COelim.tmptmtpmd	1.190e+45	7.84	7.84	2.309e+39	0.000319
15182	TS.triHPacyl.COelim.pmtmmpmpd	2.403e+44	6.89	6.89	2.301e+39	0.000318
15183	TS.triHPacyl.COelim.mppmtmmpmd	1.607e+44	6.65	6.65	2.296e+39	0.000317
15184	TS.triHPacyl.COelim.mmtmpmpmd	2.075e+44	6.80	6.80	2.292e+39	0.000316
15185	TS.triHPacyl.COelim.tpmmtmpmd	2.811e+45	8.36	8.36	2.291e+39	0.000316
15186	TS.triHPacyl.COelim.ppmtptmmd	1.147e+45	7.82	7.82	2.291e+39	0.000316
15187	TS.triHPacyl.COelim.pmtmmpmpd	2.519e+44	6.92	6.92	2.278e+39	0.000315
15188	TS.triHPacyl.COelim.tmttmmtmpd	1.847e+45	8.11	8.11	2.273e+39	0.000314
15189	TS.triHPacyl.COelim.tpmptmmd	4.915e+44	7.32	7.32	2.269e+39	0.000313
15190	TS.triHPacyl.COelim.mmpmpmpd	1.704e+44	6.69	6.69	2.268e+39	0.000313
15191	TS.triHPacyl.COelim.pmttptppd	1.846e+45	8.12	8.12	2.258e+39	0.000312
15192	TS.triHPacyl.COelim.mppmtpppd	4.308e+44	7.25	7.25	2.250e+39	0.000311
15193	TS.triHPacyl.COelim.tptmmpmpd	5.000e+44	7.34	7.34	2.241e+39	0.000309
15194	TS.triHPacyl.COelim.tpmtmpmpd	8.064e+44	7.63	7.63	2.239e+39	0.000309
15195	TS.triHPacyl.COelim.tppmpmpd	2.120e+44	6.83	6.83	2.236e+39	0.000309
15196	TS.triHPacyl.COelim.ptttptmpd	3.548e+44	7.14	7.14	2.233e+39	0.000308
15197	TS.triHPacyl.COelim.ttmptmpmd	1.002e+45	7.76	7.76	2.231e+39	0.000308
15198	TS.triHPacyl.COelim.tmmmpmtmpd	2.610e+45	8.33	8.33	2.228e+39	0.000308
15199	TS.triHPacyl.COelim.mmpptmmd	1.624e+45	8.05	8.05	2.210e+39	0.000305
15200	TS.triHPacyl.COelim.tpttpmmd	1.742e+45	8.10	8.10	2.187e+39	0.000302
15201	TS.triHPacyl.COelim.tpptptmpd	2.233e+45	8.25	8.25	2.186e+39	0.000302
15202	TS.triHPacyl.COelim.tttmtpmmd	5.811e+44	7.45	7.45	2.175e+39	0.0003
15203	TS.triHPacyl.COelim.ttmmtmmd	6.894e+44	7.56	7.56	2.159e+39	0.000298
15204	TS.triHPacyl.COelim.ptttmmpd	5.759e+44	7.45	7.45	2.157e+39	0.000298
15205	TS.triHPacyl.COelim.pmpptmpd	2.337e+44	6.91	6.91	2.157e+39	0.000298
15206	TS.triHPacyl.COelim.tpptmpmpd	1.012e+45	7.79	7.79	2.143e+39	0.000296
15207	TS.triHPacyl.COelim.mttmmpmpd	2.472e+44	6.95	6.95	2.141e+39	0.000296
15208	TS.triHPacyl.COelim.tpmtptmpd	4.078e+44	7.25	7.25	2.135e+39	0.000295
15209	TS.triHPacyl.COelim.pmtptmmd	1.074e+45	7.83	7.83	2.130e+39	0.000294
15210	TS.triHPacyl.COelim.mtptmpmpd	1.115e+44	6.48	6.48	2.129e+39	0.000294
15211	TS.triHPacyl.COelim.mppmptmmd	3.712e+44	7.20	7.20	2.122e+39	0.000293
15212	TS.triHPacyl.COelim.mmtppmmd	2.013e+44	6.83	6.83	2.116e+39	0.000292
15213	TS.triHPacyl.COelim.mppmmpmmd	1.756e+44	6.75	6.75	2.114e+39	0.000292
15214	TS.triHPacyl.COelim.mpttpmpd	4.018e+44	7.25	7.25	2.101e+39	0.00029
15215	TS.triHPacyl.COelim.ptppmmpd	1.162e+44	6.51	6.51	2.097e+39	0.00029
15216	TS.triHPacyl.COelim.tmmmtmpmd	4.525e+44	7.32	7.32	2.097e+39	0.00029
15217	TS.triHPacyl.COelim.mtptmpmpd	8.839e+43	6.36	6.36	2.066e+39	0.000285
15218	TS.triHPacyl.COelim.mmtmpmtmpd	1.027e+45	7.82	7.82	2.060e+39	0.000284
15219	TS.triHPacyl.COelim.pmtmtpd	2.843e+44	7.06	7.06	2.032e+39	0.000281
15220	TS.triHPacyl.COelim.tmmmpmpd	1.195e+45	7.93	7.93	2.013e+39	0.000278
15221	TS.triHPacyl.COelim.ptttmtpmd	3.218e+44	7.15	7.15	2.007e+39	0.000277
15222	TS.triHPacyl.COelim.tttmtmpd	1.919e+44	6.84	6.84	2.001e+39	0.000276
15223	TS.triHPacyl.COelim.mttmmpmd	1.597e+44	6.73	6.73	1.996e+39	0.000276
15224	TS.triHPacyl.COelim.tptmtpd	5.427e+45	8.84	8.84	1.987e+39	0.000274
15225	TS.triHPacyl.COelim.pmtmmpmd	2.065e+45	8.26	8.26	1.984e+39	0.000274
15226	TS.triHPacyl.COelim.mptpmmtmmd	9.101e+44	7.78	7.78	1.963e+39	0.000271
15227	TS.triHPacyl.COelim.mppmpptmpd	2.513e+44	7.01	7.01	1.952e+39	0.00027
15228	TS.triHPacyl.COelim.tpmppmmd	1.376e+44	6.66	6.66	1.948e+39	0.000269
15229	TS.triHPacyl.COelim.pttpmtmmd	1.460e+44	6.69	6.69	1.948e+39	0.000269
15230	TS.triHPacyl.COelim.tmpppmpmd	7.067e+44	7.64	7.64	1.913e+39	0.000264
15231	TS.triHPacyl.COelim.pmttppmpd	4.510e+44	7.38	7.38	1.913e+39	0.000264
15232	TS.triHPacyl.COelim.mtmmmtmpmd	2.693e+44	7.07	7.07	1.910e+39	0.000264
15233	TS.triHPacyl.COelim.pmttptppd	1.051e+45	7.88	7.88	1.902e+39	0.000263
15234	TS.triHPacyl.COelim.tpmppmtmmd	1.077e+45	7.90	7.90	1.891e+39	0.000261
15235	TS.triHPacyl.COelim.mtmmmtmpmd	8.502e+44	7.76	7.76	1.889e+39	0.000261
15236	TS.triHPacyl.COelim.ttmptmpmd	1.327e+44	6.65	6.65	1.884e+39	0.00026
15237	TS.triHPacyl.COelim.pmpmpmtmpd	6.227e+43	6.21	6.21	1.875e+39	0.000259
15238	TS.triHPacyl.COelim.tptmpppd	2.437e+45	8.39	8.39	1.870e+39	0.000258
15239	TS.triHPacyl.COelim.pmpptmpd	3.401e+44	7.22	7.22	1.866e+39	0.000258

15240	TS.triHPacyl.COelim.ttpmmpppd	1.709e+44	6.81	6.81	1.864e+39	0.000257
15241	TS.triHPacyl.COelim.tmtmmmpmd	1.878e+44	6.87	6.87	1.860e+39	0.000257
15242	TS.triHPacyl.COelim.mtppppmmd	5.626e+43	6.15	6.15	1.858e+39	0.000256
15243	TS.triHPacyl.COelim.tpppppppd	5.429e+44	7.50	7.50	1.857e+39	0.000256
15244	TS.triHPacyl.COelim.mmpptmmmd	3.379e+44	7.22	7.22	1.853e+39	0.000256
15245	TS.triHPacyl.COelim.mppmtppmd	7.320e+44	7.68	7.68	1.848e+39	0.000255
15246	TS.triHPacyl.COelim.tptmmtmpmd	2.421e+44	7.03	7.03	1.844e+39	0.000255
15247	TS.triHPacyl.COelim.tmmmpmtmmd	1.640e+45	8.17	8.17	1.844e+39	0.000255
15248	TS.triHPacyl.COelim.tmmppmtmd	2.800e+44	7.12	7.12	1.831e+39	0.000253
15249	TS.triHPacyl.COelim.tmmtmmpmd	7.345e+44	7.69	7.69	1.830e+39	0.000253
15250	TS.triHPacyl.COelim.mptmmppmd	1.897e+44	6.89	6.89	1.826e+39	0.000252
15251	TS.triHPacyl.COelim.tptmppppmd	4.905e+44	7.46	7.46	1.816e+39	0.000251
15252	TS.triHPacyl.COelim.mmtmptmpd	1.712e+45	8.21	8.21	1.801e+39	0.000249
15253	TS.triHPacyl.COelim.pmmmpmpmd	2.239e+43	5.62	5.62	1.795e+39	0.000248
15254	TS.triHPacyl.COelim.pmmpptpmd	7.260e+43	6.32	6.32	1.794e+39	0.000248
15255	TS.triHPacyl.COelim.tmmtmpppd	9.012e+44	7.83	7.83	1.790e+39	0.000247
15256	TS.triHPacyl.COelim.mtppmtmpmd	1.033e+44	6.54	6.54	1.790e+39	0.000247
15257	TS.triHPacyl.COelim.pmmmpmtmmd	8.044e+44	7.76	7.76	1.779e+39	0.000246
15258	TS.triHPacyl.COelim.tmpppppmd	3.311e+44	7.23	7.23	1.776e+39	0.000245
15259	TS.triHPacyl.COelim.tmmtmppmd	5.704e+44	7.56	7.56	1.770e+39	0.000244
15260	TS.triHPacyl.COelim.pttptmmmd	1.372e+44	6.71	6.71	1.768e+39	0.000244
15261	TS.triHPacyl.COelim.mttmtpmpd	4.549e+44	7.43	7.43	1.766e+39	0.000244
15262	TS.triHPacyl.COelim.pmmtmmpmd	2.697e+44	7.12	7.12	1.762e+39	0.000243
15263	TS.triHPacyl.COelim.mtptppmmd	1.371e+44	6.72	6.72	1.757e+39	0.000243
15264	TS.triHPacyl.COelim.pmmtptppd	7.139e+44	7.70	7.70	1.756e+39	0.000242
15265	TS.triHPacyl.COelim.tptmmmpmd	1.621e+44	6.82	6.82	1.751e+39	0.000242
15266	TS.triHPacyl.COelim.mppmmpmpmd	2.789e+44	7.14	7.14	1.749e+39	0.000242
15267	TS.triHPacyl.COelim.mptmpmpmd	6.742e+44	7.67	7.67	1.745e+39	0.000241
15268	TS.triHPacyl.COelim.tmmpmtmpmd	2.696e+44	7.12	7.12	1.743e+39	0.000241
15269	TS.triHPacyl.COelim.tptmppppmd	1.656e+44	6.84	6.84	1.735e+39	0.00024
15270	TS.triHPacyl.COelim.pttptppd	1.567e+44	6.81	6.81	1.706e+39	0.000236
15271	TS.triHPacyl.COelim.tmtmtmmd	4.947e+44	7.50	7.50	1.695e+39	0.000234
15272	TS.triHPacyl.COelim.pmmtmmmmmd	4.173e+44	7.40	7.40	1.688e+39	0.000233
15273	TS.triHPacyl.COelim.tppmmmpmd	3.103e+45	8.60	8.60	1.680e+39	0.000232
15274	TS.triHPacyl.COelim.tmmttpppd	6.497e+44	7.67	7.67	1.673e+39	0.000231
15275	TS.triHPacyl.COelim.ptmtpmmd	6.821e+43	6.33	6.33	1.661e+39	0.000229
15276	TS.triHPacyl.COelim.tttmmmpmd	2.482e+44	7.10	7.10	1.657e+39	0.000229
15277	TS.triHPacyl.COelim.tmtpppppd	3.238e+45	8.64	8.64	1.657e+39	0.000229
15278	TS.triHPacyl.COelim.tpmtppppd	3.408e+44	7.29	7.29	1.656e+39	0.000229
15279	TS.triHPacyl.COelim.ptmtpppd	6.943e+44	7.72	7.72	1.652e+39	0.000228
15280	TS.triHPacyl.COelim.tmmmmppmd	7.874e+44	7.80	7.80	1.645e+39	0.000227
15281	TS.triHPacyl.COelim.ttpmtppmd	8.918e+43	6.50	6.50	1.629e+39	0.000225
15282	TS.triHPacyl.COelim.tmmtptmpmd	2.519e+44	7.12	7.12	1.628e+39	0.000225
15283	TS.triHPacyl.COelim.mtmmpmpmd	1.309e+45	8.11	8.11	1.625e+39	0.000224
15284	TS.triHPacyl.COelim.pmmmtpppd	5.812e+43	6.25	6.25	1.622e+39	0.000224
15285	TS.triHPacyl.COelim.ptppppppmd	9.803e+43	6.56	6.56	1.620e+39	0.000224
15286	TS.triHPacyl.COelim.tppmmmmmd	1.052e+44	6.61	6.61	1.618e+39	0.000223
15287	TS.triHPacyl.COelim.ttptmtmpd	3.974e+43	6.03	6.03	1.606e+39	0.000222
15288	TS.triHPacyl.COelim.ptptptppd	2.217e+44	7.06	7.06	1.602e+39	0.000221
15289	TS.triHPacyl.COelim.tttppppmd	1.751e+44	6.92	6.92	1.601e+39	0.000221
15290	TS.triHPacyl.COelim.mppppmpmd	1.300e+45	8.11	8.11	1.598e+39	0.000221
15291	TS.triHPacyl.COelim.tmmtptppd	1.908e+46	9.72	9.72	1.592e+39	0.00022
15292	TS.triHPacyl.COelim.tmmpmmpmd	1.295e+44	6.74	6.74	1.590e+39	0.00022
15293	TS.triHPacyl.COelim.pmtmmtmpd	7.987e+44	7.83	7.83	1.589e+39	0.000219
15294	TS.triHPacyl.COelim.tmmpppppmd	2.405e+44	7.11	7.11	1.589e+39	0.000219
15295	TS.triHPacyl.COelim.ttpmmtmmpd	1.772e+43	5.56	5.56	1.577e+39	0.000218
15296	TS.triHPacyl.COelim.mmtppmmpmd	1.981e+44	7.00	7.00	1.573e+39	0.000217
15297	TS.triHPacyl.COelim.pptmpptmmd	9.133e+44	7.92	7.92	1.562e+39	0.000216
15298	TS.triHPacyl.COelim.mtmtmpmd	1.456e+44	6.82	6.82	1.559e+39	0.000215
15299	TS.triHPacyl.COelim.pmmpppppd	2.792e+45	8.60	8.60	1.510e+39	0.000209
15300	TS.triHPacyl.COelim.mmtmmtmpmd	1.224e+45	8.11	8.11	1.506e+39	0.000208
15301	TS.triHPacyl.COelim.ppttpptmmd	3.565e+45	8.75	8.75	1.498e+39	0.000207
15302	TS.triHPacyl.COelim.pmptmtpmmd	3.590e+44	7.39	7.39	1.492e+39	0.000206
15303	TS.triHPacyl.COelim.pttptmppd	3.147e+44	7.31	7.31	1.480e+39	0.000204
15304	TS.triHPacyl.COelim.tptmmpppmd	2.221e+45	8.48	8.48	1.478e+39	0.000204
15305	TS.triHPacyl.COelim.mtmmpmpppd	1.447e+45	8.23	8.23	1.474e+39	0.000204
15306	TS.triHPacyl.COelim.mpppmtmpmd	1.879e+44	7.02	7.02	1.453e+39	0.000201
15307	TS.triHPacyl.COelim.pmmtmmmpmd	3.385e+44	7.37	7.37	1.450e+39	0.0002
15308	TS.triHPacyl.COelim.mppppptmpd	6.275e+44	7.74	7.74	1.443e+39	0.000199
15309	TS.triHPacyl.COelim.pmtmmpmpd	2.748e+44	7.25	7.25	1.443e+39	0.000199
15310	TS.triHPacyl.COelim.mpppmtmpmd	1.217e+45	8.14	8.14	1.438e+39	0.000199
15311	TS.triHPacyl.COelim.mmmmpmtmpmd	1.643e+44	6.95	6.95	1.428e+39	0.000197

15312	TS.triHPacyl.COelim.tptmmtmmd	2.117e+45	8.47	8.47	1.426e+39	0.000197
15313	TS.triHPacyl.COelim.pmmppppmd	2.222e+44	7.13	7.13	1.411e+39	0.000195
15314	TS.triHPacyl.COelim.tmmmtppmd	8.623e+44	7.95	7.95	1.403e+39	0.000194
15315	TS.triHPacyl.COelim.pppmmpppd	1.981e+44	7.08	7.08	1.386e+39	0.000191
15316	TS.triHPacyl.COelim.tmtpptmpd	1.508e+45	8.29	8.29	1.384e+39	0.000191
15317	TS.triHPacyl.COelim.tmmmmpppd	9.846e+44	8.04	8.04	1.369e+39	0.000189
15318	TS.triHPacyl.COelim.ptptmtpmd	3.321e+45	8.77	8.77	1.365e+39	0.000189
15319	TS.triHPacyl.COelim.pmttppppd	9.731e+44	8.04	8.04	1.362e+39	0.000188
15320	TS.triHPacyl.COelim.tppppptmpd	4.572e+44	7.59	7.59	1.357e+39	0.000187
15321	TS.triHPacyl.COelim.ptmmppmmd	4.940e+44	7.64	7.64	1.345e+39	0.000186
15322	TS.triHPacyl.COelim.ppmtpptmpd	2.665e+45	8.65	8.65	1.335e+39	0.000184
15323	TS.triHPacyl.COelim.ptmmmtmmd	8.335e+44	7.96	7.96	1.335e+39	0.000184
15324	TS.triHPacyl.COelim.tttppmpppd	1.466e+45	8.29	8.29	1.333e+39	0.000184
15325	TS.triHPacyl.COelim.tppmptmmd	1.724e+44	7.02	7.02	1.332e+39	0.000184
15326	TS.triHPacyl.COelim.pmtptpmpd	1.678e+45	8.38	8.38	1.325e+39	0.000183
15327	TS.triHPacyl.COelim.tmtmtpmd	1.094e+45	8.12	8.12	1.323e+39	0.000183
15328	TS.triHPacyl.COelim.tpmptpmpd	1.568e+44	6.97	6.97	1.314e+39	0.000181
15329	TS.triHPacyl.COelim.mtttppmmd	3.388e+44	7.43	7.43	1.313e+39	0.000181
15330	TS.triHPacyl.COelim.mpmtppmmpd	1.846e+44	7.07	7.07	1.305e+39	0.00018
15331	TS.triHPacyl.COelim.mttmtpmmd	2.203e+44	7.18	7.18	1.304e+39	0.00018
15332	TS.triHPacyl.COelim.tmpmtmmpd	1.663e+44	7.01	7.01	1.293e+39	0.000179
15333	TS.triHPacyl.COelim.ptmtptppd	5.707e+44	7.75	7.75	1.290e+39	0.000178
15334	TS.triHPacyl.COelim.tpttmpppd	1.670e+45	8.39	8.39	1.282e+39	0.000177
15335	TS.triHPacyl.COelim.tmmptpppd	2.880e+44	7.35	7.35	1.276e+39	0.000176
15336	TS.triHPacyl.COelim.tpptmtmmd	2.155e+44	7.18	7.18	1.274e+39	0.000176
15337	TS.triHPacyl.COelim.mmmppttmmd	7.144e+43	6.52	6.52	1.263e+39	0.000174
15338	TS.triHPacyl.COelim.tpmtmmd	3.464e+44	7.47	7.47	1.257e+39	0.000174
15339	TS.triHPacyl.COelim.mmmtpmmpd	9.990e+44	8.10	8.10	1.255e+39	0.000173
15340	TS.triHPacyl.COelim.tmtmtpmmd	1.434e+45	8.32	8.32	1.249e+39	0.000173
15341	TS.triHPacyl.COelim.mmtptmmd	6.344e+44	7.84	7.84	1.241e+39	0.000171
15342	TS.triHPacyl.COelim.pmttmpppd	7.458e+44	7.93	7.93	1.238e+39	0.000171
15343	TS.triHPacyl.COelim.tpptmmpd	1.769e+45	8.45	8.45	1.230e+39	0.00017
15344	TS.triHPacyl.COelim.tppmppmd	3.449e+44	7.48	7.48	1.220e+39	0.000168
15345	TS.triHPacyl.COelim.ptppmppmd	4.354e+43	6.25	6.25	1.216e+39	0.000168
15346	TS.triHPacyl.COelim.tmtmpmtpd	3.184e+45	8.81	8.81	1.214e+39	0.000168
15347	TS.triHPacyl.COelim.mmtmmmpmd	2.279e+44	7.24	7.24	1.206e+39	0.000167
15348	TS.triHPacyl.COelim.pmptptppd	1.147e+44	6.84	6.84	1.203e+39	0.000166
15349	TS.triHPacyl.COelim.mttptmmd	9.431e+43	6.72	6.72	1.202e+39	0.000166
15350	TS.triHPacyl.COelim.mpmmptppd	3.151e+44	7.44	7.44	1.196e+39	0.000165
15351	TS.triHPacyl.COelim.ppmtpmtpd	9.799e+44	8.12	8.12	1.196e+39	0.000165
15352	TS.triHPacyl.COelim.pmtptmmpd	1.729e+44	7.08	7.08	1.196e+39	0.000165
15353	TS.triHPacyl.COelim.mmmppmppd	1.615e+44	7.04	7.04	1.195e+39	0.000165
15354	TS.triHPacyl.COelim.pppmtpmmd	1.994e+44	7.17	7.17	1.183e+39	0.000163
15355	TS.triHPacyl.COelim.pppmmtmmd	2.203e+44	7.23	7.23	1.182e+39	0.000163
15356	TS.triHPacyl.COelim.pmmppmmd	6.483e+43	6.51	6.51	1.177e+39	0.000163
15357	TS.triHPacyl.COelim.pmtptmmd	1.813e+44	7.12	7.12	1.170e+39	0.000162
15358	TS.triHPacyl.COelim.tmmppmtpd	2.396e+44	7.29	7.29	1.168e+39	0.000161
15359	TS.triHPacyl.COelim.mmmmpmmd	2.275e+44	7.26	7.26	1.166e+39	0.000161
15360	TS.triHPacyl.COelim.tmpmmpmmd	1.731e+44	7.10	7.10	1.166e+39	0.000161
15361	TS.triHPacyl.COelim.mptmmpmmd	2.643e+44	7.35	7.35	1.164e+39	0.000161
15362	TS.triHPacyl.COelim.mmtptmtpd	1.152e+45	8.23	8.23	1.158e+39	0.00016
15363	TS.triHPacyl.COelim.tmpmtpppd	4.449e+44	7.67	7.67	1.155e+39	0.000159
15364	TS.triHPacyl.COelim.ppmtpmmd	4.342e+45	9.03	9.03	1.142e+39	0.000158
15365	TS.triHPacyl.COelim.mtmtptmmd	2.696e+44	7.38	7.38	1.138e+39	0.000157
15366	TS.triHPacyl.COelim.tmpmmpmmd	2.505e+44	7.33	7.33	1.137e+39	0.000157
15367	TS.triHPacyl.COelim.tmmppmppd	8.175e+44	8.04	8.04	1.135e+39	0.000157
15368	TS.triHPacyl.COelim.tttmtmtpd	1.871e+44	7.16	7.16	1.134e+39	0.000157
15369	TS.triHPacyl.COelim.tttptmmpd	6.964e+44	7.95	7.95	1.134e+39	0.000157
15370	TS.triHPacyl.COelim.tmpmmpmmd	5.775e+44	7.84	7.84	1.126e+39	0.000155
15371	TS.triHPacyl.COelim.tpptmmd	1.010e+45	8.17	8.17	1.126e+39	0.000155
15372	TS.triHPacyl.COelim.tmtmmtmmd	3.633e+45	8.94	8.94	1.125e+39	0.000155
15373	TS.triHPacyl.COelim.pppmmtmmd	3.050e+44	7.46	7.46	1.120e+39	0.000155
15374	TS.triHPacyl.COelim.tmpmmpmmd	1.082e+44	6.84	6.84	1.119e+39	0.000155
15375	TS.triHPacyl.COelim.tpmmpmmd	6.899e+44	7.96	7.96	1.095e+39	0.000151
15376	TS.triHPacyl.COelim.pmmppmtpd	5.766e+44	7.85	7.85	1.094e+39	0.000151
15377	TS.triHPacyl.COelim.mmmmpmtpd	4.807e+43	6.37	6.37	1.093e+39	0.000151
15378	TS.triHPacyl.COelim.tmpmtpmmd	4.119e+44	7.66	7.66	1.091e+39	0.000151
15379	TS.triHPacyl.COelim.mmmppmtpd	1.190e+44	6.92	6.92	1.090e+39	0.000151
15380	TS.triHPacyl.COelim.pptmtmmpd	6.172e+44	7.91	7.91	1.075e+39	0.000148
15381	TS.triHPacyl.COelim.mpmtptmmd	1.192e+44	6.93	6.93	1.073e+39	0.000148
15382	TS.triHPacyl.COelim.tmmppmmd	6.417e+44	7.93	7.93	1.071e+39	0.000148
15383	TS.triHPacyl.COelim.mttmmpmmd	6.829e+44	7.97	7.97	1.071e+39	0.000148

15384	TS.triHPacyl.COelim.tttmtmmmd	1.725e+44	7.15	7.15	1.070e+39	0.000148
15385	TS.triHPacyl.COelim.mtprmtpppd	4.766e+43	6.38	6.38	1.067e+39	0.000147
15386	TS.triHPacyl.COelim.mptmmpppd	3.488e+44	7.58	7.58	1.057e+39	0.000146
15387	TS.triHPacyl.COelim.ppppppppd	1.971e+44	7.24	7.24	1.056e+39	0.000146
15388	TS.triHPacyl.COelim.mppppmtmmd	1.994e+44	7.24	7.24	1.055e+39	0.000146
15389	TS.triHPacyl.COelim.tpttmmppmd	2.377e+45	8.72	8.72	1.054e+39	0.000145
15390	TS.triHPacyl.COelim.ttmtmmmmmd	1.022e+45	8.26	8.26	1.053e+39	0.000145
15391	TS.triHPacyl.COelim.pmpmtppmd	4.852e+44	7.77	7.77	1.053e+39	0.000145
15392	TS.triHPacyl.COelim.pttmtmmmd	5.611e+43	6.49	6.49	1.051e+39	0.000145
15393	TS.triHPacyl.COelim.tmpmtmmppd	3.347e+44	7.55	7.55	1.050e+39	0.000145
15394	TS.triHPacyl.COelim.pmmppppmd	1.677e+44	7.14	7.14	1.048e+39	0.000145
15395	TS.triHPacyl.COelim.ttmtppppmd	9.114e+44	8.15	8.15	1.046e+39	0.000144
15396	TS.triHPacyl.COelim.ptmpmpmpd	9.920e+43	6.83	6.83	1.046e+39	0.000144
15397	TS.triHPacyl.COelim.pmtppppmd	1.190e+45	8.31	8.31	1.045e+39	0.000144
15398	TS.triHPacyl.COelim.mmmmppppd	1.028e+44	6.85	6.85	1.045e+39	0.000144
15399	TS.triHPacyl.COelim.pmtpppppd	3.160e+44	7.52	7.52	1.043e+39	0.000144
15400	TS.triHPacyl.COelim.tmpmtppmd	1.598e+44	7.12	7.12	1.042e+39	0.000144
15401	TS.triHPacyl.COelim.tpmtppmd	5.186e+44	7.82	7.82	1.039e+39	0.000143
15402	TS.triHPacyl.COelim.pmmmtmmmd	2.838e+44	7.47	7.47	1.033e+39	0.000143
15403	TS.triHPacyl.COelim.pppmppppd	1.099e+44	6.90	6.90	1.033e+39	0.000143
15404	TS.triHPacyl.COelim.mpmtpmmmd	1.496e+45	8.46	8.46	1.033e+39	0.000143
15405	TS.triHPacyl.COelim.tttptppmd	1.677e+45	8.53	8.53	1.031e+39	0.000142
15406	TS.triHPacyl.COelim.tppmpmpmd	1.084e+45	8.27	8.27	1.023e+39	0.000141
15407	TS.triHPacyl.COelim.ptmtppmd	6.885e+44	8.00	8.00	1.018e+39	0.000141
15408	TS.triHPacyl.COelim.mmmmpmtmd	2.446e+44	7.39	7.39	1.017e+39	0.00014
15409	TS.triHPacyl.COelim.mttpppppd	2.423e+45	8.75	8.75	1.017e+39	0.00014
15410	TS.triHPacyl.COelim.mttptppmd	2.922e+44	7.50	7.50	1.010e+39	0.00014
15411	TS.triHPacyl.COelim.ppppppppd	1.441e+45	8.45	8.45	1.009e+39	0.000139
15412	TS.triHPacyl.COelim.mttppppmd	7.849e+43	6.72	6.72	1.002e+39	0.000138
15413	TS.triHPacyl.COelim.tttppppmd	1.561e+45	8.51	8.51	9.946e+38	0.000137
15414	TS.triHPacyl.COelim.tppmpppmd	1.478e+44	7.10	7.10	9.895e+38	0.000137
15415	TS.triHPacyl.COelim.mppppppmd	1.798e+44	7.22	7.22	9.889e+38	0.000137
15416	TS.triHPacyl.COelim.tpptppppmd	8.471e+44	8.15	8.15	9.766e+38	0.000135
15417	TS.triHPacyl.COelim.ptmmmtmmmd	5.018e+44	7.84	7.84	9.716e+38	0.000134
15418	TS.triHPacyl.COelim.mmttmmppd	2.307e+45	8.76	8.76	9.611e+38	0.000133
15419	TS.triHPacyl.COelim.tmtppppmd	2.684e+45	8.85	8.85	9.589e+38	0.000132
15420	TS.triHPacyl.COelim.ptppptmpd	2.573e+44	7.45	7.45	9.579e+38	0.000132
15421	TS.triHPacyl.COelim.tmpmptmpd	3.795e+44	7.69	7.69	9.560e+38	0.000132
15422	TS.triHPacyl.COelim.mttppmmppd	1.175e+45	8.36	8.36	9.551e+38	0.000132
15423	TS.triHPacyl.COelim.mpppppppd	1.362e+45	8.45	8.45	9.502e+38	0.000131
15424	TS.triHPacyl.COelim.ttmppmmmd	1.020e+44	6.91	6.91	9.493e+38	0.000131
15425	TS.triHPacyl.COelim.tpptppppd	1.078e+45	8.31	8.31	9.457e+38	0.000131
15426	TS.triHPacyl.COelim.tppmmtpmd	9.338e+44	8.23	8.23	9.453e+38	0.000131
15427	TS.triHPacyl.COelim.ptppppppd	3.302e+43	6.24	6.24	9.389e+38	0.00013
15428	TS.triHPacyl.COelim.ttmpttmd	5.791e+44	7.95	7.95	9.383e+38	0.00013
15429	TS.triHPacyl.COelim.mttmtmmmd	1.237e+44	7.03	7.03	9.367e+38	0.000129
15430	TS.triHPacyl.COelim.tppmptppd	3.114e+44	7.58	7.58	9.362e+38	0.000129
15431	TS.triHPacyl.COelim.pmtmmmtmmd	5.998e+44	7.97	7.97	9.348e+38	0.000129
15432	TS.triHPacyl.COelim.tptpppppd	4.126e+44	7.75	7.75	9.329e+38	0.000129
15433	TS.triHPacyl.COelim.mtmtmmppd	2.764e+45	8.89	8.89	9.297e+38	0.000128
15434	TS.triHPacyl.COelim.ttppmmppd	2.123e+44	7.36	7.36	9.276e+38	0.000128
15435	TS.triHPacyl.COelim.mtppmmtd	4.296e+44	7.78	7.78	9.269e+38	0.000128
15436	TS.triHPacyl.COelim.pttpmpppd	6.932e+44	8.07	8.07	9.189e+38	0.000127
15437	TS.triHPacyl.COelim.pmmptmmmd	4.367e+43	6.42	6.42	9.148e+38	0.000126
15438	TS.triHPacyl.COelim.mmmmpmtmmd	1.299e+45	8.45	8.45	9.148e+38	0.000126
15439	TS.triHPacyl.COelim.tttptppmd	2.516e+45	8.84	8.84	9.100e+38	0.000126
15440	TS.triHPacyl.COelim.tppmpmtmd	5.308e+44	7.92	7.92	9.080e+38	0.000125
15441	TS.triHPacyl.COelim.ttptmtmmd	5.195e+44	7.91	7.91	9.054e+38	0.000125
15442	TS.triHPacyl.COelim.ttmtppppd	6.881e+44	8.07	8.07	9.045e+38	0.000125
15443	TS.triHPacyl.COelim.tpmtmmtd	5.350e+45	9.30	9.30	9.021e+38	0.000125
15444	TS.triHPacyl.COelim.mmtmmtd	3.750e+45	9.09	9.09	9.004e+38	0.000124
15445	TS.triHPacyl.COelim.pmpmtpppd	1.462e+45	8.53	8.53	8.996e+38	0.000124
15446	TS.triHPacyl.COelim.pttpppppd	4.841e+44	7.87	7.87	8.984e+38	0.000124
15447	TS.triHPacyl.COelim.pppmmpppd	2.867e+44	7.56	7.56	8.974e+38	0.000124
15448	TS.triHPacyl.COelim.mttppmmmd	6.169e+44	8.01	8.01	8.954e+38	0.000124
15449	TS.triHPacyl.COelim.mttppmmmd	2.544e+44	7.49	7.49	8.876e+38	0.000123
15450	TS.triHPacyl.COelim.tpttppppd	1.515e+45	8.56	8.56	8.871e+38	0.000122
15451	TS.triHPacyl.COelim.mmpptppmd	4.581e+44	7.85	7.85	8.797e+38	0.000121
15452	TS.triHPacyl.COelim.pmmptpppd	1.197e+45	8.42	8.42	8.794e+38	0.000121
15453	TS.triHPacyl.COelim.ttptppppmd	4.222e+44	7.81	7.81	8.702e+38	0.00012
15454	TS.triHPacyl.COelim.tppmtppd	5.138e+44	7.92	7.92	8.690e+38	0.00012
15455	TS.triHPacyl.COelim.tttppppd	5.169e+44	7.93	7.93	8.688e+38	0.00012

15456	TS.triHPacyl.COelim.tmtmpmpmmd	9.858e+45	9.68	9.68	8.683e+38	0.00012
15457	TS.triHPacyl.COelim.mmmmpptmpd	1.250e+44	7.08	7.08	8.635e+38	0.000119
15458	TS.triHPacyl.COelim.mpmtptmpd	8.402e+44	8.22	8.22	8.611e+38	0.000119
15459	TS.triHPacyl.COelim.mmmmmmtmpd	1.673e+45	8.64	8.64	8.543e+38	0.000118
15460	TS.triHPacyl.COelim.ptptpmpd	2.596e+44	7.53	7.53	8.530e+38	0.000118
15461	TS.triHPacyl.COelim.pmtmmmpd	5.726e+44	8.00	8.00	8.505e+38	0.000117
15462	TS.triHPacyl.COelim.mmtmmmtmmd	2.350e+45	8.84	8.84	8.473e+38	0.000117
15463	TS.triHPacyl.COelim.mmtpmmtmmd	1.014e+45	8.35	8.35	8.440e+38	0.000117
15464	TS.triHPacyl.COelim.mpmtpppppd	3.912e+44	7.78	7.78	8.436e+38	0.000116
15465	TS.triHPacyl.COelim.mppppmmpd	7.045e+44	8.13	8.13	8.400e+38	0.000116
15466	TS.triHPacyl.COelim.tmtppptmpd	1.159e+45	8.43	8.43	8.381e+38	0.000116
15467	TS.triHPacyl.COelim.pmpppptmpd	5.987e+44	8.04	8.04	8.344e+38	0.000115
15468	TS.triHPacyl.COelim.pmpptpppd	2.721e+45	8.94	8.94	8.288e+38	0.000114
15469	TS.triHPacyl.COelim.tttmtpppd	2.428e+44	7.50	7.50	8.282e+38	0.000114
15470	TS.triHPacyl.COelim.mptmtpmpd	5.843e+44	8.03	8.03	8.228e+38	0.000114
15471	TS.triHPacyl.COelim.tmtppmpd	4.104e+44	7.82	7.82	8.219e+38	0.000113
15472	TS.triHPacyl.COelim.mpppmtmpd	1.021e+44	7.00	7.00	8.189e+38	0.000113
15473	TS.triHPacyl.COelim.mmtmmmtmpd	1.322e+45	8.53	8.53	8.136e+38	0.000112
15474	TS.triHPacyl.COelim.mptmmtmpd	2.452e+44	7.52	7.52	8.110e+38	0.000112
15475	TS.triHPacyl.COelim.mtpppppmd	5.736e+43	6.66	6.66	8.096e+38	0.000112
15476	TS.triHPacyl.COelim.tppmmpmpd	2.590e+44	7.56	7.56	8.093e+38	0.000112
15477	TS.triHPacyl.COelim.mptmmtpmd	1.478e+45	8.60	8.60	8.034e+38	0.000111
15478	TS.triHPacyl.COelim.mpmmtppd	3.197e+44	7.69	7.69	8.016e+38	0.000111
15479	TS.triHPacyl.COelim.tttmmmmmd	1.953e+44	7.40	7.40	7.946e+38	0.00011
15480	TS.triHPacyl.COelim.ptmtpmpd	5.943e+44	8.07	8.07	7.921e+38	0.000109
15481	TS.triHPacyl.COelim.ptmmtpmpd	7.346e+44	8.19	8.19	7.910e+38	0.000109
15482	TS.triHPacyl.COelim.mmmmpmtmpd	7.580e+44	8.21	8.21	7.868e+38	0.000109
15483	TS.triHPacyl.COelim.mmpmtpmpd	9.971e+43	7.01	7.01	7.863e+38	0.000109
15484	TS.triHPacyl.COelim.mppppmmpd	6.675e+43	6.77	6.77	7.810e+38	0.000108
15485	TS.triHPacyl.COelim.pmpmtpmpd	1.517e+43	5.89	5.89	7.739e+38	0.000107
15486	TS.triHPacyl.COelim.tppppmmpd	9.230e+43	6.97	6.97	7.727e+38	0.000107
15487	TS.triHPacyl.COelim.tptmmpmpd	1.036e+44	7.04	7.04	7.718e+38	0.000107
15488	TS.triHPacyl.COelim.mtmmpmmpd	8.559e+44	8.30	8.30	7.677e+38	0.000106
15489	TS.triHPacyl.COelim.pttppmmpd	9.021e+43	6.96	6.96	7.668e+38	0.000106
15490	TS.triHPacyl.COelim.ptmmpmpd	9.045e+43	6.96	6.96	7.635e+38	0.000105
15491	TS.triHPacyl.COelim.tmtmtpmd	7.029e+44	8.19	8.19	7.614e+38	0.000105
15492	TS.triHPacyl.COelim.mtmppmpd	1.017e+44	7.04	7.04	7.581e+38	0.000105
15493	TS.triHPacyl.COelim.pppmmmpd	1.608e+44	7.31	7.31	7.562e+38	0.000104
15494	TS.triHPacyl.COelim.mmmmmmtppd	6.806e+44	8.17	8.17	7.557e+38	0.000104
15495	TS.triHPacyl.COelim.tpptpmpd	2.050e+45	8.83	8.83	7.551e+38	0.000104
15496	TS.triHPacyl.COelim.mmtmpmpd	6.607e+45	9.53	9.53	7.545e+38	0.000104
15497	TS.triHPacyl.COelim.tptmmtmpd	7.888e+45	9.64	9.64	7.541e+38	0.000104
15498	TS.triHPacyl.COelim.mmtpmmpd	3.265e+44	7.74	7.74	7.476e+38	0.000103
15499	TS.triHPacyl.COelim.tpptmmpd	2.680e+45	9.00	9.00	7.448e+38	0.000103
15500	TS.triHPacyl.COelim.tptmmtmpd	5.327e+44	8.04	8.04	7.448e+38	0.000103
15501	TS.triHPacyl.COelim.mptpmtmpd	7.748e+44	8.26	8.26	7.406e+38	0.000102
15502	TS.triHPacyl.COelim.ttppppmpd	2.021e+45	8.84	8.84	7.308e+38	0.000101
15503	TS.triHPacyl.COelim.mmtmpmpd	6.327e+44	8.15	8.15	7.291e+38	0.000101
15504	TS.triHPacyl.COelim.tttmtpmpd	5.203e+44	8.04	8.04	7.215e+38	9.96e-05
15505	TS.triHPacyl.COelim.pmtptmpd	1.088e+44	7.11	7.11	7.197e+38	9.94e-05
15506	TS.triHPacyl.COelim.mpmmpmpd	1.700e+44	7.38	7.38	7.185e+38	9.92e-05
15507	TS.triHPacyl.COelim.pmtppmpd	4.479e+44	7.96	7.96	7.142e+38	9.86e-05
15508	TS.triHPacyl.COelim.mpmmpmpd	7.356e+43	6.88	6.88	7.139e+38	9.86e-05
15509	TS.triHPacyl.COelim.pmtptmpd	3.089e+44	7.74	7.74	7.138e+38	9.86e-05
15510	TS.triHPacyl.COelim.pmtptmpd	1.894e+44	7.45	7.45	7.131e+38	9.85e-05
15511	TS.triHPacyl.COelim.ptppppmpd	1.262e+44	7.21	7.21	7.040e+38	9.72e-05
15512	TS.triHPacyl.COelim.pmtptmpd	8.898e+43	7.01	7.01	6.954e+38	9.6e-05
15513	TS.triHPacyl.COelim.mtmtpmpd	1.203e+44	7.19	7.19	6.946e+38	9.59e-05
15514	TS.triHPacyl.COelim.tmtptmpd	7.305e+44	8.27	8.27	6.933e+38	9.57e-05
15515	TS.triHPacyl.COelim.tpmtmtpd	9.386e+45	9.79	9.79	6.883e+38	9.5e-05
15516	TS.triHPacyl.COelim.tppmmmpd	9.883e+43	7.08	7.08	6.870e+38	9.49e-05
15517	TS.triHPacyl.COelim.mpmtpmpd	1.893e+45	8.84	8.84	6.863e+38	9.48e-05
15518	TS.triHPacyl.COelim.mppppmpd	9.940e+43	7.09	7.09	6.812e+38	9.41e-05
15519	TS.triHPacyl.COelim.ttpmtmpd	4.228e+43	6.58	6.58	6.808e+38	9.4e-05
15520	TS.triHPacyl.COelim.ptppmpd	9.986e+43	7.09	7.09	6.791e+38	9.38e-05
15521	TS.triHPacyl.COelim.mptmtpmpd	1.242e+45	8.60	8.60	6.764e+38	9.34e-05
15522	TS.triHPacyl.COelim.ptmmtpmpd	5.049e+44	8.06	8.06	6.762e+38	9.34e-05
15523	TS.triHPacyl.COelim.tptmmmpd	4.699e+44	8.02	8.02	6.760e+38	9.33e-05
15524	TS.triHPacyl.COelim.tpmtmtpd	1.410e+45	8.67	8.67	6.757e+38	9.33e-05
15525	TS.triHPacyl.COelim.ptmmtpmpd	8.157e+44	8.35	8.35	6.736e+38	9.3e-05
15526	TS.triHPacyl.COelim.mtmtpmpd	2.893e+44	7.74	7.74	6.696e+38	9.25e-05
15527	TS.triHPacyl.COelim.tptmmmpd	1.524e+45	8.73	8.73	6.653e+38	9.19e-05

15528	TS.triHPacyl.COelim.tmpmpmpmd	8.788e+43	7.03	7.03	6.648e+38	9.18e-05
15529	TS.triHPacyl.COelim.ptttppppmd	3.409e+44	7.84	7.84	6.633e+38	9.16e-05
15530	TS.triHPacyl.COelim.tmttmtmmd	2.043e+45	8.91	8.91	6.626e+38	9.15e-05
15531	TS.triHPacyl.COelim.mmmmmtppd	5.769e+44	8.15	8.15	6.624e+38	9.15e-05
15532	TS.triHPacyl.COelim.mttppppmd	2.094e+44	7.55	7.55	6.614e+38	9.13e-05
15533	TS.triHPacyl.COelim.ttmmpmtmmd	1.370e+45	8.67	8.67	6.596e+38	9.11e-05
15534	TS.triHPacyl.COelim.mpptmmpmd	4.068e+44	7.95	7.95	6.576e+38	9.08e-05
15535	TS.triHPacyl.COelim.ptttmmmmmd	3.358e+44	7.84	7.84	6.518e+38	9e-05
15536	TS.triHPacyl.COelim.ttmtpmtpmd	1.241e+45	8.62	8.62	6.514e+38	8.99e-05
15537	TS.triHPacyl.COelim.tttppptmmd	3.681e+44	7.90	7.90	6.511e+38	8.99e-05
15538	TS.triHPacyl.COelim.pmmtpmmpmd	3.168e+43	6.44	6.44	6.441e+38	8.89e-05
15539	TS.triHPacyl.COelim.pmpptmtpmd	2.576e+44	7.69	7.69	6.399e+38	8.84e-05
15540	TS.triHPacyl.COelim.ptttppmpmd	8.446e+44	8.40	8.40	6.383e+38	8.81e-05
15541	TS.triHPacyl.COelim.mtmtppppmd	1.799e+44	7.48	7.48	6.354e+38	8.77e-05
15542	TS.triHPacyl.COelim.tpttpmppmd	1.667e+45	8.81	8.81	6.351e+38	8.77e-05
15543	TS.triHPacyl.COelim.tttmmpppd	2.550e+44	7.69	7.69	6.343e+38	8.76e-05
15544	TS.triHPacyl.COelim.mmmtpmmpmd	8.664e+43	7.05	7.05	6.293e+38	8.69e-05
15545	TS.triHPacyl.COelim.mpptmtpmd	2.040e+45	8.94	8.94	6.270e+38	8.66e-05
15546	TS.triHPacyl.COelim.tmtmtpppd	3.897e+45	9.33	9.33	6.266e+38	8.65e-05
15547	TS.triHPacyl.COelim.tmmtptmmpd	2.234e+45	9.00	9.00	6.247e+38	8.63e-05
15548	TS.triHPacyl.COelim.mmmmtmmpd	6.383e+44	8.25	8.25	6.225e+38	8.59e-05
15549	TS.triHPacyl.COelim.mmpmmmpmd	5.028e+43	6.74	6.74	6.175e+38	8.53e-05
15550	TS.triHPacyl.COelim.tmttptmmd	1.543e+46	10.16	10.16	6.168e+38	8.52e-05
15551	TS.triHPacyl.COelim.ttpmmpmpd	2.976e+43	6.43	6.43	6.166e+38	8.51e-05
15552	TS.triHPacyl.COelim.tmpmpmpd	2.988e+44	7.80	7.80	6.165e+38	8.51e-05
15553	TS.triHPacyl.COelim.ptpppmpd	3.192e+44	7.84	7.84	6.163e+38	8.51e-05
15554	TS.triHPacyl.COelim.pmttmtmpd	7.390e+45	9.72	9.72	6.111e+38	8.44e-05
15555	TS.triHPacyl.COelim.mpttmmmmmd	1.430e+45	8.75	8.75	5.994e+38	8.28e-05
15556	TS.triHPacyl.COelim.pmpptmpd	6.320e+43	6.90	6.90	5.994e+38	8.28e-05
15557	TS.triHPacyl.COelim.mmtmtmtpd	1.133e+45	8.62	8.62	5.980e+38	8.26e-05
15558	TS.triHPacyl.COelim.ptttmmpmd	8.031e+44	8.42	8.42	5.914e+38	8.17e-05
15559	TS.triHPacyl.COelim.pmtptmpd	3.631e+45	9.32	9.32	5.900e+38	8.15e-05
15560	TS.triHPacyl.COelim.mpttmmmpmd	1.280e+45	8.70	8.70	5.865e+38	8.1e-05
15561	TS.triHPacyl.COelim.tpmppppmd	4.785e+44	8.12	8.12	5.767e+38	7.96e-05
15562	TS.triHPacyl.COelim.mmmmpmmmpd	2.802e+44	7.81	7.81	5.750e+38	7.94e-05
15563	TS.triHPacyl.COelim.pppmpppmd	4.888e+44	8.14	8.14	5.710e+38	7.88e-05
15564	TS.triHPacyl.COelim.mmtmptppd	1.115e+45	8.64	8.64	5.696e+38	7.86e-05
15565	TS.triHPacyl.COelim.ttpmtpmpd	7.573e+43	7.03	7.03	5.693e+38	7.86e-05
15566	TS.triHPacyl.COelim.tmpmtpmpd	1.110e+44	7.26	7.26	5.682e+38	7.85e-05
15567	TS.triHPacyl.COelim.ttpmmmmmd	5.091e+43	6.81	6.81	5.615e+38	7.75e-05
15568	TS.triHPacyl.COelim.mmpptmpmd	1.521e+44	7.46	7.46	5.592e+38	7.72e-05
15569	TS.triHPacyl.COelim.mmmmmtpppd	1.123e+45	8.66	8.66	5.553e+38	7.67e-05
15570	TS.triHPacyl.COelim.ttmmpmtmpd	4.530e+44	8.12	8.12	5.548e+38	7.66e-05
15571	TS.triHPacyl.COelim.pttmppmmmd	7.581e+43	7.05	7.05	5.546e+38	7.66e-05
15572	TS.triHPacyl.COelim.tttmmpmmd	3.723e+44	8.00	8.00	5.543e+38	7.65e-05
15573	TS.triHPacyl.COelim.pmtmptmmd	2.047e+44	7.65	7.65	5.447e+38	7.52e-05
15574	TS.triHPacyl.COelim.tpppmtmmd	1.522e+45	8.85	8.85	5.424e+38	7.49e-05
15575	TS.triHPacyl.COelim.mppmmppmd	4.108e+44	8.07	8.07	5.418e+38	7.48e-05
15576	TS.triHPacyl.COelim.tmpmmmpmmd	2.360e+44	7.74	7.74	5.409e+38	7.47e-05
15577	TS.triHPacyl.COelim.tmtppppmd	1.267e+46	10.12	10.12	5.372e+38	7.42e-05
15578	TS.triHPacyl.COelim.mmmmpmpmd	7.330e+43	7.05	7.05	5.371e+38	7.42e-05
15579	TS.triHPacyl.COelim.ptmmmmppmd	2.223e+44	7.71	7.71	5.365e+38	7.41e-05
15580	TS.triHPacyl.COelim.mptmmpmmd	1.696e+45	8.92	8.92	5.358e+38	7.4e-05
15581	TS.triHPacyl.COelim.mpptmtpmd	1.339e+45	8.79	8.79	5.290e+38	7.3e-05
15582	TS.triHPacyl.COelim.mttmmpppd	6.265e+44	8.34	8.34	5.289e+38	7.3e-05
15583	TS.triHPacyl.COelim.pmpmmmpmd	1.557e+44	7.51	7.51	5.245e+38	7.24e-05
15584	TS.triHPacyl.COelim.ttmptmmd	1.038e+45	8.64	8.64	5.238e+38	7.23e-05
15585	TS.triHPacyl.COelim.ptmppptmpd	6.111e+44	8.33	8.33	5.200e+38	7.18e-05
15586	TS.triHPacyl.COelim.mpptpmpmd	3.239e+44	7.96	7.96	5.153e+38	7.12e-05
15587	TS.triHPacyl.COelim.pttpmtpmd	2.121e+44	7.71	7.71	5.151e+38	7.11e-05
15588	TS.triHPacyl.COelim.tppppppmd	3.512e+44	8.01	8.01	5.146e+38	7.1e-05
15589	TS.triHPacyl.COelim.tmpppmtmmd	1.045e+45	8.66	8.66	5.103e+38	7.05e-05
15590	TS.triHPacyl.COelim.mpptmmtmpd	1.552e+45	8.90	8.90	5.078e+38	7.01e-05
15591	TS.triHPacyl.COelim.pttmmpppd	4.372e+44	8.15	8.15	5.071e+38	7e-05
15592	TS.triHPacyl.COelim.pmmtpmmpd	3.016e+44	7.93	7.93	5.034e+38	6.95e-05
15593	TS.triHPacyl.COelim.tmpmtpmpd	8.386e+43	7.17	7.17	5.029e+38	6.94e-05
15594	TS.triHPacyl.COelim.pmpmmmpmd	2.858e+44	7.90	7.90	5.024e+38	6.94e-05
15595	TS.triHPacyl.COelim.pmptppmpd	1.094e+44	7.33	7.33	5.023e+38	6.94e-05
15596	TS.triHPacyl.COelim.mtmmmmtmd	7.033e+45	9.82	9.82	4.978e+38	6.87e-05
15597	TS.triHPacyl.COelim.pmmmpmmpmd	2.728e+43	6.52	6.52	4.875e+38	6.73e-05
15598	TS.triHPacyl.COelim.ptmtmtpmd	6.295e+44	8.39	8.39	4.871e+38	6.73e-05
15599	TS.triHPacyl.COelim.tpmtmtpmd	4.321e+45	9.54	9.54	4.840e+38	6.68e-05

15600	TS.triHPacyl.COelim.ptppmptmmd	6.454e+43	7.04	7.04	4.803e+38	6.63e-05
15601	TS.triHPacyl.COelim.mmmmpmtpdp	3.079e+44	7.97	7.97	4.785e+38	6.61e-05
15602	TS.triHPacyl.COelim.tppmpmmmd	3.894e+44	8.11	8.11	4.782e+38	6.6e-05
15603	TS.triHPacyl.COelim.tmtpttpdp	6.750e+44	8.44	8.44	4.772e+38	6.59e-05
15604	TS.triHPacyl.COelim.tmmtpmtpmd	3.396e+45	9.41	9.41	4.751e+38	6.56e-05
15605	TS.triHPacyl.COelim.pmpmtmtpdp	9.091e+44	8.62	8.62	4.751e+38	6.56e-05
15606	TS.triHPacyl.COelim.pmmppmtpdp	3.320e+44	8.03	8.03	4.713e+38	6.51e-05
15607	TS.triHPacyl.COelim.mptmtpmtpdp	6.887e+44	8.46	8.46	4.710e+38	6.5e-05
15608	TS.triHPacyl.COelim.pmmtpmtpmd	6.990e+43	7.10	7.10	4.691e+38	6.48e-05
15609	TS.triHPacyl.COelim.mpmtpmtpmd	2.158e+44	7.77	7.77	4.689e+38	6.47e-05
15610	TS.triHPacyl.COelim.ptmmmpmtpdp	4.862e+44	8.26	8.26	4.679e+38	6.46e-05
15611	TS.triHPacyl.COelim.ttmmpmtpdp	1.224e+44	7.44	7.44	4.674e+38	6.45e-05
15612	TS.triHPacyl.COelim.mtpmtpmtpdp	2.929e+43	6.59	6.59	4.642e+38	6.41e-05
15613	TS.triHPacyl.COelim.mmmmmtpmmd	2.611e+44	7.90	7.90	4.618e+38	6.38e-05
15614	TS.triHPacyl.COelim.mptppmtpdp	1.013e+45	8.71	8.71	4.588e+38	6.33e-05
15615	TS.triHPacyl.COelim.mptmtpmtpdp	2.071e+45	9.14	9.14	4.564e+38	6.3e-05
15616	TS.triHPacyl.COelim.ptmtpmtpmd	3.948e+43	6.78	6.78	4.550e+38	6.28e-05
15617	TS.triHPacyl.COelim.tttmtpmtpdp	1.095e+45	8.76	8.76	4.533e+38	6.26e-05
15618	TS.triHPacyl.COelim.mmmppmtpdp	7.488e+43	7.17	7.17	4.506e+38	6.22e-05
15619	TS.triHPacyl.COelim.ttpmtpmtpdp	5.799e+44	8.39	8.39	4.500e+38	6.21e-05
15620	TS.triHPacyl.COelim.tmmtpmtpdp	2.264e+44	7.83	7.83	4.492e+38	6.2e-05
15621	TS.triHPacyl.COelim.tppmtpmtpdp	1.907e+45	9.10	9.10	4.488e+38	6.2e-05
15622	TS.triHPacyl.COelim.mmtmmtpmtpdp	3.406e+45	9.45	9.45	4.471e+38	6.17e-05
15623	TS.triHPacyl.COelim.mtmtmtpdp	8.604e+44	8.63	8.63	4.467e+38	6.17e-05
15624	TS.triHPacyl.COelim.tpmmpmtpdp	5.132e+44	8.32	8.32	4.437e+38	6.13e-05
15625	TS.triHPacyl.COelim.mmtmtpmtpdp	2.109e+45	9.17	9.17	4.427e+38	6.11e-05
15626	TS.triHPacyl.COelim.mptmtpmtpdp	2.500e+44	7.90	7.90	4.424e+38	6.11e-05
15627	TS.triHPacyl.COelim.mmmmmtpmtpdp	5.215e+43	6.96	6.96	4.411e+38	6.09e-05
15628	TS.triHPacyl.COelim.tmmtpmtpmd	6.191e+43	7.07	7.07	4.406e+38	6.08e-05
15629	TS.triHPacyl.COelim.tttmtpmtpdp	2.563e+44	7.91	7.91	4.403e+38	6.08e-05
15630	TS.triHPacyl.COelim.ttptmtpdp	4.123e+44	8.20	8.20	4.386e+38	6.06e-05
15631	TS.triHPacyl.COelim.mpptmtpmtpdp	2.701e+44	7.95	7.95	4.368e+38	6.03e-05
15632	TS.triHPacyl.COelim.ptmtpmtpmd	5.642e+44	8.39	8.39	4.361e+38	6.02e-05
15633	TS.triHPacyl.COelim.tppmtpmtpdp	1.944e+45	9.13	9.13	4.353e+38	6.01e-05
15634	TS.triHPacyl.COelim.mmmppmtpdp	3.182e+44	8.05	8.05	4.321e+38	5.97e-05
15635	TS.triHPacyl.COelim.mtmmpmtpmtpdp	7.920e+44	8.60	8.60	4.308e+38	5.95e-05
15636	TS.triHPacyl.COelim.ptmtmtpdp	1.157e+45	8.83	8.83	4.293e+38	5.93e-05
15637	TS.triHPacyl.COelim.mmtmtpmtpdp	3.011e+45	9.41	9.41	4.232e+38	5.84e-05
15638	TS.triHPacyl.COelim.ptmtmtpmd	1.555e+45	9.02	9.02	4.202e+38	5.8e-05
15639	TS.triHPacyl.COelim.pmtmtpmtpdp	1.122e+44	7.45	7.45	4.199e+38	5.8e-05
15640	TS.triHPacyl.COelim.ttmtpmtpmd	1.262e+44	7.52	7.52	4.193e+38	5.79e-05
15641	TS.triHPacyl.COelim.pmmmmtpmtpdp	1.425e+44	7.60	7.60	4.141e+38	5.72e-05
15642	TS.triHPacyl.COelim.mmpmtpmtpdp	1.597e+44	7.67	7.67	4.103e+38	5.67e-05
15643	TS.triHPacyl.COelim.ttpmtpmtpdp	5.474e+43	7.04	7.04	4.069e+38	5.62e-05
15644	TS.triHPacyl.COelim.mmtppmtpdp	1.607e+45	9.06	9.06	4.060e+38	5.61e-05
15645	TS.triHPacyl.COelim.tmmtpmtpmd	2.792e+45	9.39	9.39	4.059e+38	5.6e-05
15646	TS.triHPacyl.COelim.tpmmmtpmtpdp	2.244e+45	9.26	9.26	4.057e+38	5.6e-05
15647	TS.triHPacyl.COelim.mtpmtpmtpdp	1.577e+44	7.68	7.68	4.031e+38	5.57e-05
15648	TS.triHPacyl.COelim.pmmtpmtpmd	6.858e+43	7.19	7.19	3.994e+38	5.51e-05
15649	TS.triHPacyl.COelim.pttmtmtpdp	2.715e+44	8.01	8.01	3.983e+38	5.5e-05
15650	TS.triHPacyl.COelim.mppmtpmtpdp	2.657e+44	8.00	8.00	3.979e+38	5.49e-05
15651	TS.triHPacyl.COelim.pmtmtpmtpdp	7.513e+44	8.62	8.62	3.977e+38	5.49e-05
15652	TS.triHPacyl.COelim.tpmmtmtpdp	2.893e+43	6.68	6.68	3.957e+38	5.46e-05
15653	TS.triHPacyl.COelim.pppmtpmtpdp	2.147e+44	7.87	7.87	3.954e+38	5.46e-05
15654	TS.triHPacyl.COelim.mppmtpmtpdp	2.187e+44	7.88	7.88	3.951e+38	5.45e-05
15655	TS.triHPacyl.COelim.pmmmmtpmtpdp	8.243e+43	7.31	7.31	3.924e+38	5.42e-05
15656	TS.triHPacyl.COelim.pmmppmtpmd	2.081e+44	7.86	7.86	3.921e+38	5.41e-05
15657	TS.triHPacyl.COelim.tttptmtpmd	2.343e+44	7.93	7.93	3.905e+38	5.39e-05
15658	TS.triHPacyl.COelim.mmmppmtpmd	2.169e+44	7.89	7.89	3.903e+38	5.39e-05
15659	TS.triHPacyl.COelim.tppmtpmtpmd	3.862e+45	9.61	9.61	3.886e+38	5.36e-05
15660	TS.triHPacyl.COelim.ttptmtpmtpmd	1.185e+44	7.53	7.53	3.869e+38	5.34e-05
15661	TS.triHPacyl.COelim.mmmmpmtpdp	1.631e+44	7.73	7.73	3.787e+38	5.23e-05
15662	TS.triHPacyl.COelim.tmtptmtpdp	5.301e+45	9.81	9.81	3.785e+38	5.23e-05
15663	TS.triHPacyl.COelim.mmmmmtpmtpdp	9.193e+43	7.40	7.40	3.763e+38	5.2e-05
15664	TS.triHPacyl.COelim.pttptmtpmd	4.054e+44	8.28	8.28	3.745e+38	5.17e-05
15665	TS.triHPacyl.COelim.mmmmpmtpdp	3.924e+44	8.27	8.27	3.740e+38	5.16e-05
15666	TS.triHPacyl.COelim.pmmtpmtpdp	7.985e+44	8.69	8.69	3.702e+38	5.11e-05
15667	TS.triHPacyl.COelim.tppmtpmtpdp	3.983e+44	8.28	8.28	3.693e+38	5.1e-05
15668	TS.triHPacyl.COelim.mppmtpmtpdp	2.783e+45	9.45	9.45	3.663e+38	5.06e-05
15669	TS.triHPacyl.COelim.mttmtpmtpdp	3.447e+44	8.21	8.21	3.633e+38	5.02e-05
15670	TS.triHPacyl.COelim.mppmtpmtpdp	1.560e+44	7.73	7.73	3.629e+38	5.01e-05
15671	TS.triHPacyl.COelim.tpmmtmtpdp	1.477e+45	9.07	9.07	3.629e+38	5.01e-05

15672	TS.triHPacyl.COelim.mppmptmpmd	4.066e+43	6.93	6.93	3.628e+38	5.01e-05
15673	TS.triHPacyl.COelim.tppmpptmpd	6.002e+44	8.54	8.54	3.620e+38	5e-05
15674	TS.triHPacyl.COelim.mmmmmmtmpd	7.293e+44	8.66	8.66	3.611e+38	4.99e-05
15675	TS.triHPacyl.COelim.ptmtppmmpmd	1.798e+44	7.82	7.82	3.601e+38	4.97e-05
15676	TS.triHPacyl.COelim.ptptptmpmd	2.415e+44	8.00	8.00	3.601e+38	4.97e-05
15677	TS.triHPacyl.COelim.tpmtpttmpd	3.476e+45	9.59	9.59	3.576e+38	4.94e-05
15678	TS.triHPacyl.COelim.pmmtpptmpd	1.201e+44	7.59	7.59	3.575e+38	4.94e-05
15679	TS.triHPacyl.COelim.ttpmptmpmd	1.063e+44	7.52	7.52	3.564e+38	4.92e-05
15680	TS.triHPacyl.COelim.mmtmmmpmd	2.393e+45	9.38	9.38	3.540e+38	4.89e-05
15681	TS.triHPacyl.COelim.pmpmptmpmd	2.110e+44	7.93	7.93	3.509e+38	4.85e-05
15682	TS.triHPacyl.COelim.pmpmptmpmd	6.129e+43	7.20	7.20	3.505e+38	4.84e-05
15683	TS.triHPacyl.COelim.ptmpmmpmd	6.574e+43	7.24	7.24	3.495e+38	4.83e-05
15684	TS.triHPacyl.COelim.pmmtpmmpmd	6.526e+43	7.25	7.25	3.439e+38	4.75e-05
15685	TS.triHPacyl.COelim.tppmmpmmpmd	3.281e+44	8.21	8.21	3.438e+38	4.75e-05
15686	TS.triHPacyl.COelim.mmmmpmmpmd	8.234e+44	8.76	8.76	3.427e+38	4.73e-05
15687	TS.triHPacyl.COelim.pmmtpmmpmd	5.741e+44	8.55	8.55	3.414e+38	4.71e-05
15688	TS.triHPacyl.COelim.mtmtmmmpmd	1.700e+45	9.20	9.20	3.401e+38	4.7e-05
15689	TS.triHPacyl.COelim.pmtptmpmd	4.398e+44	8.39	8.39	3.401e+38	4.7e-05
15690	TS.triHPacyl.COelim.pmtppmmpmd	6.444e+44	8.62	8.62	3.388e+38	4.68e-05
15691	TS.triHPacyl.COelim.tptptmmpmd	1.516e+46	10.50	10.50	3.384e+38	4.67e-05
15692	TS.triHPacyl.COelim.mmtppmmpmd	1.101e+45	8.94	8.94	3.375e+38	4.66e-05
15693	TS.triHPacyl.COelim.tpmtmtpmd	2.107e+45	9.33	9.33	3.358e+38	4.64e-05
15694	TS.triHPacyl.COelim.pmtmmpmmpmd	2.055e+44	7.94	7.94	3.335e+38	4.6e-05
15695	TS.triHPacyl.COelim.tpptptmmpmd	1.442e+45	9.12	9.12	3.296e+38	4.55e-05
15696	TS.triHPacyl.COelim.tpptppmmpmd	8.717e+44	8.82	8.82	3.295e+38	4.55e-05
15697	TS.triHPacyl.COelim.pttpmmpmmpmd	6.179e+44	8.61	8.61	3.294e+38	4.55e-05
15698	TS.triHPacyl.COelim.mptpmmpmmpmd	7.694e+44	8.74	8.74	3.289e+38	4.54e-05
15699	TS.triHPacyl.COelim.tttptmmpmd	9.309e+44	8.86	8.86	3.287e+38	4.54e-05
15700	TS.triHPacyl.COelim.mtptmmpmmpmd	4.411e+44	8.41	8.41	3.280e+38	4.53e-05
15701	TS.triHPacyl.COelim.mtptmmpmmpmd	2.028e+45	9.32	9.32	3.280e+38	4.53e-05
15702	TS.triHPacyl.COelim.ptpmtmmpmd	4.301e+43	7.03	7.03	3.275e+38	4.52e-05
15703	TS.triHPacyl.COelim.pmmmtmmpmd	5.158e+44	8.51	8.51	3.266e+38	4.51e-05
15704	TS.triHPacyl.COelim.mmmmtmmpmd	2.825e+44	8.15	8.15	3.266e+38	4.51e-05
15705	TS.triHPacyl.COelim.ttptmmpmmpmd	5.460e+44	8.54	8.54	3.260e+38	4.5e-05
15706	TS.triHPacyl.COelim.tppmmpmmpmd	1.652e+44	7.84	7.84	3.235e+38	4.47e-05
15707	TS.triHPacyl.COelim.mppmptmmpmd	2.339e+45	9.42	9.42	3.216e+38	4.44e-05
15708	TS.triHPacyl.COelim.mmpmptmmpmd	1.867e+44	7.91	7.91	3.205e+38	4.43e-05
15709	TS.triHPacyl.COelim.ppmtpmmpmmpmd	8.628e+44	8.83	8.83	3.191e+38	4.41e-05
15710	TS.triHPacyl.COelim.mmtpmmpmmpmd	1.856e+44	7.92	7.92	3.166e+38	4.37e-05
15711	TS.triHPacyl.COelim.ptttmmpmmpmd	5.588e+44	8.58	8.58	3.160e+38	4.36e-05
15712	TS.triHPacyl.COelim.ptmmpmmpmmpmd	3.478e+44	8.29	8.29	3.156e+38	4.36e-05
15713	TS.triHPacyl.COelim.pmtppmmpmmpmd	5.894e+44	8.61	8.61	3.132e+38	4.32e-05
15714	TS.triHPacyl.COelim.ttpmptmmpmd	1.001e+44	7.56	7.56	3.106e+38	4.29e-05
15715	TS.triHPacyl.COelim.ptppmtpmmpmd	3.769e+43	6.99	6.99	3.037e+38	4.19e-05
15716	TS.triHPacyl.COelim.tttmmpmmpmd	2.733e+44	8.18	8.18	2.981e+38	4.12e-05
15717	TS.triHPacyl.COelim.mptmptmmpmd	4.748e+44	8.52	8.52	2.974e+38	4.11e-05
15718	TS.triHPacyl.COelim.pmtpmmpmmpmd	1.683e+44	7.91	7.91	2.920e+38	4.03e-05
15719	TS.triHPacyl.COelim.mtpmmpmmpmd	3.843e+43	7.03	7.03	2.885e+38	3.98e-05
15720	TS.triHPacyl.COelim.tmpmmtmmpmd	1.081e+44	7.65	7.65	2.883e+38	3.98e-05
15721	TS.triHPacyl.COelim.pppmtpmmpmd	1.402e+44	7.82	7.82	2.815e+38	3.89e-05
15722	TS.triHPacyl.COelim.pmmtpmmpmd	1.040e+44	7.65	7.65	2.786e+38	3.85e-05
15723	TS.triHPacyl.COelim.ptpmmpmmpmd	3.369e+43	6.98	6.98	2.782e+38	3.84e-05
15724	TS.triHPacyl.COelim.pmptmmpmmpmd	7.308e+44	8.81	8.81	2.770e+38	3.83e-05
15725	TS.triHPacyl.COelim.ptmmpmmpmmpmd	5.450e+44	8.65	8.65	2.732e+38	3.77e-05
15726	TS.triHPacyl.COelim.ttptmmpmmpmd	1.608e+44	7.92	7.92	2.719e+38	3.75e-05
15727	TS.triHPacyl.COelim.tpmmpmmpmmpmd	3.622e+44	8.41	8.41	2.699e+38	3.73e-05
15728	TS.triHPacyl.COelim.mmmmpmmpmmpmd	3.010e+44	8.31	8.31	2.663e+38	3.68e-05
15729	TS.triHPacyl.COelim.mmtmmpmmpmd	4.503e+44	8.56	8.56	2.615e+38	3.61e-05
15730	TS.triHPacyl.COelim.mmmmmmtmpmd	2.236e+45	9.52	9.52	2.611e+38	3.61e-05
15731	TS.triHPacyl.COelim.mmpmtmmpmd	2.236e+44	8.15	8.15	2.593e+38	3.58e-05
15732	TS.triHPacyl.COelim.mtppmptmmpmd	1.183e+44	7.78	7.78	2.562e+38	3.54e-05
15733	TS.triHPacyl.COelim.mmpmmpmmpmd	3.449e+43	7.05	7.05	2.535e+38	3.5e-05
15734	TS.triHPacyl.COelim.pmpmptmmpmd	2.389e+44	8.20	8.20	2.526e+38	3.49e-05
15735	TS.triHPacyl.COelim.pmtmmtmmpmd	3.122e+45	9.74	9.74	2.512e+38	3.47e-05
15736	TS.triHPacyl.COelim.tpmtmtpmmpmd	1.010e+45	9.07	9.07	2.508e+38	3.46e-05
15737	TS.triHPacyl.COelim.ttmppmmpmmpmd	2.996e+44	8.34	8.34	2.508e+38	3.46e-05
15738	TS.triHPacyl.COelim.mtmmptmmpmd	1.125e+45	9.13	9.13	2.502e+38	3.45e-05
15739	TS.triHPacyl.COelim.ptttmmpmmpmd	2.522e+44	8.24	8.24	2.488e+38	3.44e-05
15740	TS.triHPacyl.COelim.ptmtpmmpmmpmd	1.040e+44	7.73	7.73	2.452e+38	3.39e-05
15741	TS.triHPacyl.COelim.mmtppmmpmmpmd	1.578e+45	9.35	9.35	2.450e+38	3.38e-05
15742	TS.triHPacyl.COelim.ttmtmmpmmpmd	1.402e+45	9.28	9.28	2.439e+38	3.37e-05
15743	TS.triHPacyl.COelim.mmmmpmmpmmpmd	1.754e+45	9.41	9.41	2.433e+38	3.36e-05

15744	TS.triHPacyl.COelim.mmmppptmnd	6.818e+43	7.48	7.48	2.431e+38	3.36e-05
15745	TS.triHPacyl.COelim.pptmmtmpmd	6.689e+44	8.84	8.84	2.416e+38	3.34e-05
15746	TS.triHPacyl.COelim.ttpmmtmpd	3.805e+44	8.51	8.51	2.415e+38	3.33e-05
15747	TS.triHPacyl.COelim.mpttmmtppd	1.738e+45	9.41	9.41	2.411e+38	3.33e-05
15748	TS.triHPacyl.COelim.pttpmmtmnd	2.287e+44	8.21	8.21	2.399e+38	3.31e-05
15749	TS.triHPacyl.COelim.tpmtmtmpmd	3.745e+45	9.87	9.87	2.398e+38	3.31e-05
15750	TS.triHPacyl.COelim.mmmmpmtppd	5.454e+44	8.73	8.73	2.396e+38	3.31e-05
15751	TS.triHPacyl.COelim.pmtmmtmnd	2.777e+44	8.33	8.33	2.393e+38	3.3e-05
15752	TS.triHPacyl.COelim.mtmmtmnd	9.959e+44	9.10	9.10	2.357e+38	3.25e-05
15753	TS.triHPacyl.COelim.mmmmmmtmnd	2.463e+45	9.64	9.64	2.346e+38	3.24e-05
15754	TS.triHPacyl.COelim.pmmmpmtmpd	2.970e+44	8.38	8.38	2.320e+38	3.2e-05
15755	TS.triHPacyl.COelim.ptpmmtpppd	6.609e+43	7.49	7.49	2.298e+38	3.17e-05
15756	TS.triHPacyl.COelim.ptttmtpppd	2.530e+44	8.30	8.30	2.291e+38	3.16e-05
15757	TS.triHPacyl.COelim.mpppmppmpd	1.074e+45	9.16	9.16	2.288e+38	3.16e-05
15758	TS.triHPacyl.COelim.mtpmpppppd	1.244e+44	7.88	7.88	2.264e+38	3.13e-05
15759	TS.triHPacyl.COelim.mttmmtmnd	7.654e+44	8.98	8.98	2.211e+38	3.05e-05
15760	TS.triHPacyl.COelim.mmpmmtmpmd	4.613e+43	7.30	7.30	2.210e+38	3.05e-05
15761	TS.triHPacyl.COelim.ptttppmmpd	1.328e+44	7.93	7.93	2.206e+38	3.05e-05
15762	TS.triHPacyl.COelim.tpmmmppppd	4.150e+44	8.62	8.62	2.198e+38	3.03e-05
15763	TS.triHPacyl.COelim.mppppppppd	1.143e+45	9.22	9.22	2.196e+38	3.03e-05
15764	TS.triHPacyl.COelim.mpmtpmmpmd	1.647e+44	8.07	8.07	2.179e+38	3.01e-05
15765	TS.triHPacyl.COelim.mmpmtpmmpd	8.240e+44	9.03	9.03	2.174e+38	3e-05
15766	TS.triHPacyl.COelim.mtmmtmpmd	1.380e+45	9.35	9.35	2.143e+38	2.96e-05
15767	TS.triHPacyl.COelim.mpmtpmmpmd	1.135e+44	7.86	7.86	2.133e+38	2.95e-05
15768	TS.triHPacyl.COelim.mppppmmpmd	1.227e+44	7.91	7.91	2.120e+38	2.93e-05
15769	TS.triHPacyl.COelim.ptpppmmpmd	3.601e+43	7.18	7.18	2.109e+38	2.91e-05
15770	TS.triHPacyl.COelim.tmpmtmpmd	7.468e+43	7.62	7.62	2.104e+38	2.9e-05
15771	TS.triHPacyl.COelim.pmtmtpmnd	1.416e+44	8.00	8.00	2.098e+38	2.9e-05
15772	TS.triHPacyl.COelim.ptmmtmpmnd	7.588e+44	9.00	9.00	2.096e+38	2.89e-05
15773	TS.triHPacyl.COelim.ttptmmpmd	3.102e+44	8.47	8.47	2.089e+38	2.88e-05
15774	TS.triHPacyl.COelim.ptttmmpmd	6.573e+44	8.92	8.92	2.084e+38	2.88e-05
15775	TS.triHPacyl.COelim.mttppmmpmd	1.086e+45	9.22	9.22	2.082e+38	2.87e-05
15776	TS.triHPacyl.COelim.mtppppmmpmd	6.067e+43	7.50	7.50	2.074e+38	2.86e-05
15777	TS.triHPacyl.COelim.mptpmmpmd	1.047e+45	9.21	9.21	2.047e+38	2.83e-05
15778	TS.triHPacyl.COelim.mmmmpmtmnd	8.231e+44	9.07	9.07	2.037e+38	2.81e-05
15779	TS.triHPacyl.COelim.tpmmmmtmpd	2.859e+44	8.44	8.44	2.015e+38	2.78e-05
15780	TS.triHPacyl.COelim.mtttppmmpd	2.054e+45	9.63	9.63	1.978e+38	2.73e-05
15781	TS.triHPacyl.COelim.mmmppppmnd	5.737e+43	7.50	7.50	1.968e+38	2.72e-05
15782	TS.triHPacyl.COelim.tpmtmmpmd	6.426e+44	8.94	8.94	1.958e+38	2.7e-05
15783	TS.triHPacyl.COelim.pmmmmppmpd	1.438e+44	8.06	8.06	1.947e+38	2.69e-05
15784	TS.triHPacyl.COelim.tpmtmtpppd	2.963e+45	9.86	9.86	1.931e+38	2.67e-05
15785	TS.triHPacyl.COelim.mppmtmtpmd	2.456e+45	9.76	9.76	1.906e+38	2.63e-05
15786	TS.triHPacyl.COelim.mmmppptppd	2.254e+44	8.34	8.34	1.901e+38	2.62e-05
15787	TS.triHPacyl.COelim.tpmtmmpmd	1.097e+45	9.28	9.28	1.893e+38	2.61e-05
15788	TS.triHPacyl.COelim.mppmmmtmpd	1.956e+44	8.26	8.26	1.879e+38	2.59e-05
15789	TS.triHPacyl.COelim.mtmmtppppd	9.771e+44	9.22	9.22	1.878e+38	2.59e-05
15790	TS.triHPacyl.COelim.tmmtpmtpd	4.456e+45	10.13	10.13	1.849e+38	2.55e-05
15791	TS.triHPacyl.COelim.ptmmtmtpmd	4.676e+45	10.17	10.17	1.833e+38	2.53e-05
15792	TS.triHPacyl.COelim.pttmppppmd	5.228e+44	8.87	8.87	1.815e+38	2.51e-05
15793	TS.triHPacyl.COelim.mtmmtmmpmd	2.007e+45	9.68	9.68	1.790e+38	2.47e-05
15794	TS.triHPacyl.COelim.mmttppmmpd	2.262e+45	9.75	9.75	1.772e+38	2.45e-05
15795	TS.triHPacyl.COelim.ptmtmmpmd	1.032e+45	9.29	9.29	1.748e+38	2.41e-05
15796	TS.triHPacyl.COelim.tpmtptppd	5.041e+45	10.24	10.24	1.742e+38	2.41e-05
15797	TS.triHPacyl.COelim.tppmmtmpd	2.293e+44	8.41	8.41	1.722e+38	2.38e-05
15798	TS.triHPacyl.COelim.tpmmtmpmd	2.223e+44	8.39	8.39	1.704e+38	2.35e-05
15799	TS.triHPacyl.COelim.ptmmtmmpmd	8.026e+44	9.16	9.16	1.693e+38	2.34e-05
15800	TS.triHPacyl.COelim.tppmmtmmpmd	1.189e+45	9.40	9.40	1.691e+38	2.33e-05
15801	TS.triHPacyl.COelim.ptpmpptmpd	4.525e+43	7.46	7.46	1.672e+38	2.31e-05
15802	TS.triHPacyl.COelim.mttmptppd	9.494e+43	7.90	7.90	1.665e+38	2.3e-05
15803	TS.triHPacyl.COelim.mtttppmmpmd	6.557e+44	9.05	9.05	1.661e+38	2.29e-05
15804	TS.triHPacyl.COelim.mtptppmmpd	8.441e+44	9.21	9.21	1.659e+38	2.29e-05
15805	TS.triHPacyl.COelim.mtppptmmpmd	3.675e+43	7.36	7.36	1.611e+38	2.22e-05
15806	TS.triHPacyl.COelim.tppmmpmmpmd	4.513e+44	8.85	8.85	1.605e+38	2.22e-05
15807	TS.triHPacyl.COelim.ptpmmtmpd	8.270e+44	9.21	9.21	1.603e+38	2.21e-05
15808	TS.triHPacyl.COelim.ptmmtmmpd	4.603e+44	8.87	8.87	1.600e+38	2.21e-05
15809	TS.triHPacyl.COelim.tppmmtmpd	4.523e+44	8.86	8.86	1.596e+38	2.2e-05
15810	TS.triHPacyl.COelim.pmtmmtmnd	2.565e+45	9.90	9.90	1.584e+38	2.19e-05
15811	TS.triHPacyl.COelim.mtttptppmd	5.590e+45	10.36	10.36	1.576e+38	2.18e-05
15812	TS.triHPacyl.COelim.ptpmmppppd	1.209e+44	8.08	8.08	1.567e+38	2.16e-05
15813	TS.triHPacyl.COelim.tmpmmtmnd	2.740e+45	9.94	9.94	1.563e+38	2.16e-05
15814	TS.triHPacyl.COelim.mppmmtmnd	3.063e+45	10.01	10.01	1.550e+38	2.14e-05
15815	TS.triHPacyl.COelim.mpttmtppd	1.260e+45	9.49	9.49	1.546e+38	2.13e-05

15816	TS.triHPacyl.COelim.ttttmmpppd	1.366e+45	9.54	9.54	1.538e+38	2.12e-05
15817	TS.triHPacyl.COelim.tmmppptmmpd	2.936e+44	8.62	8.62	1.534e+38	2.12e-05
15818	TS.triHPacyl.COelim.ptpmtmmmd	4.767e+43	7.54	7.54	1.531e+38	2.11e-05
15819	TS.triHPacyl.COelim.pmpmtttmpd	5.539e+44	9.01	9.01	1.509e+38	2.08e-05
15820	TS.triHPacyl.COelim.mmpptptmmd	3.286e+44	8.70	8.70	1.507e+38	2.08e-05
15821	TS.triHPacyl.COelim.mmtmtmpmd	2.882e+45	10.00	10.00	1.487e+38	2.05e-05
15822	TS.triHPacyl.COelim.ttttmtpppd	1.251e+45	9.51	9.51	1.475e+38	2.04e-05
15823	TS.triHPacyl.COelim.pttmtptmmd	2.202e+44	8.48	8.48	1.474e+38	2.04e-05
15824	TS.triHPacyl.COelim.mmtmpppppd	6.141e+44	9.09	9.09	1.473e+38	2.03e-05
15825	TS.triHPacyl.COelim.ttmttppmd	1.241e+45	9.51	9.51	1.461e+38	2.02e-05
15826	TS.triHPacyl.COelim.mtmtpppppd	1.995e+45	9.80	9.80	1.456e+38	2.01e-05
15827	TS.triHPacyl.COelim.mttmtmmpd	2.180e+44	8.48	8.48	1.451e+38	2e-05
15828	TS.triHPacyl.COelim.ttptmtppmd	1.233e+45	9.51	9.51	1.444e+38	1.99e-05
15829	TS.triHPacyl.COelim.mmpmpmmpmd	2.968e+44	8.67	8.67	1.437e+38	1.98e-05
15830	TS.triHPacyl.COelim.ptmtmmpmd	1.117e+45	9.46	9.46	1.434e+38	1.98e-05
15831	TS.triHPacyl.COelim.tmpmtmmpd	3.509e+45	10.14	10.14	1.431e+38	1.98e-05
15832	TS.triHPacyl.COelim.ptmtmmmmmd	7.809e+44	9.25	9.25	1.428e+38	1.97e-05
15833	TS.triHPacyl.COelim.tttptttmpd	5.249e+44	9.01	9.01	1.424e+38	1.97e-05
15834	TS.triHPacyl.COelim.mmmmmttmmd	1.391e+45	9.60	9.60	1.407e+38	1.94e-05
15835	TS.triHPacyl.COelim.mtppppmmpd	1.357e+44	8.22	8.22	1.384e+38	1.91e-05
15836	TS.triHPacyl.COelim.tpptptmmd	3.699e+44	8.82	8.82	1.382e+38	1.91e-05
15837	TS.triHPacyl.COelim.tmttppppmd	3.631e+44	8.82	8.82	1.372e+38	1.89e-05
15838	TS.triHPacyl.COelim.ptpmpmpmd	5.912e+43	7.07	7.07	1.345e+38	1.86e-05
15839	TS.triHPacyl.COelim.mmpmtpmmd	5.501e+44	9.08	9.08	1.338e+38	1.85e-05
15840	TS.triHPacyl.COelim.tmttppmmd	3.500e+45	10.18	10.18	1.337e+38	1.85e-05
15841	TS.triHPacyl.COelim.mttptmmpd	2.784e+44	8.68	8.68	1.324e+38	1.83e-05
15842	TS.triHPacyl.COelim.mptptmmpd	3.120e+44	8.75	8.75	1.321e+38	1.82e-05
15843	TS.triHPacyl.COelim.mttpttmmmd	8.171e+45	10.70	10.70	1.319e+38	1.82e-05
15844	TS.triHPacyl.COelim.pmpptppmpd	5.685e+43	7.75	7.75	1.296e+38	1.79e-05
15845	TS.triHPacyl.COelim.mtppmmpmd	2.397e+44	8.60	8.60	1.295e+38	1.79e-05
15846	TS.triHPacyl.COelim.mtptmmpmd	6.028e+44	9.15	9.15	1.293e+38	1.79e-05
15847	TS.triHPacyl.COelim.tmttppmmd	6.378e+45	10.56	10.56	1.289e+38	1.78e-05
15848	TS.triHPacyl.COelim.mppmptmmd	2.246e+45	9.95	9.95	1.276e+38	1.76e-05
15849	TS.triHPacyl.COelim.mttptmmmpd	1.025e+45	9.49	9.49	1.250e+38	1.73e-05
15850	TS.triHPacyl.COelim.mmmmmttmmd	1.223e+45	9.60	9.60	1.247e+38	1.72e-05
15851	TS.triHPacyl.COelim.mtptppmmpd	1.497e+44	8.35	8.35	1.236e+38	1.71e-05
15852	TS.triHPacyl.COelim.mmpppptmmpd	1.624e+44	8.40	8.40	1.233e+38	1.7e-05
15853	TS.triHPacyl.COelim.mtmtppmmpd	2.105e+45	9.93	9.93	1.232e+38	1.7e-05
15854	TS.triHPacyl.COelim.mppmppppmd	2.065e+44	8.56	8.56	1.194e+38	1.65e-05
15855	TS.triHPacyl.COelim.ttttmmppmd	2.572e+45	10.07	10.07	1.186e+38	1.64e-05
15856	TS.triHPacyl.COelim.ptttmmmmmd	2.989e+44	8.79	8.79	1.183e+38	1.63e-05
15857	TS.triHPacyl.COelim.mtttppppmd	1.640e+44	8.43	8.43	1.183e+38	1.63e-05
15858	TS.triHPacyl.COelim.mtttmmmpmd	2.686e+45	10.10	10.10	1.178e+38	1.63e-05
15859	TS.triHPacyl.COelim.tpmtptmmpd	9.158e+44	9.46	9.46	1.175e+38	1.62e-05
15860	TS.triHPacyl.COelim.tmpmtttmpd	2.943e+45	10.16	10.16	1.167e+38	1.61e-05
15861	TS.triHPacyl.COelim.mtppmtpmmd	3.003e+43	7.43	7.43	1.153e+38	1.59e-05
15862	TS.triHPacyl.COelim.pppppppppd	4.356e+44	9.03	9.03	1.146e+38	1.58e-05
15863	TS.triHPacyl.COelim.mmtptptmmd	1.432e+44	8.37	8.37	1.138e+38	1.57e-05
15864	TS.triHPacyl.COelim.mmmppppppmd	6.204e+43	7.88	7.88	1.137e+38	1.57e-05
15865	TS.triHPacyl.COelim.mtppppmmmpd	1.476e+44	8.39	8.39	1.135e+38	1.57e-05
15866	TS.triHPacyl.COelim.mttptmmmd	1.699e+44	8.48	8.48	1.133e+38	1.56e-05
15867	TS.triHPacyl.COelim.mtttptpppd	3.120e+45	10.21	10.21	1.132e+38	1.56e-05
15868	TS.triHPacyl.COelim.mtmtmtpmmd	1.965e+45	9.94	9.94	1.126e+38	1.55e-05
15869	TS.triHPacyl.COelim.pmpmmpmmpd	1.070e+44	8.21	8.21	1.116e+38	1.54e-05
15870	TS.triHPacyl.COelim.ptpmmmpmd	3.735e+43	7.59	7.59	1.103e+38	1.52e-05
15871	TS.triHPacyl.COelim.ptmttpppd	1.651e+45	9.85	9.85	1.101e+38	1.52e-05
15872	TS.triHPacyl.COelim.mtmtmmmpd	9.676e+44	9.56	9.56	1.057e+38	1.46e-05
15873	TS.triHPacyl.COelim.ptmttppd	6.984e+44	9.37	9.37	1.049e+38	1.45e-05
15874	TS.triHPacyl.COelim.mmpmpmmpmd	1.110e+44	8.27	8.27	1.047e+38	1.45e-05
15875	TS.triHPacyl.COelim.mpttmmmmmd	1.905e+45	9.97	9.97	1.044e+38	1.44e-05
15876	TS.triHPacyl.COelim.tpptpmmpmd	1.739e+45	9.92	9.92	1.040e+38	1.44e-05
15877	TS.triHPacyl.COelim.tpptppmmpd	3.863e+44	9.02	9.02	1.034e+38	1.43e-05
15878	TS.triHPacyl.COelim.mptpmpmmpd	2.071e+45	10.03	10.03	1.030e+38	1.42e-05
15879	TS.triHPacyl.COelim.ptptmtpmmd	6.565e+44	9.34	9.34	1.026e+38	1.42e-05
15880	TS.triHPacyl.COelim.mmpmmtmmpd	3.342e+44	8.94	8.94	1.022e+38	1.41e-05
15881	TS.triHPacyl.COelim.mpppmtmmpd	4.654e+44	9.15	9.15	1.011e+38	1.4e-05
15882	TS.triHPacyl.COelim.mppppmmpd	6.826e+44	9.38	9.38	1.011e+38	1.4e-05
15883	TS.triHPacyl.COelim.mppmmpmmpd	1.164e+44	8.32	8.32	1.007e+38	1.39e-05
15884	TS.triHPacyl.COelim.mppmptmmd	2.489e+44	8.78	8.78	9.974e+37	1.38e-05
15885	TS.triHPacyl.COelim.mppppptmmd	9.736e+43	8.23	8.23	9.884e+37	1.36e-05
15886	TS.triHPacyl.COelim.ptmtmmtmmpd	1.095e+45	9.67	9.67	9.867e+37	1.36e-05
15887	TS.triHPacyl.COelim.mmmtpmmpd	2.468e+44	8.78	8.78	9.865e+37	1.36e-05

15888	TS.triHPacyl.COelim.mptmmppmd	1.072e+45	9.66	9.66	9.813e+37	1.35e-05
15889	TS.triHPacyl.COelim.ptmtmtmmpd	8.897e+44	9.55	9.55	9.810e+37	1.35e-05
15890	TS.triHPacyl.COelim.mttmmpppd	6.598e+44	9.38	9.38	9.757e+37	1.35e-05
15891	TS.triHPacyl.COelim.mttmtpmmd	4.521e+44	9.15	9.15	9.709e+37	1.34e-05
15892	TS.triHPacyl.COelim.mppmmtppd	5.589e+44	9.28	9.28	9.708e+37	1.34e-05
15893	TS.triHPacyl.COelim.pmtptmtpmd	1.697e+44	8.57	8.57	9.632e+37	1.33e-05
15894	TS.triHPacyl.COelim.mttmmmtmpd	1.389e+45	9.83	9.83	9.605e+37	1.33e-05
15895	TS.triHPacyl.COelim.mppmmpmpd	5.408e+44	9.27	9.27	9.587e+37	1.32e-05
15896	TS.triHPacyl.COelim.mppmnmmpd	2.723e+44	8.86	8.86	9.570e+37	1.32e-05
15897	TS.triHPacyl.COelim.ptmtmtmmd	1.588e+45	9.91	9.91	9.517e+37	1.31e-05
15898	TS.triHPacyl.COelim.mmtmmtmmd	1.143e+46	11.09	11.09	9.514e+37	1.31e-05
15899	TS.triHPacyl.COelim.tmtmmpmpd	9.351e+44	9.60	9.60	9.513e+37	1.31e-05
15900	TS.triHPacyl.COelim.mppmptpmd	1.759e+44	8.61	8.61	9.435e+37	1.3e-05
15901	TS.triHPacyl.COelim.pmttptmpd	1.048e+45	9.67	9.67	9.425e+37	1.3e-05
15902	TS.triHPacyl.COelim.tmtmmtmmd	2.043e+45	10.07	10.07	9.394e+37	1.3e-05
15903	TS.triHPacyl.COelim.mmtmmtmpd	5.725e+45	10.69	10.69	9.285e+37	1.28e-05
15904	TS.triHPacyl.COelim.mtptmmpmd	1.515e+45	9.91	9.91	9.193e+37	1.27e-05
15905	TS.triHPacyl.COelim.mmmppmtmmd	2.131e+44	8.74	8.74	9.151e+37	1.26e-05
15906	TS.triHPacyl.COelim.pttmtppppd	7.496e+44	9.49	9.49	9.150e+37	1.26e-05
15907	TS.triHPacyl.COelim.pmtmmpppd	6.525e+44	9.42	9.42	9.008e+37	1.24e-05
15908	TS.triHPacyl.COelim.mpppppppd	4.891e+44	9.25	9.25	8.996e+37	1.24e-05
15909	TS.triHPacyl.COelim.tttmmpmpd	4.994e+44	9.26	9.26	8.964e+37	1.24e-05
15910	TS.triHPacyl.COelim.mptmmpppd	6.859e+44	9.45	9.45	8.924e+37	1.23e-05
15911	TS.triHPacyl.COelim.pmttptppd	5.764e+45	10.73	10.73	8.836e+37	1.22e-05
15912	TS.triHPacyl.COelim.mmtppppmd	2.681e+43	7.53	7.53	8.808e+37	1.22e-05
15913	TS.triHPacyl.COelim.mtmptmmpd	5.877e+44	9.37	9.37	8.749e+37	1.21e-05
15914	TS.triHPacyl.COelim.mppmtmmpd	1.483e+45	9.93	9.93	8.702e+37	1.2e-05
15915	TS.triHPacyl.COelim.tmpmmtmmd	2.368e+44	8.84	8.84	8.639e+37	1.19e-05
15916	TS.triHPacyl.COelim.pmtmmpmpd	2.607e+44	8.90	8.90	8.628e+37	1.19e-05
15917	TS.triHPacyl.COelim.mptmppppd	4.247e+44	9.19	9.19	8.600e+37	1.19e-05
15918	TS.triHPacyl.COelim.mtmtmtmmpd	1.059e+44	8.36	8.36	8.578e+37	1.18e-05
15919	TS.triHPacyl.COelim.mtppmmpmd	6.075e+44	9.41	9.41	8.460e+37	1.17e-05
15920	TS.triHPacyl.COelim.tpmtmmpmd	2.995e+45	10.37	10.37	8.427e+37	1.16e-05
15921	TS.triHPacyl.COelim.mtmtmtmmpd	1.022e+46	11.10	11.10	8.411e+37	1.16e-05
15922	TS.triHPacyl.COelim.mmpmmpmpd	1.681e+44	8.66	8.66	8.309e+37	1.15e-05
15923	TS.triHPacyl.COelim.mmmppmmpd	1.650e+44	8.65	8.65	8.304e+37	1.15e-05
15924	TS.triHPacyl.COelim.tttmtttmpd	9.593e+44	9.70	9.70	8.302e+37	1.15e-05
15925	TS.triHPacyl.COelim.mmmptmmpd	1.109e+44	8.41	8.41	8.291e+37	1.14e-05
15926	TS.triHPacyl.COelim.pmtmmtmpd	1.583e+44	9.12	9.12	8.207e+37	1.13e-05
15927	TS.triHPacyl.COelim.tmttptppd	4.912e+45	10.68	10.68	8.161e+37	1.13e-05
15928	TS.triHPacyl.COelim.mtptmmpmd	5.803e+44	9.41	9.41	8.075e+37	1.11e-05
15929	TS.triHPacyl.COelim.tmpmmtmmd	2.931e+44	9.01	9.01	8.058e+37	1.11e-05
15930	TS.triHPacyl.COelim.tppmmmpmd	3.928e+44	9.20	9.20	7.816e+37	1.08e-05
15931	TS.triHPacyl.COelim.pmtmppppd	1.179e+45	9.86	9.86	7.773e+37	1.07e-05
15932	TS.triHPacyl.COelim.pppmmmpd	8.233e+43	8.27	8.27	7.718e+37	1.07e-05
15933	TS.triHPacyl.COelim.mppmmpmpd	7.143e+44	9.58	9.58	7.544e+37	1.04e-05
15934	TS.triHPacyl.COelim.mptmppppd	9.322e+44	9.74	9.74	7.505e+37	1.04e-05
15935	TS.triHPacyl.COelim.pmttptmpd	1.032e+45	9.80	9.80	7.453e+37	1.03e-05
15936	TS.triHPacyl.COelim.mptmmpppd	1.234e+45	9.91	9.91	7.453e+37	1.03e-05
15937	TS.triHPacyl.COelim.mtppmtpmd	3.129e+44	9.10	9.10	7.352e+37	1.02e-05
15938	TS.triHPacyl.COelim.tttmmtmpd	1.129e+45	9.87	9.87	7.257e+37	1e-05
15939	TS.triHPacyl.COelim.tmmppmmpd	2.559e+44	8.99	8.99	7.242e+37	1e-05
15940	TS.triHPacyl.COelim.mmtmmpmpd	3.697e+45	10.58	10.58	7.226e+37	9.98e-06
15941	TS.triHPacyl.COelim.mtmmpmmpd	1.395e+44	8.63	8.63	7.213e+37	9.96e-06
15942	TS.triHPacyl.COelim.mtmmpmpd	2.875e+44	9.07	9.07	7.126e+37	9.84e-06
15943	TS.triHPacyl.COelim.ptmtmtpmd	1.640e+45	10.11	10.11	7.070e+37	9.76e-06
15944	TS.triHPacyl.COelim.mppmptpmd	1.135e+45	9.89	9.89	7.027e+37	9.7e-06
15945	TS.triHPacyl.COelim.mmmppptpmd	3.262e+44	9.15	9.15	7.020e+37	9.69e-06
15946	TS.triHPacyl.COelim.mtmtmtpd	7.941e+44	9.70	9.70	6.849e+37	9.46e-06
15947	TS.triHPacyl.COelim.mtmmtmmd	1.447e+45	10.07	10.07	6.723e+37	9.28e-06
15948	TS.triHPacyl.COelim.pttmtmmpd	3.017e+44	9.13	9.13	6.690e+37	9.24e-06
15949	TS.triHPacyl.COelim.mmtmtpppd	7.917e+45	11.08	11.08	6.663e+37	9.2e-06
15950	TS.triHPacyl.COelim.mppmmpmpd	8.404e+44	9.75	9.75	6.633e+37	9.16e-06
15951	TS.triHPacyl.COelim.tmttptmpd	1.677e+45	10.17	10.17	6.537e+37	9.03e-06
15952	TS.triHPacyl.COelim.mppmmpmpd	1.295e+45	10.02	10.02	6.506e+37	8.98e-06
15953	TS.triHPacyl.COelim.tmmppptppd	8.931e+44	9.80	9.80	6.436e+37	8.89e-06
15954	TS.triHPacyl.COelim.ptmptmmpd	4.973e+43	8.08	8.08	6.433e+37	8.88e-06
15955	TS.triHPacyl.COelim.pmtmtpmpd	5.277e+44	9.49	9.49	6.431e+37	8.88e-06
15956	TS.triHPacyl.COelim.mppmmtmmd	1.752e+45	10.21	10.21	6.415e+37	8.86e-06
15957	TS.triHPacyl.COelim.ptppmmpmd	6.869e+43	8.28	8.28	6.405e+37	8.84e-06
15958	TS.triHPacyl.COelim.ptmtpmpd	4.461e+44	9.40	9.40	6.358e+37	8.78e-06
15959	TS.triHPacyl.COelim.pmtmmpmpd	1.546e+44	8.77	8.77	6.301e+37	8.7e-06

15960	TS.triHPacyl.COelim.mtptppmpmd	2.064e+44	8.95	8.95	6.253e+37	8.63e-06
15961	TS.triHPacyl.COelim.mmmtptmtpmd	4.578e+45	10.80	10.80	6.223e+37	8.59e-06
15962	TS.triHPacyl.COelim.mmmtmtpmmd	1.938e+44	8.92	8.92	6.157e+37	8.5e-06
15963	TS.triHPacyl.COelim.mttmmtmtpmd	9.627e+44	9.88	9.88	6.136e+37	8.47e-06
15964	TS.triHPacyl.COelim.mmmtpppmmd	4.516e+43	8.08	8.08	5.912e+37	8.16e-06
15965	TS.triHPacyl.COelim.pttmtptmmd	3.072e+44	9.22	9.22	5.874e+37	8.11e-06
15966	TS.triHPacyl.COelim.mppppptpmd	2.119e+44	9.00	9.00	5.854e+37	8.08e-06
15967	TS.triHPacyl.COelim.tmtptpmpmd	2.410e+44	9.08	9.08	5.849e+37	8.08e-06
15968	TS.triHPacyl.COelim.mtttptpmpd	1.856e+44	8.93	8.93	5.820e+37	8.04e-06
15969	TS.triHPacyl.COelim.mtptpptpmd	6.078e+44	9.64	9.64	5.813e+37	8.03e-06
15970	TS.triHPacyl.COelim.tmtpttmmd	2.407e+45	10.46	10.46	5.787e+37	7.99e-06
15971	TS.triHPacyl.COelim.pmtptmtpmd	1.500e+44	8.81	8.81	5.778e+37	7.98e-06
15972	TS.triHPacyl.COelim.ptmtmtpmd	6.674e+44	9.70	9.70	5.759e+37	7.95e-06
15973	TS.triHPacyl.COelim.mtmtmmpmmd	8.110e+44	9.82	9.82	5.738e+37	7.92e-06
15974	TS.triHPacyl.COelim.tpppmtmtpd	4.872e+44	9.52	9.52	5.630e+37	7.77e-06
15975	TS.triHPacyl.COelim.mpttmpppmd	9.898e+44	9.95	9.95	5.581e+37	7.71e-06
15976	TS.triHPacyl.COelim.mmmpmmpmmd	2.796e+44	9.20	9.20	5.561e+37	7.68e-06
15977	TS.triHPacyl.COelim.mmtpmtpmmd	1.674e+45	10.27	10.27	5.552e+37	7.67e-06
15978	TS.triHPacyl.COelim.tmtmtmmd	1.438e+44	8.80	8.80	5.545e+37	7.66e-06
15979	TS.triHPacyl.COelim.ptppmtmtpd	7.345e+43	8.41	8.41	5.512e+37	7.61e-06
15980	TS.triHPacyl.COelim.mmppmtpmd	6.062e+44	9.68	9.68	5.424e+37	7.49e-06
15981	TS.triHPacyl.COelim.mtttmtmtpd	3.990e+45	10.80	10.80	5.406e+37	7.46e-06
15982	TS.triHPacyl.COelim.ptmtmmpmmd	1.384e+44	8.80	8.80	5.367e+37	7.41e-06
15983	TS.triHPacyl.COelim.pmtmmtmmd	1.089e+45	10.03	10.03	5.342e+37	7.38e-06
15984	TS.triHPacyl.COelim.tpptmtpmd	3.213e+45	10.68	10.68	5.289e+37	7.3e-06
15985	TS.triHPacyl.COelim.ptptmtpmd	1.014e+44	8.63	8.63	5.250e+37	7.25e-06
15986	TS.triHPacyl.COelim.ptmtmtpmmd	5.323e+44	9.62	9.62	5.211e+37	7.19e-06
15987	TS.triHPacyl.COelim.tmpmtpmmd	6.132e+44	9.71	9.71	5.202e+37	7.18e-06
15988	TS.triHPacyl.COelim.mpmtmpppmd	1.429e+44	8.84	8.84	5.162e+37	7.13e-06
15989	TS.triHPacyl.COelim.mmtpptmtpd	4.891e+44	9.58	9.58	5.120e+37	7.07e-06
15990	TS.triHPacyl.COelim.mmmtptpmd	2.638e+44	9.22	9.22	5.067e+37	7e-06
15991	TS.triHPacyl.COelim.mtptppmmd	1.666e+44	8.95	8.95	5.054e+37	6.98e-06
15992	TS.triHPacyl.COelim.mmmtpppmd	1.140e+44	8.72	8.72	5.044e+37	6.96e-06
15993	TS.triHPacyl.COelim.pmtmmtmtpd	4.613e+44	9.56	9.56	5.024e+37	6.94e-06
15994	TS.triHPacyl.COelim.ptpmpmpmd	1.477e+44	8.88	8.88	4.982e+37	6.88e-06
15995	TS.triHPacyl.COelim.ptptmtpmd	1.570e+44	8.92	8.92	4.967e+37	6.86e-06
15996	TS.triHPacyl.COelim.pttptmtpmd	5.043e+44	9.62	9.62	4.959e+37	6.85e-06
15997	TS.triHPacyl.COelim.tmtptmmpmd	1.028e+46	11.42	11.42	4.953e+37	6.84e-06
15998	TS.triHPacyl.COelim.mmtpmmpmmd	8.994e+44	9.96	9.96	4.952e+37	6.84e-06
15999	TS.triHPacyl.COelim.mtppmmpmd	2.363e+44	9.18	9.18	4.890e+37	6.75e-06
16000	TS.triHPacyl.COelim.mpmtmtpmmd	6.679e+44	9.79	9.79	4.889e+37	6.75e-06
16001	TS.triHPacyl.COelim.mtttmtmtpd	5.530e+44	9.69	9.69	4.860e+37	6.71e-06
16002	TS.triHPacyl.COelim.pmtmtpmmd	5.173e+44	9.65	9.65	4.851e+37	6.7e-06
16003	TS.triHPacyl.COelim.pttmtmtpmd	4.777e+44	9.60	9.60	4.839e+37	6.68e-06
16004	TS.triHPacyl.COelim.pttpppmmd	2.777e+44	9.29	9.29	4.739e+37	6.54e-06
16005	TS.triHPacyl.COelim.ptptmmpmmd	2.055e+44	9.12	9.12	4.652e+37	6.42e-06
16006	TS.triHPacyl.COelim.ppppmpmpd	5.609e+43	8.35	8.35	4.642e+37	6.41e-06
16007	TS.triHPacyl.COelim.pttmtpppmd	7.172e+44	9.87	9.87	4.618e+37	6.38e-06
16008	TS.triHPacyl.COelim.mmtmtpmmd	8.012e+44	9.94	9.94	4.608e+37	6.36e-06
16009	TS.triHPacyl.COelim.mptmmpmmd	1.180e+45	10.17	10.17	4.605e+37	6.36e-06
16010	TS.triHPacyl.COelim.mppmtmmpmd	1.292e+45	10.23	10.23	4.584e+37	6.33e-06
16011	TS.triHPacyl.COelim.mmmpptpmd	9.925e+43	8.70	8.70	4.529e+37	6.25e-06
16012	TS.triHPacyl.COelim.mttmmmpmmd	4.546e+44	9.62	9.62	4.478e+37	6.18e-06
16013	TS.triHPacyl.COelim.tmtptmtpmd	1.403e+45	10.29	10.29	4.461e+37	6.16e-06
16014	TS.triHPacyl.COelim.tppppppmd	7.633e+43	8.56	8.56	4.455e+37	6.15e-06
16015	TS.triHPacyl.COelim.mtmtmmpmmd	1.084e+45	10.14	10.14	4.449e+37	6.14e-06
16016	TS.triHPacyl.COelim.mmtpmtpmmd	1.353e+45	10.27	10.27	4.437e+37	6.13e-06
16017	TS.triHPacyl.COelim.mttmmmpmmd	1.807e+45	10.45	10.45	4.415e+37	6.1e-06
16018	TS.triHPacyl.COelim.tmtptmtpmd	1.141e+46	11.56	11.56	4.336e+37	5.99e-06
16019	TS.triHPacyl.COelim.ttptmmpmmd	1.327e+44	8.91	8.91	4.322e+37	5.97e-06
16020	TS.triHPacyl.COelim.mmppmmtmmd	5.212e+44	9.73	9.73	4.288e+37	5.92e-06
16021	TS.triHPacyl.COelim.mmpmmpmmd	4.598e+43	8.28	8.28	4.279e+37	5.91e-06
16022	TS.triHPacyl.COelim.mmmtmmpmmd	6.000e+43	8.44	8.44	4.245e+37	5.86e-06
16023	TS.triHPacyl.COelim.mpmtpmmpmd	3.995e+44	9.58	9.58	4.161e+37	5.75e-06
16024	TS.triHPacyl.COelim.pmpmtpmmd	6.851e+43	8.54	8.54	4.147e+37	5.73e-06
16025	TS.triHPacyl.COelim.ptmtppmmd	7.320e+44	9.95	9.95	4.106e+37	5.67e-06
16026	TS.triHPacyl.COelim.tmtptmmd	1.640e+45	10.44	10.44	4.089e+37	5.65e-06
16027	TS.triHPacyl.COelim.mppmtpmmd	3.190e+44	9.46	9.46	4.063e+37	5.61e-06
16028	TS.triHPacyl.COelim.tppmtpmmd	8.328e+43	8.67	8.67	4.004e+37	5.53e-06
16029	TS.triHPacyl.COelim.mtppmmpmmd	1.020e+44	8.79	8.79	4.003e+37	5.53e-06
16030	TS.triHPacyl.COelim.ptptpmpmd	1.226e+44	8.91	8.91	3.985e+37	5.5e-06
16031	TS.triHPacyl.COelim.pmtmtpmmd	5.139e+44	9.77	9.77	3.927e+37	5.42e-06

16032	TS.triHPacyl.COelim.pttptmptmmd	1.408e+44	9.00	9.00	3.911e+37	5.4e-06
16033	TS.triHPacyl.COelim.tmtptmmpdpd	1.541e+45	10.43	10.43	3.900e+37	5.39e-06
16034	TS.triHPacyl.COelim.mtptptmmpd	6.981e+43	8.58	8.58	3.896e+37	5.38e-06
16035	TS.triHPacyl.COelim.pttmptmtpd	3.932e+44	9.62	9.62	3.887e+37	5.37e-06
16036	TS.triHPacyl.COelim.mtmptmmmmmd	2.899e+44	9.44	9.44	3.870e+37	5.34e-06
16037	TS.triHPacyl.COelim.mmmptmmmmmd	2.877e+44	9.43	9.43	3.858e+37	5.33e-06
16038	TS.triHPacyl.COelim.tmmppmtmpd	5.265e+44	9.80	9.80	3.833e+37	5.29e-06
16039	TS.triHPacyl.COelim.ptptmtmmpd	2.173e+44	9.27	9.27	3.812e+37	5.26e-06
16040	TS.triHPacyl.COelim.tpmppmpppd	1.486e+44	9.05	9.05	3.769e+37	5.2e-06
16041	TS.triHPacyl.COelim.mptpmmtmpd	3.913e+45	11.00	11.00	3.768e+37	5.2e-06
16042	TS.triHPacyl.COelim.mmmptmmmmmd	3.004e+44	9.48	9.48	3.743e+37	5.17e-06
16043	TS.triHPacyl.COelim.ttmtpmtmmd	1.779e+45	10.54	10.54	3.714e+37	5.13e-06
16044	TS.triHPacyl.COelim.mtmptmmmmmd	1.803e+44	9.18	9.18	3.701e+37	5.11e-06
16045	TS.triHPacyl.COelim.tpmtppppppd	6.331e+44	9.93	9.93	3.679e+37	5.08e-06
16046	TS.triHPacyl.COelim.pmptptpppd	1.769e+44	9.18	9.18	3.658e+37	5.05e-06
16047	TS.triHPacyl.COelim.ptptmtmmd	7.087e+44	10.01	10.01	3.603e+37	4.97e-06
16048	TS.triHPacyl.COelim.mmmtpptmmd	1.486e+44	9.09	9.09	3.563e+37	4.92e-06
16049	TS.triHPacyl.COelim.mmmmtmtpmpd	2.328e+44	9.37	9.37	3.462e+37	4.78e-06
16050	TS.triHPacyl.COelim.pmtmpptmmd	1.218e+44	9.48	9.48	3.430e+37	4.74e-06
16051	TS.triHPacyl.COelim.ttmppmtpmpd	1.801e+44	9.23	9.23	3.419e+37	4.72e-06
16052	TS.triHPacyl.COelim.mpmmtmmmmmd	5.502e+44	9.90	9.90	3.399e+37	4.69e-06
16053	TS.triHPacyl.COelim.tmmppttmtpd	3.022e+44	9.54	9.54	3.375e+37	4.66e-06
16054	TS.triHPacyl.COelim.pmppptpppd	7.629e+43	8.73	8.73	3.354e+37	4.63e-06
16055	TS.triHPacyl.COelim.ptmtmmpmpd	2.689e+44	9.49	9.49	3.293e+37	4.55e-06
16056	TS.triHPacyl.COelim.mmpmptpmmd	8.281e+43	8.80	8.80	3.208e+37	4.43e-06
16057	TS.triHPacyl.COelim.mtmptmtpmpd	6.693e+44	10.05	10.05	3.206e+37	4.43e-06
16058	TS.triHPacyl.COelim.mptmptmtpd	7.104e+45	11.46	11.46	3.195e+37	4.41e-06
16059	TS.triHPacyl.COelim.mptmptmtpd	2.130e+45	10.75	10.75	3.154e+37	4.36e-06
16060	TS.triHPacyl.COelim.mtptmppmpd	7.836e+44	10.16	10.16	3.117e+37	4.3e-06
16061	TS.triHPacyl.COelim.mmpmmmtppd	5.423e+44	9.96	9.96	3.017e+37	4.17e-06
16062	TS.triHPacyl.COelim.mtppmtmtpd	1.218e+45	10.45	10.45	2.961e+37	4.09e-06
16063	TS.triHPacyl.COelim.ptptmmpmpd	6.894e+44	10.11	10.11	2.959e+37	4.09e-06
16064	TS.triHPacyl.COelim.mtmmtmtpd	1.790e+45	10.68	10.68	2.946e+37	4.07e-06
16065	TS.triHPacyl.COelim.ptppmmpppd	6.622e+44	10.09	10.09	2.936e+37	4.05e-06
16066	TS.triHPacyl.COelim.mtmpppmmd	1.578e+44	9.25	9.25	2.873e+37	3.97e-06
16067	TS.triHPacyl.COelim.mmmmtmtpd	5.285e+45	11.35	11.35	2.857e+37	3.94e-06
16068	TS.triHPacyl.COelim.mmtppptmtpd	3.429e+44	9.72	9.72	2.844e+37	3.93e-06
16069	TS.triHPacyl.COelim.mmttptmtpd	3.856e+45	11.17	11.17	2.826e+37	3.9e-06
16070	TS.triHPacyl.COelim.mmmtpppmpd	1.769e+44	9.34	9.34	2.790e+37	3.85e-06
16071	TS.triHPacyl.COelim.tmmppmtppd	7.112e+44	10.17	10.17	2.785e+37	3.84e-06
16072	TS.triHPacyl.COelim.mtmppppmpd	2.759e+44	9.61	9.61	2.750e+37	3.8e-06
16073	TS.triHPacyl.COelim.ptptppmpd	9.418e+43	8.97	8.97	2.747e+37	3.79e-06
16074	TS.triHPacyl.COelim.mmttptmtpd	3.683e+45	11.16	11.16	2.745e+37	3.79e-06
16075	TS.triHPacyl.COelim.mttmmmmmpd	8.591e+44	10.29	10.29	2.735e+37	3.78e-06
16076	TS.triHPacyl.COelim.mmmtpptmmd	4.347e+44	9.89	9.89	2.712e+37	3.74e-06
16077	TS.triHPacyl.COelim.mptmmtmtpd	8.450e+45	11.67	11.67	2.678e+37	3.7e-06
16078	TS.triHPacyl.COelim.mtptppmmmd	1.060e+45	10.44	10.44	2.644e+37	3.65e-06
16079	TS.triHPacyl.COelim.mtptptppd	7.585e+43	8.87	8.87	2.640e+37	3.64e-06
16080	TS.triHPacyl.COelim.mmttptmmd	1.876e+45	10.81	10.81	2.518e+37	3.48e-06
16081	TS.triHPacyl.COelim.mmpmtmmpmd	4.145e+44	9.91	9.91	2.507e+37	3.46e-06
16082	TS.triHPacyl.COelim.mttmtmtpmd	4.487e+44	9.96	9.96	2.506e+37	3.46e-06
16083	TS.triHPacyl.COelim.mmpmtmmpmd	6.217e+44	10.16	10.16	2.484e+37	3.43e-06
16084	TS.triHPacyl.COelim.tpppmtppd	4.553e+44	9.98	9.98	2.454e+37	3.39e-06
16085	TS.triHPacyl.COelim.mtmptmtpd	3.015e+44	9.74	9.74	2.423e+37	3.35e-06
16086	TS.triHPacyl.COelim.ptpmmtmmpd	2.514e+43	8.27	8.27	2.378e+37	3.28e-06
16087	TS.triHPacyl.COelim.tppmmmtmtpd	7.696e+44	10.32	10.32	2.322e+37	3.21e-06
16088	TS.triHPacyl.COelim.mptmptmmd	2.306e+45	10.98	10.98	2.320e+37	3.2e-06
16089	TS.triHPacyl.COelim.pmptpmmpmd	6.354e+44	10.22	10.22	2.285e+37	3.16e-06
16090	TS.triHPacyl.COelim.mmmtpptmtpd	9.211e+44	10.44	10.44	2.283e+37	3.15e-06
16091	TS.triHPacyl.COelim.mmttptmmd	5.320e+45	11.50	11.50	2.249e+37	3.11e-06
16092	TS.triHPacyl.COelim.ttpmmmmmmmd	7.974e+43	9.01	9.01	2.186e+37	3.02e-06
16093	TS.triHPacyl.COelim.mttmmtmtpmd	2.847e+45	11.14	11.14	2.173e+37	3e-06
16094	TS.triHPacyl.COelim.tpmppppppd	4.198e+44	10.00	10.00	2.172e+37	3e-06
16095	TS.triHPacyl.COelim.mpmtpmmpmd	2.828e+44	9.77	9.77	2.171e+37	3e-06
16096	TS.triHPacyl.COelim.mttmmtmmd	5.197e+44	10.14	10.14	2.119e+37	2.93e-06
16097	TS.triHPacyl.COelim.tmpmptmtpd	1.025e+45	10.55	10.55	2.098e+37	2.9e-06
16098	TS.triHPacyl.COelim.ttpmptmtpd	8.016e+43	9.04	9.04	2.087e+37	2.88e-06
16099	TS.triHPacyl.COelim.mmmtpptpmd	1.965e+44	9.57	9.57	2.086e+37	2.88e-06
16100	TS.triHPacyl.COelim.mtmppptppd	3.173e+44	9.87	9.87	2.051e+37	2.83e-06
16101	TS.triHPacyl.COelim.pmmmtmtpmd	3.205e+44	9.88	9.88	2.032e+37	2.81e-06
16102	TS.triHPacyl.COelim.pmptmppppd	1.937e+44	9.58	9.58	2.030e+37	2.8e-06
16103	TS.triHPacyl.COelim.pmmppmmppd	5.076e+44	10.16	10.16	2.025e+37	2.8e-06

16104	TS.triHPacyl.COelim.mmmtpppppd	1.041e+45	10.59	10.59	2.002e+37	2.76e-06
16105	TS.triHPacyl.COelim.mmmmpmmtppd	4.590e+44	10.12	10.12	1.944e+37	2.68e-06
16106	TS.triHPacyl.COelim.tmptmmpmd	6.162e+44	10.30	10.30	1.942e+37	2.68e-06
16107	TS.triHPacyl.COelim.mpttptmppd	1.251e+45	10.72	10.72	1.934e+37	2.67e-06
16108	TS.triHPacyl.COelim.pmpppmmmpd	5.500e+43	8.86	8.86	1.930e+37	2.67e-06
16109	TS.triHPacyl.COelim.mmpmmmmppd	5.651e+43	8.88	8.88	1.909e+37	2.64e-06
16110	TS.triHPacyl.COelim.ptpmmmtmpd	1.472e+44	9.46	9.46	1.895e+37	2.62e-06
16111	TS.triHPacyl.COelim.mtpmmppmmd	1.880e+44	9.61	9.61	1.890e+37	2.61e-06
16112	TS.triHPacyl.COelim.mpmtmmtmpd	1.062e+45	10.65	10.65	1.854e+37	2.56e-06
16113	TS.triHPacyl.COelim.pmmtpppppd	1.046e+44	9.27	9.27	1.847e+37	2.55e-06
16114	TS.triHPacyl.COelim.ptmtmtpmd	6.619e+44	10.37	10.37	1.844e+37	2.55e-06
16115	TS.triHPacyl.COelim.mttmtmmpmd	5.696e+45	11.66	11.66	1.836e+37	2.54e-06
16116	TS.triHPacyl.COelim.mmmmtppmpd	2.352e+44	9.76	9.76	1.816e+37	2.51e-06
16117	TS.triHPacyl.COelim.mmmmtmmtmpd	7.789e+45	11.88	11.88	1.739e+37	2.4e-06
16118	TS.triHPacyl.COelim.mtppmtmmmd	9.417e+43	9.25	9.25	1.712e+37	2.36e-06
16119	TS.triHPacyl.COelim.pmpppptppd	6.506e+43	9.04	9.04	1.692e+37	2.34e-06
16120	TS.triHPacyl.COelim.mmmtpptppd	6.039e+44	10.37	10.37	1.691e+37	2.33e-06
16121	TS.triHPacyl.COelim.mpppppmpd	9.851e+43	9.29	9.29	1.686e+37	2.33e-06
16122	TS.triHPacyl.COelim.ptmtmtpmd	1.302e+44	9.46	9.46	1.678e+37	2.32e-06
16123	TS.triHPacyl.COelim.mtmppmmpmd	2.879e+44	9.94	9.94	1.666e+37	2.3e-06
16124	TS.triHPacyl.COelim.mmmtpptmpd	8.175e+44	10.56	10.56	1.654e+37	2.28e-06
16125	TS.triHPacyl.COelim.ptmtmmpppd	4.728e+44	10.24	10.24	1.642e+37	2.27e-06
16126	TS.triHPacyl.COelim.mttmtmmpmd	8.383e+44	10.60	10.60	1.601e+37	2.21e-06
16127	TS.triHPacyl.COelim.ttmtpmpmmd	3.494e+44	10.08	10.08	1.591e+37	2.2e-06
16128	TS.triHPacyl.COelim.mmmmpmtmmpd	1.664e+44	9.64	9.64	1.577e+37	2.18e-06
16129	TS.triHPacyl.COelim.mtppmmtppd	5.987e+44	10.41	10.41	1.554e+37	2.15e-06
16130	TS.triHPacyl.COelim.pmmppppmd	6.574e+43	9.10	9.10	1.548e+37	2.14e-06
16131	TS.triHPacyl.COelim.mtmtptpppd	1.372e+45	10.91	10.91	1.541e+37	2.13e-06
16132	TS.triHPacyl.COelim.mptmmmtmmd	2.723e+45	11.33	11.33	1.525e+37	2.11e-06
16133	TS.triHPacyl.COelim.mmmtpptppd	1.959e+45	11.13	11.13	1.516e+37	2.09e-06
16134	TS.triHPacyl.COelim.mtpmmpmmd	1.127e+44	9.44	9.44	1.495e+37	2.06e-06
16135	TS.triHPacyl.COelim.tppmtmpd	8.017e+44	10.63	10.63	1.455e+37	2.01e-06
16136	TS.triHPacyl.COelim.ptmmpmtppd	2.030e+44	9.81	9.81	1.448e+37	2e-06
16137	TS.triHPacyl.COelim.ptttmmtmpd	9.698e+44	10.75	10.75	1.441e+37	1.99e-06
16138	TS.triHPacyl.COelim.mtptmtpmd	6.265e+45	11.88	11.88	1.388e+37	1.92e-06
16139	TS.triHPacyl.COelim.mtmtptppmd	1.224e+45	10.91	10.91	1.372e+37	1.89e-06
16140	TS.triHPacyl.COelim.ptmmpmtmpd	1.701e+44	9.74	9.74	1.366e+37	1.89e-06
16141	TS.triHPacyl.COelim.ptmtmptmmd	7.871e+44	10.66	10.66	1.342e+37	1.85e-06
16142	TS.triHPacyl.COelim.mtmppmpmmd	8.272e+43	9.33	9.33	1.323e+37	1.83e-06
16143	TS.triHPacyl.COelim.mmmtpptppd	1.488e+45	11.06	11.06	1.308e+37	1.81e-06
16144	TS.triHPacyl.COelim.mmtmmpmmpmd	7.152e+44	10.62	10.62	1.307e+37	1.8e-06
16145	TS.triHPacyl.COelim.mtmtptmmpd	1.042e+45	10.86	10.86	1.285e+37	1.77e-06
16146	TS.triHPacyl.COelim.pmptpmtmpd	7.413e+44	10.66	10.66	1.267e+37	1.75e-06
16147	TS.triHPacyl.COelim.pmpppmtmmpd	6.234e+43	9.21	9.21	1.216e+37	1.68e-06
16148	TS.triHPacyl.COelim.pmmptmmd	1.118e+44	9.56	9.56	1.215e+37	1.68e-06
16149	TS.triHPacyl.COelim.mttmptmmd	7.265e+44	10.68	10.68	1.198e+37	1.65e-06
16150	TS.triHPacyl.COelim.mmtmmpmmpd	1.103e+45	10.94	10.94	1.191e+37	1.64e-06
16151	TS.triHPacyl.COelim.pmmmtmmpmd	1.863e+44	9.89	9.89	1.170e+37	1.61e-06
16152	TS.triHPacyl.COelim.mmmtpptmpd	4.595e+44	10.44	10.44	1.147e+37	1.58e-06
16153	TS.triHPacyl.COelim.mtppmtppmd	1.313e+44	9.69	9.69	1.146e+37	1.58e-06
16154	TS.triHPacyl.COelim.mmmppmtmpd	4.075e+44	10.37	10.37	1.128e+37	1.56e-06
16155	TS.triHPacyl.COelim.mtppmptppd	7.797e+44	10.76	10.76	1.127e+37	1.56e-06
16156	TS.triHPacyl.COelim.mptmmtmmpd	1.505e+45	11.16	11.16	1.125e+37	1.55e-06
16157	TS.triHPacyl.COelim.mppppmmpd	1.019e+44	9.57	9.57	1.097e+37	1.51e-06
16158	TS.triHPacyl.COelim.tppmmtmmd	3.148e+43	8.87	8.87	1.090e+37	1.51e-06
16159	TS.triHPacyl.COelim.mtmmtmtpd	3.022e+45	11.60	11.60	1.069e+37	1.48e-06
16160	TS.triHPacyl.COelim.ptptmppmd	3.126e+44	10.26	10.26	1.052e+37	1.45e-06
16161	TS.triHPacyl.COelim.ptpmmppppd	8.592e+43	9.50	9.50	1.038e+37	1.43e-06
16162	TS.triHPacyl.COelim.tpmtptppmd	3.027e+45	11.62	11.62	1.037e+37	1.43e-06
16163	TS.triHPacyl.COelim.mtpmmtmmpd	1.226e+44	9.71	9.71	1.032e+37	1.43e-06
16164	TS.triHPacyl.COelim.mtptptmmpd	5.109e+44	10.56	10.56	1.030e+37	1.42e-06
16165	TS.triHPacyl.COelim.mmmmtmtpd	2.484e+45	11.51	11.51	1.029e+37	1.42e-06
16166	TS.triHPacyl.COelim.mptmptmmd	4.549e+45	11.87	11.87	1.028e+37	1.42e-06
16167	TS.triHPacyl.COelim.mtppmmtppd	1.386e+44	9.79	9.79	1.026e+37	1.42e-06
16168	TS.triHPacyl.COelim.ttptptmmd	1.492e+45	11.22	11.22	1.006e+37	1.39e-06
16169	TS.triHPacyl.COelim.mtptmmtmmd	2.296e+45	11.48	11.48	1.002e+37	1.38e-06
16170	TS.triHPacyl.COelim.mmpmtmmpmd	2.324e+44	10.11	10.11	9.983e+36	1.38e-06
16171	TS.triHPacyl.COelim.mmpptmpppd	2.104e+45	11.43	11.43	9.971e+36	1.38e-06
16172	TS.triHPacyl.COelim.mppmmppmd	1.911e+44	10.01	10.01	9.694e+36	1.34e-06
16173	TS.triHPacyl.COelim.tmptmtpmd	5.194e+44	10.62	10.62	9.464e+36	1.31e-06
16174	TS.triHPacyl.COelim.mmpmmtpppd	5.097e+44	10.65	10.65	8.962e+36	1.24e-06
16175	TS.triHPacyl.COelim.pmmmtppmpd	2.449e+45	11.58	11.58	8.961e+36	1.24e-06

16176	TS.triHPacyl.COelim.pmpmpmpmd	5.088e+43	9.28	9.28	8.794e+36	1.21e-06
16177	TS.triHPacyl.COelim.mtptppppmd	4.952e+44	10.64	10.64	8.730e+36	1.21e-06
16178	TS.triHPacyl.COelim.mmmmtmtmpd	3.303e+45	11.78	11.78	8.621e+36	1.19e-06
16179	TS.triHPacyl.COelim.mmttmtppmd	1.197e+45	11.18	11.18	8.538e+36	1.18e-06
16180	TS.triHPacyl.COelim.mmmmpmtppd	2.831e+44	10.33	10.33	8.490e+36	1.17e-06
16181	TS.triHPacyl.COelim.mtppmtppd	2.754e+44	10.31	10.31	8.439e+36	1.17e-06
16182	TS.triHPacyl.COelim.mpttmtmmd	6.025e+45	12.15	12.15	8.421e+36	1.16e-06
16183	TS.triHPacyl.COelim.ptpmpmmpmd	3.418e+43	9.08	9.08	8.352e+36	1.15e-06
16184	TS.triHPacyl.COelim.mtmtmtmpd	1.616e+45	11.42	11.42	7.781e+36	1.07e-06
16185	TS.triHPacyl.COelim.mttprmmppmd	2.402e+46	13.05	13.05	7.481e+36	1.03e-06
16186	TS.triHPacyl.COelim.mmpmmtmpd	6.917e+44	10.94	10.94	7.410e+36	1.02e-06
16187	TS.triHPacyl.COelim.ptpmpmpppd	9.257e+43	9.75	9.75	7.337e+36	1.01e-06
16188	TS.triHPacyl.COelim.mmmppptmpd	3.980e+44	10.64	10.64	7.059e+36	9.75e-07
16189	TS.triHPacyl.COelim.mtmmmmppmd	5.512e+45	12.22	12.22	6.903e+36	9.53e-07
16190	TS.triHPacyl.COelim.ptptmptmmd	3.075e+44	10.64	10.64	6.837e+36	9.44e-07
16191	TS.triHPacyl.COelim.mmmmpmtmpd	2.081e+44	10.30	10.30	6.560e+36	9.06e-07
16192	TS.triHPacyl.COelim.ttmpmptmmd	2.514e+44	10.42	10.42	6.483e+36	8.95e-07
16193	TS.triHPacyl.COelim.mtptmptmmd	3.346e+45	11.96	11.96	6.463e+36	8.92e-07
16194	TS.triHPacyl.COelim.mmttmmpmmd	1.687e+45	11.56	11.56	6.447e+36	8.9e-07
16195	TS.triHPacyl.COelim.tppppmmpd	6.691e+44	10.65	10.65	6.420e+36	8.86e-07
16196	TS.triHPacyl.COelim.mmpmtmmppd	4.760e+44	10.81	10.81	6.384e+36	8.82e-07
16197	TS.triHPacyl.COelim.mtmtmtmmd	2.412e+45	11.79	11.79	6.180e+36	8.53e-07
16198	TS.triHPacyl.COelim.ptpmpmmpd	2.058e+44	10.34	10.34	6.039e+36	8.34e-07
16199	TS.triHPacyl.COelim.tmpmpmmpmd	2.366e+44	10.44	10.44	5.887e+36	8.13e-07
16200	TS.triHPacyl.COelim.mmpmmpmmpmd	9.544e+43	9.90	9.90	5.830e+36	8.05e-07
16201	TS.triHPacyl.COelim.mtmtpmmpmmd	2.486e+44	10.48	10.48	5.796e+36	8e-07
16202	TS.triHPacyl.COelim.mtmtptmmd	1.208e+44	10.05	10.05	5.771e+36	7.97e-07
16203	TS.triHPacyl.COelim.mmpmtmpmmd	5.622e+44	10.97	10.97	5.700e+36	7.87e-07
16204	TS.triHPacyl.COelim.mtppmppmd	2.748e+44	10.55	10.55	5.640e+36	7.79e-07
16205	TS.triHPacyl.COelim.mmpmmtmppd	1.018e+44	9.96	9.96	5.609e+36	7.74e-07
16206	TS.triHPacyl.COelim.mtppmptppd	1.686e+44	10.27	10.27	5.559e+36	7.68e-07
16207	TS.triHPacyl.COelim.tmpmmpmmd	5.791e+44	11.03	11.03	5.365e+36	7.41e-07
16208	TS.triHPacyl.COelim.mptmptmmd	8.133e+44	11.23	11.23	5.327e+36	7.36e-07
16209	TS.triHPacyl.COelim.mtptmmpmd	3.880e+44	10.80	10.80	5.298e+36	7.32e-07
16210	TS.triHPacyl.COelim.mmmmpmtmmd	1.155e+44	10.09	10.09	5.136e+36	7.09e-07
16211	TS.triHPacyl.COelim.mmmppmtppd	8.668e+44	11.31	11.31	5.038e+36	6.96e-07
16212	TS.triHPacyl.COelim.mtppmmpmmd	1.551e+44	10.29	10.29	4.926e+36	6.8e-07
16213	TS.triHPacyl.COelim.mtmtmptppd	2.653e+44	10.61	10.61	4.922e+36	6.8e-07
16214	TS.triHPacyl.COelim.mppmtmmpd	5.231e+44	11.03	11.03	4.809e+36	6.64e-07
16215	TS.triHPacyl.COelim.ptpmpmmpd	9.766e+43	10.04	10.04	4.760e+36	6.57e-07
16216	TS.triHPacyl.COelim.mtppppppmd	6.417e+43	9.79	9.79	4.718e+36	6.51e-07
16217	TS.triHPacyl.COelim.tmpmptmmd	7.727e+44	11.29	11.29	4.590e+36	6.34e-07
16218	TS.triHPacyl.COelim.mtptmtpd	8.435e+45	12.73	12.73	4.488e+36	6.2e-07
16219	TS.triHPacyl.COelim.ttmpmtmmd	4.111e+44	10.93	10.93	4.461e+36	6.16e-07
16220	TS.triHPacyl.COelim.mmttmtmmd	1.776e+45	11.84	11.84	4.211e+36	5.81e-07
16221	TS.triHPacyl.COelim.tmpmtpppd	1.049e+45	11.54	11.54	4.121e+36	5.69e-07
16222	TS.triHPacyl.COelim.tppppmppd	4.936e+44	11.09	11.09	4.109e+36	5.67e-07
16223	TS.triHPacyl.COelim.mtppmmpmmd	1.526e+44	10.40	10.40	4.030e+36	5.56e-07
16224	TS.triHPacyl.COelim.ptttmptmpd	7.512e+44	11.36	11.36	3.988e+36	5.51e-07
16225	TS.triHPacyl.COelim.pmpptmmd	6.045e+44	11.24	11.24	3.947e+36	5.45e-07
16226	TS.triHPacyl.COelim.ptmpmptppd	1.638e+44	10.46	10.46	3.917e+36	5.41e-07
16227	TS.triHPacyl.COelim.mtttmtmmd	1.437e+45	11.76	11.76	3.864e+36	5.33e-07
16228	TS.triHPacyl.COelim.mtmmmmpppd	5.268e+45	12.57	12.57	3.641e+36	5.03e-07
16229	TS.triHPacyl.COelim.ptmpmptmmd	1.556e+44	10.49	10.49	3.537e+36	4.88e-07
16230	TS.triHPacyl.COelim.mtppmpppd	8.781e+43	10.15	10.15	3.528e+36	4.87e-07
16231	TS.triHPacyl.COelim.mtppmtmmd	1.632e+45	11.91	11.91	3.452e+36	4.77e-07
16232	TS.triHPacyl.COelim.ptmtmpppd	5.986e+44	11.32	11.32	3.418e+36	4.72e-07
16233	TS.triHPacyl.COelim.mtppppppmd	1.224e+44	10.42	10.42	3.155e+36	4.36e-07
16234	TS.triHPacyl.COelim.mmpmptpppd	2.692e+45	12.28	12.28	3.025e+36	4.18e-07
16235	TS.triHPacyl.COelim.pmpptmmd	4.302e+44	11.19	11.19	3.022e+36	4.17e-07
16236	TS.triHPacyl.COelim.tmpmptpppd	3.887e+44	11.15	11.15	2.953e+36	4.08e-07
16237	TS.triHPacyl.COelim.mtmmmmpppd	2.050e+45	12.17	12.17	2.800e+36	3.87e-07
16238	TS.triHPacyl.COelim.mtppmmtmmd	3.049e+44	11.04	11.04	2.769e+36	3.82e-07
16239	TS.triHPacyl.COelim.mtppmmpmmd	1.373e+44	10.57	10.57	2.734e+36	3.78e-07
16240	TS.triHPacyl.COelim.ptmmpmmpmd	1.246e+45	11.90	11.90	2.652e+36	3.66e-07
16241	TS.triHPacyl.COelim.mmpmptmmd	2.140e+44	10.86	10.86	2.638e+36	3.64e-07
16242	TS.triHPacyl.COelim.ttmpmtpmd	1.913e+44	10.80	10.80	2.579e+36	3.56e-07
16243	TS.triHPacyl.COelim.pttpmppmd	1.885e+45	12.17	12.17	2.564e+36	3.54e-07
16244	TS.triHPacyl.COelim.mtppmptmmd	1.887e+45	12.18	12.18	2.545e+36	3.51e-07
16245	TS.triHPacyl.COelim.mtmmmtpppd	2.962e+45	12.45	12.45	2.537e+36	3.5e-07
16246	TS.triHPacyl.COelim.pmpmptmmd	1.466e+45	12.05	12.05	2.444e+36	3.37e-07
16247	TS.triHPacyl.COelim.mtptmmpmd	7.298e+44	11.65	11.65	2.363e+36	3.26e-07

16248	TS.triHPacyl.COelim.ttpmmpmpmd	1.793e+44	10.82	10.82	2.349e+36	3.24e-07
16249	TS.triHPacyl.COelim.ptmpmmpmpmd	7.475e+43	10.30	10.30	2.348e+36	3.24e-07
16250	TS.triHPacyl.COelim.mmpmmpmpmd	1.204e+45	11.98	11.98	2.257e+36	3.12e-07
16251	TS.triHPacyl.COelim.pmppttppmd	6.365e+44	11.64	11.64	2.100e+36	2.9e-07
16252	TS.triHPacyl.COelim.pmpptppmd	1.358e+45	12.10	12.10	2.073e+36	2.86e-07
16253	TS.triHPacyl.COelim.mtpmmtmmpd	4.349e+43	10.05	10.05	2.073e+36	2.86e-07
16254	TS.triHPacyl.COelim.ptmpmmpmpd	1.326e+44	10.72	10.72	2.064e+36	2.85e-07
16255	TS.triHPacyl.COelim.mtpmmpmpmd	3.376e+44	11.31	11.31	1.942e+36	2.68e-07
16256	TS.triHPacyl.COelim.mtpmmpmmd	4.102e+44	11.43	11.43	1.933e+36	2.67e-07
16257	TS.triHPacyl.COelim.mttmtmmpmd	7.504e+44	11.80	11.80	1.897e+36	2.62e-07
16258	TS.triHPacyl.COelim.pmpptpppd	2.133e+44	11.06	11.06	1.864e+36	2.57e-07
16259	TS.triHPacyl.COelim.mtpmmpmpd	9.027e+43	10.56	10.56	1.819e+36	2.51e-07
16260	TS.triHPacyl.COelim.ptptmmpmpd	1.826e+44	10.99	10.99	1.795e+36	2.48e-07
16261	TS.triHPacyl.COelim.tmpmmpmpd	4.191e+44	11.49	11.49	1.792e+36	2.47e-07
16262	TS.triHPacyl.COelim.mtpmtpmpd	4.776e+45	12.95	12.95	1.761e+36	2.43e-07
16263	TS.triHPacyl.COelim.ttpmmtmpmd	3.773e+44	11.45	11.45	1.730e+36	2.39e-07
16264	TS.triHPacyl.COelim.mtmtmtpmd	3.762e+45	12.83	12.83	1.701e+36	2.35e-07
16265	TS.triHPacyl.COelim.mmpmtpmpd	2.048e+44	11.09	11.09	1.694e+36	2.34e-07
16266	TS.triHPacyl.COelim.mttmtpmpd	1.018e+46	13.42	13.42	1.691e+36	2.34e-07
16267	TS.triHPacyl.COelim.mppmtmmpd	8.719e+44	11.99	11.99	1.610e+36	2.22e-07
16268	TS.triHPacyl.COelim.mttptmmpd	1.676e+45	12.40	12.40	1.557e+36	2.15e-07
16269	TS.triHPacyl.COelim.mmpmmpmpd	1.347e+44	10.90	10.90	1.555e+36	2.15e-07
16270	TS.triHPacyl.COelim.tttptmmpd	3.688e+45	12.89	12.89	1.507e+36	2.08e-07
16271	TS.triHPacyl.COelim.mtmppmmpd	2.210e+44	11.21	11.21	1.503e+36	2.08e-07
16272	TS.triHPacyl.COelim.mtmmtppmd	3.031e+45	12.78	12.78	1.476e+36	2.04e-07
16273	TS.triHPacyl.COelim.ptppmtpmd	3.070e+44	11.43	11.43	1.439e+36	1.99e-07
16274	TS.triHPacyl.COelim.pmpmmpmpd	1.561e+45	12.41	12.41	1.420e+36	1.96e-07
16275	TS.triHPacyl.COelim.mpmmtmmpd	1.653e+45	12.47	12.47	1.352e+36	1.87e-07
16276	TS.triHPacyl.COelim.mtmppptppd	1.751e+44	11.14	11.14	1.350e+36	1.86e-07
16277	TS.triHPacyl.COelim.mmpmmtmpmd	7.021e+43	10.59	10.59	1.345e+36	1.86e-07
16278	TS.triHPacyl.COelim.mtmppppppd	1.586e+44	11.09	11.09	1.330e+36	1.84e-07
16279	TS.triHPacyl.COelim.mtpmtpmmpd	6.001e+43	10.54	10.54	1.260e+36	1.74e-07
16280	TS.triHPacyl.COelim.tttpttppd	2.664e+45	12.81	12.81	1.247e+36	1.72e-07
16281	TS.triHPacyl.COelim.mptmmpmpd	5.654e+44	11.88	11.88	1.244e+36	1.72e-07
16282	TS.triHPacyl.COelim.tpmptpppd	1.349e+44	11.04	11.04	1.232e+36	1.7e-07
16283	TS.triHPacyl.COelim.mtpmtpmmpd	4.953e+44	11.83	11.83	1.186e+36	1.64e-07
16284	TS.triHPacyl.COelim.mtmppmmpd	9.498e+43	10.85	10.85	1.183e+36	1.63e-07
16285	TS.triHPacyl.COelim.mtmptmmpd	1.516e+45	12.53	12.53	1.121e+36	1.55e-07
16286	TS.triHPacyl.COelim.mtpmmppppd	7.000e+44	12.08	12.08	1.106e+36	1.53e-07
16287	TS.triHPacyl.COelim.mmpmtpppd	2.433e+44	11.47	11.47	1.067e+36	1.47e-07
16288	TS.triHPacyl.COelim.mtmppmmpd	1.472e+44	11.17	11.17	1.066e+36	1.47e-07
16289	TS.triHPacyl.COelim.mtmmtmmpd	8.604e+45	13.60	13.60	1.058e+36	1.46e-07
16290	TS.triHPacyl.COelim.mttmtpmpd	7.527e+45	13.53	13.53	1.050e+36	1.45e-07
16291	TS.triHPacyl.COelim.pttpmmpmpd	7.414e+44	12.15	12.15	1.041e+36	1.44e-07
16292	TS.triHPacyl.COelim.mmtmmtmmpd	8.255e+44	12.25	12.25	9.880e+35	1.36e-07
16293	TS.triHPacyl.COelim.mttmtmmpd	1.394e+45	12.56	12.56	9.865e+35	1.36e-07
16294	TS.triHPacyl.COelim.mmpmmppppd	3.808e+44	11.79	11.79	9.808e+35	1.35e-07
16295	TS.triHPacyl.COelim.pmpmmpmmpd	7.081e+43	10.80	10.80	9.642e+35	1.33e-07
16296	TS.triHPacyl.COelim.mtpmmpmmpd	1.096e+45	12.44	12.44	9.421e+35	1.3e-07
16297	TS.triHPacyl.COelim.ptptmtpppd	7.138e+43	10.83	10.83	9.166e+35	1.27e-07
16298	TS.triHPacyl.COelim.mtmppmmpd	2.736e+44	11.69	11.69	8.346e+35	1.15e-07
16299	TS.triHPacyl.COelim.pmpptppmd	1.029e+45	12.50	12.50	8.030e+35	1.11e-07
16300	TS.triHPacyl.COelim.ptmmpmpmpd	5.130e+43	10.73	10.73	7.846e+35	1.08e-07
16301	TS.triHPacyl.COelim.mttmmpmpd	1.412e+46	14.09	14.09	7.650e+35	1.06e-07
16302	TS.triHPacyl.COelim.mttmmtmpd	1.056e+46	13.95	13.95	7.261e+35	1e-07
16303	TS.triHPacyl.COelim.mtpmmpmmpd	1.975e+44	11.65	11.65	6.459e+35	8.92e-08
16304	TS.triHPacyl.COelim.mmpmtpppd	4.536e+44	12.18	12.18	6.082e+35	8.4e-08
16305	TS.triHPacyl.COelim.mtmppmmpd	8.406e+43	11.25	11.25	5.394e+35	7.45e-08
16306	TS.triHPacyl.COelim.mtmmtpppd	8.130e+45	13.97	13.97	5.376e+35	7.42e-08
16307	TS.triHPacyl.COelim.mtpmmtmpd	3.623e+44	12.17	12.17	4.902e+35	6.77e-08
16308	TS.triHPacyl.COelim.mtpmtmmpd	4.574e+44	12.34	12.34	4.675e+35	6.45e-08
16309	TS.triHPacyl.COelim.pmpmtpmmpd	5.419e+43	11.07	11.07	4.670e+35	6.45e-08
16310	TS.triHPacyl.COelim.ptmptppmd	2.179e+44	11.91	11.91	4.614e+35	6.37e-08
16311	TS.triHPacyl.COelim.mtpmtpppd	4.801e+43	11.06	11.06	4.185e+35	5.78e-08
16312	TS.triHPacyl.COelim.mpmmtmmpd	2.628e+45	13.50	13.50	3.833e+35	5.29e-08
16313	TS.triHPacyl.COelim.mtmppmmpd	8.221e+43	11.47	11.47	3.622e+35	5e-08
16314	TS.triHPacyl.COelim.mtmppptmpd	1.571e+44	11.77	11.77	3.393e+35	4.68e-08
16315	TS.triHPacyl.COelim.mtmppmmpd	5.921e+43	11.33	11.33	3.275e+35	4.52e-08
16316	TS.triHPacyl.COelim.mtmmtmmpd	6.019e+45	14.09	14.09	3.258e+35	4.5e-08
16317	TS.triHPacyl.COelim.mttptmmpd	1.913e+45	13.41	13.41	3.241e+35	4.48e-08
16318	TS.triHPacyl.COelim.mtpmmpmmpd	1.000e+45	13.19	13.19	2.479e+35	3.42e-08
16319	TS.triHPacyl.COelim.mmpmmtmmpd	1.075e+44	11.88	11.88	2.395e+35	3.31e-08

16320	TS.triHPacyl.COelim.ptttmppppd	1.044e+45	13.27	13.27	2.253e+35	3.11e-08
16321	TS.triHPacyl.COelim.mtttmtttmpd	7.430e+45	14.45	14.45	2.193e+35	3.03e-08
16322	TS.triHPacyl.COelim.ptmpppmmd	1.221e+44	12.01	12.01	2.160e+35	2.98e-08
16323	TS.triHPacyl.COelim.mtprmmtpmd	2.897e+44	12.56	12.56	2.045e+35	2.82e-08
16324	TS.triHPacyl.COelim.ptmmpmmmd	7.381e+43	11.82	11.82	1.818e+35	2.51e-08
16325	TS.triHPacyl.COelim.ptmtptmmd	3.039e+44	12.70	12.70	1.694e+35	2.34e-08
16326	TS.triHPacyl.COelim.mtmpppmmd	9.873e+43	12.06	12.06	1.628e+35	2.25e-08
16327	TS.triHPacyl.COelim.mtmttppmd	5.084e+45	14.46	14.46	1.491e+35	2.06e-08
16328	TS.triHPacyl.COelim.mtttmtpppd	5.652e+45	14.53	14.53	1.478e+35	2.04e-08
16329	TS.triHPacyl.COelim.mmpmtmmd	1.387e+46	15.29	15.29	1.004e+35	1.39e-08
16330	TS.triHPacyl.COelim.ptttmppmd	1.134e+45	13.82	13.82	9.637e+34	1.33e-08
16331	TS.triHPacyl.COelim.mtptmppmd	2.116e+45	14.24	14.24	8.932e+34	1.23e-08
16332	TS.triHPacyl.COelim.mtppmpppd	2.221e+45	14.35	14.35	7.880e+34	1.09e-08
16333	TS.triHPacyl.COelim.mtptmppmd	2.494e+45	14.44	14.44	7.524e+34	1.04e-08
16334	TS.triHPacyl.COelim.ptmptttmpd	3.651e+44	13.38	13.38	6.553e+34	9.05e-09
16335	TS.triHPacyl.COelim.mtprmmtpmd	2.879e+44	13.25	13.25	6.364e+34	8.79e-09
16336	TS.triHPacyl.COelim.pmpmmtmpd	7.850e+43	12.75	12.75	4.013e+34	5.54e-09
16337	TS.triHPacyl.COelim.mtprmmtpmd	1.303e+44	13.17	13.17	3.321e+34	4.59e-09
16338	TS.triHPacyl.COelim.mtmtmtpmd	2.728e+44	13.71	13.71	2.784e+34	3.84e-09
16339	TS.triHPacyl.COelim.pmpmmtppd	1.374e+44	13.48	13.48	2.089e+34	2.88e-09
16340	TS.triHPacyl.COelim.pmpmttmpd	7.964e+43	13.21	13.21	1.891e+34	2.61e-09
16341	TS.triHPacyl.COelim.mmpmpttmpd	2.529e+45	15.40	15.40	1.540e+34	2.13e-09
16342	TS.triHPacyl.COelim.mppmmtmpd	1.777e+45	15.25	15.25	1.383e+34	1.91e-09
16343	TS.triHPacyl.COelim.pmpmmtppd	7.096e+43	13.47	13.47	1.099e+34	1.52e-09
16344	TS.triHPacyl.COelim.pmpmtpppd	1.127e+44	13.93	13.93	8.078e+33	1.12e-09
16345	TS.triHPacyl.COelim.pmpmmtmmd	1.028e+44	16.08	16.08	1.970e+32	2.72e-11
16346	Total				7.243e+44	100

(2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)

Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
16359	triHPacyl.tmmmtttmpu	9.711e+42	0.00	0.00	9.711e+42	19.6
16360	triHPacyl.pmmmtttmpu	1.037e+43	0.24	0.24	6.980e+42	14.1
16361	triHPacyl.tmmmtttmpu	1.256e+43	0.36	0.36	6.863e+42	13.9
16362	triHPacyl.pmmmtttmpu	1.102e+43	1.04	1.04	1.935e+42	3.9
16363	triHPacyl.ptppmtmpmu	7.779e+42	1.19	1.19	1.049e+42	2.12
16364	triHPacyl.pmpmtmpmu	5.298e+42	0.99	0.99	1.010e+42	2.04
16365	triHPacyl.tmtmmpmpmu	3.922e+43	2.35	2.35	7.561e+41	1.53
16366	triHPacyl.pmpmtmpmu	8.674e+42	1.47	1.47	7.341e+41	1.48
16367	triHPacyl.pmmmtttmpu	6.916e+42	1.36	1.36	7.010e+41	1.41
16368	triHPacyl.mmmmtttmpu	1.533e+43	1.85	1.85	6.859e+41	1.38
16369	triHPacyl.pmtppppmu	2.193e+43	2.26	2.26	4.949e+41	0.999
16370	triHPacyl.pmmmtttmpu	1.018e+43	1.84	1.84	4.655e+41	0.94
16371	triHPacyl.ppppmtmpmu	7.625e+43	3.08	3.08	4.365e+41	0.881
16372	triHPacyl.tmmmtttmpu	1.407e+43	2.08	2.08	4.293e+41	0.867
16373	triHPacyl.pmpmtttmpu	9.753e+42	1.89	1.89	4.069e+41	0.821
16374	triHPacyl.pmtppppmu	4.673e+43	2.85	2.85	3.927e+41	0.793
16375	triHPacyl.pttptppmu	2.148e+43	2.42	2.42	3.723e+41	0.751
16376	triHPacyl.tmtptppmu	5.604e+43	3.01	3.01	3.582e+41	0.723
16377	triHPacyl.pmpmmpmpu	6.013e+42	1.69	1.69	3.535e+41	0.713
16378	triHPacyl.pmpmtttmpu	2.920e+43	2.76	2.76	2.870e+41	0.579
16379	triHPacyl.ppppmpmpu	5.521e+43	3.14	3.14	2.833e+41	0.572
16380	triHPacyl.ptppmmpmu	2.802e+43	2.75	2.75	2.772e+41	0.56
16381	triHPacyl.ptmmpmpmu	3.664e+43	2.92	2.92	2.754e+41	0.556
16382	triHPacyl.pmmmtttmpu	8.163e+42	2.05	2.05	2.609e+41	0.527
16383	triHPacyl.tppmmpmpu	8.602e+43	3.55	3.55	2.238e+41	0.452
16384	triHPacyl.tpppmpmpu	1.465e+44	3.93	3.93	2.010e+41	0.406
16385	triHPacyl.tpmmtttmpu	1.954e+43	2.74	2.74	1.978e+41	0.399
16386	triHPacyl.pmtppppmu	2.869e+43	2.97	2.97	1.978e+41	0.399
16387	triHPacyl.ptppmtmpmu	2.014e+43	2.82	2.82	1.792e+41	0.362
16388	triHPacyl.tmtmmpmpu	7.386e+43	3.59	3.59	1.777e+41	0.359
16389	triHPacyl.pmtppppmu	6.158e+44	4.88	4.88	1.715e+41	0.346
16390	triHPacyl.ptmmpmmpu	2.976e+43	3.08	3.08	1.703e+41	0.344
16391	triHPacyl.pmmmpmpmpu	1.182e+43	2.53	2.53	1.685e+41	0.34

16392	triHPacyl.tpmmmtmpu	1.261e+43	2.58	2.58	1.664e+41	0.336
16393	triHPacyl.pttpptmpu	4.171e+43	3.29	3.29	1.661e+41	0.335
16394	triHPacyl.ptppptmpu	1.260e+43	2.64	2.64	1.511e+41	0.305
16395	triHPacyl.tpmmmtmpu	1.280e+43	2.66	2.66	1.478e+41	0.298
16396	triHPacyl.tpmmmtmpu	8.774e+42	2.45	2.45	1.449e+41	0.293
16397	triHPacyl.tmpmmmpu	2.016e+43	2.95	2.95	1.427e+41	0.288
16398	triHPacyl.ppmmpmpu	9.057e+42	2.49	2.49	1.381e+41	0.279
16399	triHPacyl.ptmmmtmpu	2.919e+43	3.19	3.19	1.373e+41	0.277
16400	triHPacyl.tmmmtmpu	4.675e+43	3.48	3.48	1.373e+41	0.277
16401	triHPacyl.ttpmmmpu	2.284e+43	3.05	3.05	1.370e+41	0.276
16402	triHPacyl.pmmptppu	8.784e+42	2.49	2.49	1.354e+41	0.273
16403	triHPacyl.ppmmpmpu	4.412e+42	2.10	2.10	1.308e+41	0.264
16404	triHPacyl.pttpmmmpu	3.370e+43	3.35	3.35	1.226e+41	0.247
16405	triHPacyl.ptppmmmpu	1.928e+43	3.02	3.02	1.220e+41	0.246
16406	triHPacyl.ptmmmtmpu	1.157e+43	2.72	2.72	1.217e+41	0.246
16407	triHPacyl.tmmmtmpu	1.501e+43	2.87	2.87	1.215e+41	0.245
16408	triHPacyl.tmmmtppu	1.222e+43	2.81	2.81	1.091e+41	0.22
16409	triHPacyl.pptmpmpu	1.663e+43	3.00	3.00	1.083e+41	0.219
16410	triHPacyl.tmmmtmpu	3.001e+43	3.36	3.36	1.063e+41	0.215
16411	triHPacyl.mmmmtmpu	3.599e+43	3.49	3.49	1.040e+41	0.21
16412	triHPacyl.pttpmtmpu	3.131e+43	3.42	3.42	1.013e+41	0.204
16413	triHPacyl.tmtmmmtmpu	4.511e+43	3.64	3.64	1.012e+41	0.204
16414	triHPacyl.tppmtmpu	1.001e+44	4.11	4.11	1.009e+41	0.204
16415	triHPacyl.tmmmtmpu	2.131e+43	3.19	3.19	1.008e+41	0.204
16416	triHPacyl.pmtppppu	3.811e+43	3.55	3.55	9.964e+40	0.201
16417	triHPacyl.tmmmtmpu	3.525e+43	3.50	3.50	9.892e+40	0.2
16418	triHPacyl.tmtmpmpu	1.134e+44	4.21	4.21	9.678e+40	0.195
16419	triHPacyl.tmtmpppu	3.915e+43	3.58	3.58	9.656e+40	0.195
16420	triHPacyl.tmmmtmpu	3.983e+43	3.60	3.60	9.460e+40	0.191
16421	triHPacyl.tmmmtmpu	2.267e+43	3.27	3.27	9.404e+40	0.19
16422	triHPacyl.mpmptmpu	2.810e+43	3.40	3.40	9.404e+40	0.19
16423	triHPacyl.pttpmtmpu	1.366e+44	4.36	4.36	9.153e+40	0.185
16424	triHPacyl.tmpmtppu	2.100e+43	3.24	3.24	9.109e+40	0.184
16425	triHPacyl.mppptmpu	5.195e+43	3.82	3.82	8.564e+40	0.173
16426	triHPacyl.tmpmmmpu	5.029e+43	3.80	3.80	8.544e+40	0.172
16427	triHPacyl.pptmpmpu	2.557e+43	3.40	3.40	8.497e+40	0.171
16428	triHPacyl.tmmmtmpu	6.756e+43	4.00	4.00	8.288e+40	0.167
16429	triHPacyl.tmtpptpu	4.849e+43	3.82	3.82	8.051e+40	0.162
16430	triHPacyl.ptmptmpu	1.435e+43	3.09	3.09	8.039e+40	0.162
16431	triHPacyl.pptmtpu	1.811e+43	3.24	3.24	7.891e+40	0.159
16432	triHPacyl.pmmptppu	4.999e+43	3.85	3.85	7.867e+40	0.159
16433	triHPacyl.pppmtppu	8.808e+42	2.81	2.81	7.849e+40	0.158
16434	triHPacyl.ptppmpu	1.428e+43	3.11	3.11	7.700e+40	0.155
16435	triHPacyl.tmtmpppu	1.007e+44	4.29	4.29	7.567e+40	0.153
16436	triHPacyl.ptmmmtmpu	3.051e+43	3.58	3.58	7.560e+40	0.153
16437	triHPacyl.pttpmtppu	2.838e+43	3.56	3.56	7.263e+40	0.147
16438	triHPacyl.tmtmtmpu	8.635e+43	4.24	4.24	7.016e+40	0.142
16439	triHPacyl.mppppmpu	5.782e+43	4.02	4.02	6.837e+40	0.138
16440	triHPacyl.tptmtmpu	5.337e+43	3.97	3.97	6.823e+40	0.138
16441	triHPacyl.pptmpmpu	2.259e+43	3.47	3.47	6.747e+40	0.136
16442	triHPacyl.pppptmpu	5.639e+43	4.01	4.01	6.743e+40	0.136
16443	triHPacyl.tptmmmtmpu	3.241e+43	3.68	3.68	6.705e+40	0.135
16444	triHPacyl.tppmtppu	2.746e+44	4.96	4.96	6.645e+40	0.134
16445	triHPacyl.tttmmmpu	3.555e+43	3.76	3.76	6.469e+40	0.131
16446	triHPacyl.ttmmmtmpu	3.308e+43	3.72	3.72	6.453e+40	0.13
16447	triHPacyl.pppmpmpu	2.239e+43	3.49	3.49	6.384e+40	0.129
16448	triHPacyl.pppmtmpu	1.707e+43	3.34	3.34	6.339e+40	0.128
16449	triHPacyl.tmpmtmpu	2.643e+43	3.61	3.61	6.223e+40	0.126
16450	triHPacyl.tmmmttpu	3.086e+43	3.71	3.71	6.110e+40	0.123
16451	triHPacyl.ptppmmmpu	1.165e+43	3.13	3.13	6.068e+40	0.122
16452	triHPacyl.ppmmtppu	7.075e+42	2.84	2.84	5.994e+40	0.121
16453	triHPacyl.tmpmtmpu	8.446e+43	4.34	4.34	5.799e+40	0.117
16454	triHPacyl.pptppptmpu	4.736e+43	4.00	4.00	5.785e+40	0.117
16455	triHPacyl.pmpptppu	2.642e+43	3.65	3.65	5.767e+40	0.116
16456	triHPacyl.tmmmtmpu	2.827e+43	3.70	3.70	5.672e+40	0.114
16457	triHPacyl.ptmmmtmpu	3.947e+43	3.91	3.91	5.610e+40	0.113
16458	triHPacyl.ttmmtmpu	2.332e+43	3.60	3.60	5.525e+40	0.112
16459	triHPacyl.pttmtmpu	1.256e+44	4.61	4.61	5.474e+40	0.11
16460	triHPacyl.tmtmmmtmpu	1.027e+44	4.51	4.51	5.346e+40	0.108
16461	triHPacyl.tmtmtpu	5.621e+43	4.15	4.15	5.295e+40	0.107
16462	triHPacyl.pmmptmpu	2.151e+43	3.60	3.60	5.091e+40	0.103
16463	triHPacyl.tmmmtppu	3.959e+43	3.97	3.97	5.045e+40	0.102

16464	triHPacyl.tmppmtmmu	4.237e+43	4.02	4.02	5.000e+40	0.101
16465	triHPacyl.pttpmpmpu	9.092e+43	4.49	4.49	4.887e+40	0.0986
16466	triHPacyl.pttpmtppmu	1.946e+43	3.58	3.58	4.836e+40	0.0976
16467	triHPacyl.tppmpmpu	1.865e+43	3.55	3.55	4.834e+40	0.0976
16468	triHPacyl.tmtptmpu	1.864e+44	4.93	4.93	4.792e+40	0.0967
16469	triHPacyl.pmtppppu	5.925e+43	4.26	4.26	4.637e+40	0.0936
16470	triHPacyl.pmtmpppu	3.551e+43	3.97	3.97	4.586e+40	0.0926
16471	triHPacyl.ptmpptmmu	4.235e+43	4.07	4.07	4.583e+40	0.0925
16472	triHPacyl.pttmtmpu	1.035e+44	4.61	4.61	4.503e+40	0.0909
16473	triHPacyl.tmtmtmmu	2.516e+44	5.15	5.15	4.422e+40	0.0893
16474	triHPacyl.ptppptmpu	2.796e+43	3.85	3.85	4.373e+40	0.0883
16475	triHPacyl.tpmmtmpu	1.798e+43	3.59	3.59	4.330e+40	0.0874
16476	triHPacyl.ptmpmpmpu	1.687e+43	3.56	3.56	4.305e+40	0.0869
16477	triHPacyl.tmpmmmmu	2.970e+43	3.90	3.90	4.261e+40	0.086
16478	triHPacyl.tttptmpu	4.706e+43	4.19	4.19	4.199e+40	0.0848
16479	triHPacyl.pppppmpu	3.374e+43	3.99	3.99	4.152e+40	0.0838
16480	triHPacyl.pmtmmppmu	1.160e+44	4.74	4.74	4.117e+40	0.0831
16481	triHPacyl.ppmmtmpu	9.256e+42	3.24	3.24	4.044e+40	0.0816
16482	triHPacyl.ptppmpmmu	2.386e+43	3.81	3.81	4.009e+40	0.0809
16483	triHPacyl.mmtmpmpu	7.431e+43	4.49	4.49	3.987e+40	0.0805
16484	triHPacyl.ppppmtmpu	4.797e+43	4.23	4.23	3.959e+40	0.0799
16485	triHPacyl.pttpptppmu	4.120e+43	4.15	4.15	3.915e+40	0.079
16486	triHPacyl.tptmpmpmu	2.806e+43	3.92	3.92	3.911e+40	0.0789
16487	triHPacyl.ttmmmtmpu	4.542e+43	4.22	4.22	3.830e+40	0.0773
16488	triHPacyl.ptppmtppmu	1.582e+43	3.60	3.60	3.783e+40	0.0763
16489	triHPacyl.ppppmtppmu	5.963e+43	4.40	4.40	3.738e+40	0.0754
16490	triHPacyl.pttpmpmpu	4.923e+43	4.28	4.28	3.735e+40	0.0754
16491	triHPacyl.pmtmpmtmu	6.563e+43	4.45	4.45	3.732e+40	0.0753
16492	triHPacyl.pmtmpmtmpu	4.753e+43	4.27	4.27	3.666e+40	0.074
16493	triHPacyl.pmpmpmpmu	6.931e+42	3.14	3.14	3.571e+40	0.0721
16494	triHPacyl.ptppppmpu	3.166e+43	4.05	4.05	3.557e+40	0.0718
16495	triHPacyl.pmmmpmpu	2.575e+43	3.94	3.94	3.463e+40	0.0699
16496	triHPacyl.pmmmpmtmu	2.864e+43	4.03	4.03	3.342e+40	0.0675
16497	triHPacyl.pptpmtmpu	6.051e+43	4.47	4.47	3.329e+40	0.0672
16498	triHPacyl.pppppptppu	1.603e+44	5.06	5.06	3.315e+40	0.0669
16499	triHPacyl.pmmmpmpmu	2.230e+43	3.88	3.88	3.312e+40	0.0668
16500	triHPacyl.pttmtmpmu	9.061e+43	4.72	4.72	3.303e+40	0.0667
16501	triHPacyl.ppmmpmpmu	5.392e+42	3.04	3.04	3.279e+40	0.0662
16502	triHPacyl.tptmpmpmu	3.665e+43	4.19	4.19	3.247e+40	0.0655
16503	triHPacyl.tmmmtppmu	3.208e+43	4.11	4.11	3.235e+40	0.0653
16504	triHPacyl.ptmmmtppmu	2.504e+43	3.97	3.97	3.231e+40	0.0652
16505	triHPacyl.ttpmtmpmu	7.198e+43	4.60	4.60	3.228e+40	0.0651
16506	triHPacyl.tpppmtppmu	1.568e+43	3.69	3.69	3.223e+40	0.0651
16507	triHPacyl.pppppptmpu	1.707e+44	5.11	5.11	3.208e+40	0.0648
16508	triHPacyl.ptppmmmmu	2.646e+43	4.00	4.00	3.202e+40	0.0646
16509	triHPacyl.mmpmpmpu	3.288e+43	4.14	4.14	3.178e+40	0.0641
16510	triHPacyl.tmtmpppmu	7.391e+43	4.63	4.63	3.146e+40	0.0635
16511	triHPacyl.pptmptpmu	7.317e+43	4.63	4.63	3.081e+40	0.0622
16512	triHPacyl.ptmpmtmpu	3.824e+43	4.25	4.25	3.065e+40	0.0619
16513	triHPacyl.pttmtmpmu	8.539e+43	4.74	4.74	2.995e+40	0.0605
16514	triHPacyl.ppppmtmpmu	1.012e+43	3.49	3.49	2.895e+40	0.0584
16515	triHPacyl.ttpmmmpmu	1.548e+43	3.75	3.75	2.887e+40	0.0583
16516	triHPacyl.pmmmpmtmu	3.402e+43	4.23	4.23	2.815e+40	0.0568
16517	triHPacyl.pttpmtppu	8.630e+43	4.79	4.79	2.794e+40	0.0564
16518	triHPacyl.tptpmtppu	6.011e+44	5.95	5.95	2.790e+40	0.0563
16519	triHPacyl.tptmtppu	1.838e+44	5.26	5.26	2.724e+40	0.055
16520	triHPacyl.mmpmpmpmu	2.063e+43	3.96	3.96	2.702e+40	0.0545
16521	triHPacyl.ppmmmmpmu	6.830e+42	3.30	3.30	2.700e+40	0.0545
16522	triHPacyl.pmpmpmtppu	2.987e+43	4.18	4.18	2.682e+40	0.0541
16523	triHPacyl.ptmpmpmpu	6.487e+43	4.66	4.66	2.631e+40	0.0531
16524	triHPacyl.ptmmpmpmu	1.295e+43	3.70	3.70	2.597e+40	0.0524
16525	triHPacyl.ptmmpmtmpu	6.328e+43	4.65	4.65	2.583e+40	0.0521
16526	triHPacyl.ppmmttmmu	2.166e+43	4.03	4.03	2.527e+40	0.051
16527	triHPacyl.tpmmpmpmu	1.389e+43	3.77	3.77	2.505e+40	0.0506
16528	triHPacyl.pmtmpmtmpu	5.399e+43	4.59	4.59	2.467e+40	0.0498
16529	triHPacyl.ptmmpmtppu	1.382e+44	5.15	5.15	2.467e+40	0.0498
16530	triHPacyl.pmpmpmtmmu	4.021e+43	4.41	4.41	2.456e+40	0.0496
16531	triHPacyl.tpppmtppu	5.254e+44	5.95	5.95	2.441e+40	0.0493
16532	triHPacyl.tmtmpmpmu	6.742e+43	4.73	4.73	2.430e+40	0.049
16533	triHPacyl.pttpptppmu	2.282e+43	4.09	4.09	2.381e+40	0.048
16534	triHPacyl.tmmmpmpmu	5.899e+43	4.66	4.66	2.375e+40	0.0479
16535	triHPacyl.pptpptppmu	2.654e+43	4.20	4.20	2.327e+40	0.047

16536	triHPacyl.pmmmpmmpu	2.491e+43	4.16	4.16	2.317e+40	0.0468
16537	triHPacyl.ppppptompu	2.481e+44	5.54	5.54	2.292e+40	0.0463
16538	triHPacyl.ttpmmtmmu	5.314e+43	4.63	4.63	2.252e+40	0.0455
16539	triHPacyl.ttpmmpmpu	2.194e+43	4.11	4.11	2.239e+40	0.0452
16540	triHPacyl.ppmmtmmpu	1.652e+43	3.94	3.94	2.227e+40	0.0449
16541	triHPacyl.tmmmpmtmpu	2.353e+43	4.18	4.18	2.136e+40	0.0431
16542	triHPacyl.pmmmpmpmpu	1.470e+43	3.91	3.91	2.070e+40	0.0418
16543	triHPacyl.tpmmmmmmpu	1.305e+43	3.85	3.85	2.030e+40	0.041
16544	triHPacyl.pmpmpmmmpu	2.093e+43	4.14	4.14	2.021e+40	0.0408
16545	triHPacyl.pmpmpmpmpu	7.046e+42	3.49	3.49	2.015e+40	0.0407
16546	triHPacyl.tpmmpmtmmu	3.679e+43	4.49	4.49	1.968e+40	0.0397
16547	triHPacyl.tmtppptompu	5.594e+44	6.11	6.11	1.967e+40	0.0397
16548	triHPacyl.ppmmtmmpu	9.217e+42	3.67	3.67	1.964e+40	0.0396
16549	triHPacyl.pmpmpmpmpu	9.290e+43	5.05	5.05	1.955e+40	0.0395
16550	triHPacyl.pttmmtmmu	7.991e+43	4.96	4.96	1.932e+40	0.039
16551	triHPacyl.pmpmpmpmpu	2.279e+43	4.22	4.22	1.915e+40	0.0386
16552	triHPacyl.mpmmpptompu	1.179e+43	3.83	3.83	1.914e+40	0.0386
16553	triHPacyl.pttmppmpu	1.981e+43	4.14	4.14	1.907e+40	0.0385
16554	triHPacyl.pmtmpmtmmu	9.033e+43	5.05	5.05	1.906e+40	0.0385
16555	triHPacyl.pptppptompu	1.520e+44	5.36	5.36	1.899e+40	0.0383
16556	triHPacyl.tmmtpmpmpu	1.216e+43	3.86	3.86	1.880e+40	0.0379
16557	triHPacyl.tptmmpmpmpu	1.821e+44	5.47	5.47	1.878e+40	0.0379
16558	triHPacyl.tptmmtpppu	6.289e+43	4.85	4.85	1.842e+40	0.0372
16559	triHPacyl.pttpmmpmpu	2.403e+43	4.29	4.29	1.799e+40	0.0363
16560	triHPacyl.ptmmpptompu	1.920e+44	5.53	5.53	1.789e+40	0.0361
16561	triHPacyl.ptmmmtmpmpu	3.478e+43	4.52	4.52	1.782e+40	0.036
16562	triHPacyl.ptmmpptompu	4.183e+43	4.63	4.63	1.767e+40	0.0357
16563	triHPacyl.tpmmpmtmpu	1.537e+43	4.04	4.04	1.766e+40	0.0357
16564	triHPacyl.tmtppptompu	7.553e+43	4.99	4.99	1.745e+40	0.0352
16565	triHPacyl.mmpppptompu	2.285e+44	5.65	5.65	1.735e+40	0.035
16566	triHPacyl.tpmmpptompu	7.802e+43	5.03	5.03	1.681e+40	0.0339
16567	triHPacyl.mpmmpmpmpu	1.122e+43	3.88	3.88	1.680e+40	0.0339
16568	triHPacyl.pppptommpu	7.860e+43	5.04	5.04	1.666e+40	0.0336
16569	triHPacyl.tptmmmtmmu	7.856e+43	5.04	5.04	1.663e+40	0.0336
16570	triHPacyl.pttmptpppu	3.351e+43	4.54	4.54	1.656e+40	0.0334
16571	triHPacyl.tptmmtmpu	9.342e+43	5.15	5.15	1.654e+40	0.0334
16572	triHPacyl.tmpmmtmmu	8.030e+43	5.06	5.06	1.642e+40	0.0331
16573	triHPacyl.pmpppptommpu	2.639e+43	4.41	4.41	1.629e+40	0.0329
16574	triHPacyl.mmpmptompu	9.514e+43	5.18	5.18	1.607e+40	0.0324
16575	triHPacyl.ptpmmtmpu	1.342e+43	4.02	4.02	1.593e+40	0.0322
16576	triHPacyl.pptpmtmpmpu	1.887e+43	4.23	4.23	1.574e+40	0.0318
16577	triHPacyl.ttpmpmpmpu	5.985e+43	4.92	4.92	1.571e+40	0.0317
16578	triHPacyl.pttmmtpppu	2.725e+43	4.45	4.45	1.568e+40	0.0317
16579	triHPacyl.ppmmttpppu	3.039e+43	4.52	4.52	1.549e+40	0.0313
16580	triHPacyl.tptmpmpmpu	2.812e+43	4.48	4.48	1.544e+40	0.0312
16581	triHPacyl.tmtmmmpmpu	5.224e+43	4.85	4.85	1.541e+40	0.0311
16582	triHPacyl.ptmmmtmpu	3.111e+43	4.56	4.56	1.487e+40	0.03
16583	triHPacyl.pttmmtmpu	3.474e+43	4.63	4.63	1.476e+40	0.0298
16584	triHPacyl.tpmmtpppu	2.761e+43	4.49	4.49	1.469e+40	0.0297
16585	triHPacyl.pttpmmpmpu	3.268e+43	4.59	4.59	1.469e+40	0.0296
16586	triHPacyl.tmtppptompu	1.994e+43	4.30	4.30	1.467e+40	0.0296
16587	triHPacyl.tppmmtppu	2.594e+44	5.83	5.83	1.462e+40	0.0295
16588	triHPacyl.pptpmtpppu	3.240e+43	4.59	4.59	1.461e+40	0.0295
16589	triHPacyl.tmtpmtmpmpu	8.041e+43	5.14	5.14	1.460e+40	0.0295
16590	triHPacyl.pptppppmpu	1.861e+43	4.27	4.27	1.447e+40	0.0292
16591	triHPacyl.pmtmptommpu	1.291e+44	5.43	5.43	1.435e+40	0.029
16592	triHPacyl.pmmmpmtppu	3.215e+43	4.60	4.60	1.433e+40	0.0289
16593	triHPacyl.pmtppptompu	1.502e+44	5.52	5.52	1.420e+40	0.0287
16594	triHPacyl.pptppptommpu	2.085e+43	4.35	4.35	1.418e+40	0.0286
16595	triHPacyl.pttmmtmpmpu	4.886e+43	4.87	4.87	1.381e+40	0.0279
16596	triHPacyl.mmtppmpmpu	8.566e+43	5.22	5.22	1.359e+40	0.0274
16597	triHPacyl.tttmmmpmpu	6.300e+43	5.04	5.04	1.341e+40	0.0271
16598	triHPacyl.pppppmpmpu	6.965e+43	5.10	5.10	1.339e+40	0.027
16599	triHPacyl.ppppmtppu	1.802e+44	5.67	5.67	1.331e+40	0.0269
16600	triHPacyl.mmtmptommpu	8.253e+43	5.22	5.22	1.305e+40	0.0263
16601	triHPacyl.tmpmmtmmu	5.750e+43	5.01	5.01	1.282e+40	0.0259
16602	triHPacyl.tptmmtmmu	1.199e+44	5.46	5.46	1.268e+40	0.0256
16603	triHPacyl.tpmmpmpmpu	2.973e+43	4.63	4.63	1.268e+40	0.0256
16604	triHPacyl.tptmmmpmpu	3.715e+43	4.76	4.76	1.256e+40	0.0254
16605	triHPacyl.tppppptompu	1.024e+44	5.38	5.38	1.236e+40	0.0249
16606	triHPacyl.pttpptompu	9.162e+43	5.32	5.32	1.227e+40	0.0248
16607	triHPacyl.pmpmpmpmpu	1.339e+43	4.17	4.17	1.223e+40	0.0247

16608	triHPacyl.pttmtmpmu	1.031e+44	5.39	5.39	1.214e+40	0.0245
16609	triHPacyl.pptnmtppmu	3.556e+43	4.77	4.77	1.201e+40	0.0242
16610	triHPacyl.tpmppmmpmu	1.234e+43	4.14	4.14	1.192e+40	0.0241
16611	triHPacyl.mppmptmpmu	1.362e+43	4.20	4.20	1.192e+40	0.0241
16612	triHPacyl.ttmmtmtmpu	3.842e+43	4.82	4.82	1.178e+40	0.0238
16613	triHPacyl.pttppptppu	7.574e+43	5.23	5.23	1.177e+40	0.0238
16614	triHPacyl.ppptpmpmu	6.119e+43	5.10	5.10	1.175e+40	0.0237
16615	triHPacyl.ptmmmmppu	3.112e+43	4.71	4.71	1.157e+40	0.0233
16616	triHPacyl.pppmtmtmu	1.620e+43	4.32	4.32	1.147e+40	0.0231
16617	triHPacyl.tppmmpmpu	4.193e+43	4.89	4.89	1.146e+40	0.0231
16618	triHPacyl.tmtmptppu	5.404e+43	5.05	5.05	1.141e+40	0.023
16619	triHPacyl.tppmtmtmu	1.484e+45	7.03	7.03	1.124e+40	0.0227
16620	triHPacyl.pppmptmpu	3.426e+43	4.79	4.79	1.119e+40	0.0226
16621	triHPacyl.pttppmpmu	9.285e+43	5.38	5.38	1.110e+40	0.0224
16622	triHPacyl.pttmtmpu	2.857e+43	4.69	4.69	1.101e+40	0.0222
16623	triHPacyl.pmmptmpu	2.703e+43	4.66	4.66	1.093e+40	0.0221
16624	triHPacyl.tppmtmpu	6.531e+44	6.56	6.56	1.083e+40	0.0219
16625	triHPacyl.tppmtmpmu	9.841e+43	5.45	5.45	1.059e+40	0.0214
16626	triHPacyl.tmmmtmpmu	1.674e+43	4.40	4.40	1.048e+40	0.0212
16627	triHPacyl.tppmmtppu	5.801e+43	5.14	5.14	1.042e+40	0.021
16628	triHPacyl.ptmtppmmpu	1.215e+44	5.59	5.59	1.030e+40	0.0208
16629	triHPacyl.mpppmtppu	2.718e+43	4.70	4.70	1.029e+40	0.0208
16630	triHPacyl.tppmmtmpu	2.985e+44	6.13	6.13	1.028e+40	0.0208
16631	triHPacyl.tmtppppmu	6.596e+43	5.23	5.23	1.024e+40	0.0207
16632	triHPacyl.tptpmtmpu	1.283e+44	5.63	5.63	1.022e+40	0.0206
16633	triHPacyl.tppmmtmpu	5.754e+43	5.15	5.15	1.014e+40	0.0205
16634	triHPacyl.tmmmtmpmu	9.164e+43	5.43	5.43	1.007e+40	0.0203
16635	triHPacyl.pmtppmtmpu	7.063e+43	5.29	5.29	9.884e+39	0.0199
16636	triHPacyl.tmtmtpmpu	1.144e+44	5.58	5.58	9.811e+39	0.0198
16637	triHPacyl.mpppmtppu	1.194e+44	5.61	5.61	9.749e+39	0.0197
16638	triHPacyl.pptppptppu	3.539e+43	4.89	4.89	9.677e+39	0.0195
16639	triHPacyl.tppmmpmpu	4.515e+43	5.04	5.04	9.675e+39	0.0195
16640	triHPacyl.ttmmtmpmu	1.608e+43	4.43	4.43	9.609e+39	0.0194
16641	triHPacyl.mppmptmpu	1.971e+43	4.55	4.55	9.565e+39	0.0193
16642	triHPacyl.tppmmmpmpu	1.581e+43	4.43	4.43	9.420e+39	0.019
16643	triHPacyl.tppmmpmpu	5.715e+43	5.20	5.20	9.235e+39	0.0186
16644	triHPacyl.pptmmtmpu	1.689e+43	4.48	4.48	9.205e+39	0.0186
16645	triHPacyl.tmtpmtmpu	3.287e+43	4.88	4.88	9.174e+39	0.0185
16646	triHPacyl.pttmtppmu	6.029e+43	5.24	5.24	9.127e+39	0.0184
16647	triHPacyl.tttppmmpmu	6.385e+43	5.28	5.28	9.106e+39	0.0184
16648	triHPacyl.ptppmmpmu	2.773e+43	4.79	4.79	8.982e+39	0.0181
16649	triHPacyl.mmtppmmpmu	1.412e+44	5.77	5.77	8.809e+39	0.0178
16650	triHPacyl.tmtmtmpu	1.650e+44	5.87	5.87	8.750e+39	0.0177
16651	triHPacyl.pmtmptppmu	1.168e+44	5.66	5.66	8.746e+39	0.0177
16652	triHPacyl.tppmmtmpu	6.771e+43	5.34	5.34	8.721e+39	0.0176
16653	triHPacyl.pppmptmpu	2.233e+43	4.68	4.68	8.698e+39	0.0176
16654	triHPacyl.tppmmtmpu	4.315e+43	5.07	5.07	8.697e+39	0.0176
16655	triHPacyl.tppmmtmpu	6.903e+43	5.35	5.35	8.693e+39	0.0175
16656	triHPacyl.pttppptmpu	5.664e+43	5.24	5.24	8.571e+39	0.0173
16657	triHPacyl.tppmptmpu	1.462e+43	4.44	4.44	8.552e+39	0.0173
16658	triHPacyl.pptmptmpu	3.295e+43	4.93	4.93	8.472e+39	0.0171
16659	triHPacyl.pptmmtmpu	2.900e+43	4.85	4.85	8.458e+39	0.0171
16660	triHPacyl.pptmmtppu	5.504e+43	5.24	5.24	8.403e+39	0.017
16661	triHPacyl.tppmmtppu	5.699e+43	5.26	5.26	8.400e+39	0.017
16662	triHPacyl.ptmptmtmu	1.330e+44	5.77	5.77	8.373e+39	0.0169
16663	triHPacyl.tptmmpmpu	3.777e+43	5.02	5.02	8.356e+39	0.0169
16664	triHPacyl.pttmtppu	7.519e+43	5.43	5.43	8.347e+39	0.0168
16665	triHPacyl.ptppmtppu	1.889e+43	4.61	4.61	8.324e+39	0.0168
16666	triHPacyl.tppmmtmpu	4.511e+43	5.13	5.13	8.306e+39	0.0168
16667	triHPacyl.pppptppmu	1.129e+44	5.68	5.68	8.169e+39	0.0165
16668	triHPacyl.tmpmmpmpu	4.736e+43	5.17	5.17	8.127e+39	0.0164
16669	triHPacyl.mptpmtmpu	1.787e+43	4.59	4.59	8.075e+39	0.0163
16670	triHPacyl.pppmmpmu	1.062e+44	5.67	5.67	7.856e+39	0.0159
16671	triHPacyl.tmtmmpmpu	2.498e+44	6.19	6.19	7.687e+39	0.0155
16672	triHPacyl.ptmmmtmpu	4.568e+43	5.18	5.18	7.643e+39	0.0154
16673	triHPacyl.ptmmpmtmpu	7.809e+43	5.51	5.51	7.624e+39	0.0154
16674	triHPacyl.mptpmtppu	1.187e+43	4.38	4.38	7.607e+39	0.0154
16675	triHPacyl.pttmtppu	5.858e+43	5.34	5.34	7.600e+39	0.0153
16676	triHPacyl.tmmmtppu	6.932e+43	5.44	5.44	7.505e+39	0.0151
16677	triHPacyl.pptppmmpu	1.492e+43	4.53	4.53	7.453e+39	0.015
16678	triHPacyl.pmmtpppmu	1.560e+43	4.56	4.56	7.384e+39	0.0149
16679	triHPacyl.ppttptmpu	4.572e+43	5.21	5.21	7.301e+39	0.0147

16680	triHPacyl.tmtmmtppmu	3.668e+44	6.46	6.46	7.215e+39	0.0146
16681	triHPacyl.tmtmmtmmpu	4.612e+44	6.60	6.60	7.211e+39	0.0146
16682	triHPacyl.mppmpmtmpu	1.424e+43	4.52	4.52	7.209e+39	0.0146
16683	triHPacyl.pmmmpptppu	2.235e+43	4.80	4.80	7.162e+39	0.0145
16684	triHPacyl.mppmmtmpu	9.255e+42	4.27	4.27	7.154e+39	0.0144
16685	triHPacyl.mmtmppppmu	6.397e+43	5.44	5.44	7.004e+39	0.0141
16686	triHPacyl.ptmmtmmpu	4.527e+43	5.23	5.23	6.959e+39	0.014
16687	triHPacyl.tttmmtmmpu	9.119e+43	5.65	5.65	6.935e+39	0.014
16688	triHPacyl.tpptmtmpu	1.361e+44	5.90	5.90	6.906e+39	0.0139
16689	triHPacyl.ttmmttmpu	7.295e+43	5.53	5.53	6.873e+39	0.0139
16690	triHPacyl.pmpmpmpmpu	4.122e+43	5.19	5.19	6.807e+39	0.0137
16691	triHPacyl.ptppmtmpu	4.326e+43	5.23	5.23	6.745e+39	0.0136
16692	triHPacyl.pptppptmpu	5.664e+43	5.39	5.39	6.720e+39	0.0136
16693	triHPacyl.tttmmtmpu	8.536e+43	5.64	5.64	6.696e+39	0.0135
16694	triHPacyl.tmtmptmpu	8.671e+43	5.65	5.65	6.687e+39	0.0135
16695	triHPacyl.ptmtptmpu	1.101e+44	5.80	5.80	6.541e+39	0.0132
16696	triHPacyl.tptmmtmpu	5.324e+43	5.37	5.37	6.519e+39	0.0132
16697	triHPacyl.pmpmpmtmpu	2.057e+43	4.81	4.81	6.454e+39	0.013
16698	triHPacyl.ptmtmtpu	1.034e+44	5.78	5.78	6.413e+39	0.0129
16699	triHPacyl.pttmmtmmpu	8.854e+43	5.69	5.69	6.300e+39	0.0127
16700	triHPacyl.ptppppmpu	3.004e+43	5.05	5.05	6.298e+39	0.0127
16701	triHPacyl.tpmmpmtmpu	3.219e+43	5.09	5.09	6.268e+39	0.0126
16702	triHPacyl.ptppptmpu	6.220e+43	5.49	5.49	6.178e+39	0.0125
16703	triHPacyl.ptmtmtpu	1.836e+44	6.15	6.15	6.092e+39	0.0123
16704	triHPacyl.pttmmtmmpu	1.196e+44	5.89	5.89	6.088e+39	0.0123
16705	triHPacyl.mmmmttmtu	1.113e+44	5.86	5.86	6.016e+39	0.0121
16706	triHPacyl.ptppmpmpu	1.881e+43	4.80	4.80	5.966e+39	0.012
16707	triHPacyl.tptmtpmpu	6.036e+43	5.50	5.50	5.921e+39	0.012
16708	triHPacyl.pppptmpu	6.012e+43	5.51	5.51	5.816e+39	0.0117
16709	triHPacyl.pppptmpu	4.162e+43	5.30	5.30	5.706e+39	0.0115
16710	triHPacyl.tmtmmtmmpu	2.072e+44	6.26	6.26	5.688e+39	0.0115
16711	triHPacyl.mmpmpptppu	6.481e+43	5.57	5.57	5.683e+39	0.0115
16712	triHPacyl.tttmmtmpu	4.002e+43	5.28	5.28	5.680e+39	0.0115
16713	triHPacyl.tttmmtppu	2.298e+43	4.95	4.95	5.673e+39	0.0114
16714	triHPacyl.ptmmtmmpu	1.693e+43	4.77	4.77	5.638e+39	0.0114
16715	triHPacyl.ptmmtmmpu	1.330e+43	4.63	4.63	5.600e+39	0.0113
16716	triHPacyl.mppmpptppu	5.407e+43	5.47	5.47	5.578e+39	0.0113
16717	triHPacyl.tpmmpmpmu	2.355e+43	4.98	4.98	5.565e+39	0.0112
16718	triHPacyl.tmpmpmpmpu	2.619e+43	5.04	5.04	5.551e+39	0.0112
16719	triHPacyl.ppmmtmpu	4.782e+43	5.41	5.41	5.501e+39	0.0111
16720	triHPacyl.ptppppppu	6.974e+43	5.64	5.64	5.470e+39	0.011
16721	triHPacyl.mppppptmpu	4.326e+43	5.35	5.35	5.438e+39	0.011
16722	triHPacyl.tptmmtppu	5.457e+43	5.50	5.50	5.414e+39	0.0109
16723	triHPacyl.tmtmmtmpu	9.580e+43	5.83	5.83	5.408e+39	0.0109
16724	triHPacyl.tptmmtmpu	1.197e+44	5.97	5.97	5.396e+39	0.0109
16725	triHPacyl.ptmtmtpu	5.416e+43	5.49	5.49	5.383e+39	0.0109
16726	triHPacyl.tmpmpmtmpu	1.336e+44	6.03	6.03	5.367e+39	0.0108
16727	triHPacyl.tttmtpmpu	2.767e+43	5.10	5.10	5.290e+39	0.0107
16728	triHPacyl.mmtmmtppu	5.753e+43	5.54	5.54	5.260e+39	0.0106
16729	triHPacyl.tmtmmtmpu	1.424e+44	6.09	6.09	5.196e+39	0.0105
16730	triHPacyl.pttpmmpu	3.969e+43	5.33	5.33	5.161e+39	0.0104
16731	triHPacyl.pptmptmpu	2.597e+44	6.46	6.46	5.134e+39	0.0104
16732	triHPacyl.tmtmmtmpu	3.105e+44	6.57	6.57	5.081e+39	0.0103
16733	triHPacyl.pptmmpmpu	2.613e+44	6.47	6.47	5.044e+39	0.0102
16734	triHPacyl.mmtmptmpu	1.992e+44	6.31	6.31	5.025e+39	0.0101
16735	triHPacyl.tmtmptmpu	2.322e+44	6.41	6.41	4.981e+39	0.0101
16736	triHPacyl.mppppptmpu	1.837e+44	6.28	6.28	4.923e+39	0.00994
16737	triHPacyl.pptmtpmpu	1.357e+44	6.10	6.10	4.864e+39	0.00982
16738	triHPacyl.pttpptppu	8.307e+43	5.81	5.81	4.830e+39	0.00975
16739	triHPacyl.mtmmpmtmpu	3.197e+43	5.25	5.25	4.823e+39	0.00973
16740	triHPacyl.tptmmpppu	4.229e+43	5.41	5.41	4.818e+39	0.00972
16741	triHPacyl.ptttmtpmpu	1.228e+44	6.05	6.05	4.810e+39	0.00971
16742	triHPacyl.pmpppppmpu	1.485e+43	4.80	4.80	4.757e+39	0.0096
16743	triHPacyl.pptmmtmpu	5.051e+43	5.53	5.53	4.733e+39	0.00955
16744	triHPacyl.ptpmtmpu	4.717e+43	5.49	5.49	4.724e+39	0.00953
16745	triHPacyl.tmpmpmtmpu	5.896e+43	5.62	5.62	4.709e+39	0.0095
16746	triHPacyl.tmpmpmpmpu	1.692e+43	4.88	4.88	4.687e+39	0.00946
16747	triHPacyl.pttmmtmmpu	8.801e+43	5.87	5.87	4.673e+39	0.00943
16748	triHPacyl.pppmmtmmpu	2.426e+43	5.11	5.11	4.605e+39	0.00929
16749	triHPacyl.pptmptmpu	1.773e+43	4.93	4.93	4.564e+39	0.00921
16750	triHPacyl.pttpptmpu	4.050e+44	6.80	6.80	4.492e+39	0.00907
16751	triHPacyl.pptmmpmpu	1.013e+44	5.98	5.98	4.455e+39	0.00899

16752	triHPacyl.pmtppptmmu	3.748e+43	5.39	5.39	4.446e+39	0.00897
16753	triHPacyl.ttmmtmtpu	1.239e+44	6.10	6.10	4.446e+39	0.00897
16754	triHPacyl.ttmmtmmpu	3.863e+43	5.41	5.41	4.415e+39	0.00891
16755	triHPacyl.pmpppptmmu	3.890e+43	5.42	5.42	4.412e+39	0.00891
16756	triHPacyl.tpptmmpmpu	1.019e+44	6.00	6.00	4.370e+39	0.00882
16757	triHPacyl.pptppmpmpu	4.601e+43	5.53	5.53	4.332e+39	0.00874
16758	triHPacyl.ptppmtmmu	4.008e+43	5.45	5.45	4.323e+39	0.00873
16759	triHPacyl.ptttptmpu	1.443e+44	6.21	6.21	4.298e+39	0.00868
16760	triHPacyl.pppmmmpu	4.635e+43	5.54	5.54	4.281e+39	0.00864
16761	triHPacyl.ttmmtmmpu	1.345e+43	4.80	4.80	4.280e+39	0.00864
16762	triHPacyl.ttmmtmmpu	1.075e+44	6.04	6.04	4.262e+39	0.0086
16763	triHPacyl.pmpmtpmpu	1.968e+43	5.03	5.03	4.242e+39	0.00856
16764	triHPacyl.tmtmmpmpu	6.867e+43	5.78	5.78	4.219e+39	0.00852
16765	triHPacyl.mmtmmtmpu	9.407e+43	5.98	5.98	4.140e+39	0.00836
16766	triHPacyl.tmpmtmpu	1.921e+43	5.04	5.04	4.101e+39	0.00828
16767	triHPacyl.ppmmtmpu	2.968e+43	5.30	5.30	4.088e+39	0.00825
16768	triHPacyl.mmpmptmpu	5.255e+43	5.64	5.64	4.069e+39	0.00821
16769	triHPacyl.pptpmpmpu	3.610e+43	5.43	5.43	3.998e+39	0.00807
16770	triHPacyl.tmpmmmpu	2.723e+43	5.26	5.26	3.983e+39	0.00804
16771	triHPacyl.pppmtpmpu	9.902e+43	6.03	6.03	3.983e+39	0.00804
16772	triHPacyl.tmtmmpmpu	9.948e+43	6.04	6.04	3.955e+39	0.00798
16773	triHPacyl.ptptmpmpu	6.706e+43	5.81	5.81	3.947e+39	0.00797
16774	triHPacyl.ttmmtmpu	1.033e+44	6.07	6.07	3.888e+39	0.00785
16775	triHPacyl.mmtppmpu	9.702e+44	7.41	7.41	3.888e+39	0.00785
16776	triHPacyl.mmtmtpmpu	2.263e+44	6.54	6.54	3.887e+39	0.00784
16777	triHPacyl.ptmpmpmpu	4.371e+43	5.56	5.56	3.868e+39	0.00781
16778	triHPacyl.mmmmtmpu	3.845e+43	5.49	5.49	3.867e+39	0.0078
16779	triHPacyl.ptttmtmpu	1.104e+44	6.12	6.12	3.819e+39	0.00771
16780	triHPacyl.mtppmpmpu	2.739e+43	5.29	5.29	3.814e+39	0.0077
16781	triHPacyl.ptmtpmpmpu	1.388e+44	6.27	6.27	3.780e+39	0.00763
16782	triHPacyl.mmpmpmpmpu	1.501e+44	6.31	6.31	3.770e+39	0.00761
16783	triHPacyl.pptmpmpmpu	2.443e+43	5.23	5.23	3.760e+39	0.00759
16784	triHPacyl.ptttmtmpu	1.519e+44	6.32	6.32	3.753e+39	0.00757
16785	triHPacyl.pmpppptmpu	2.798e+43	5.32	5.32	3.750e+39	0.00757
16786	triHPacyl.ptpppmpmpu	9.526e+43	6.05	6.05	3.746e+39	0.00756
16787	triHPacyl.pttpmtmpmpu	1.649e+44	6.38	6.38	3.722e+39	0.00751
16788	triHPacyl.mmpmtpmpmpu	5.532e+43	5.73	5.73	3.717e+39	0.0075
16789	triHPacyl.pmpmtmpmpu	5.279e+43	5.70	5.70	3.716e+39	0.0075
16790	triHPacyl.tmtmpmpmpu	1.547e+44	6.35	6.35	3.685e+39	0.00744
16791	triHPacyl.mmmmtmpmpu	1.274e+43	4.87	4.87	3.608e+39	0.00728
16792	triHPacyl.mmpmtpmpmpu	3.162e+43	5.41	5.41	3.602e+39	0.00727
16793	triHPacyl.pptpmpmpu	6.678e+43	5.87	5.87	3.527e+39	0.00712
16794	triHPacyl.pmpptmpmpu	1.371e+44	6.30	6.30	3.525e+39	0.00711
16795	triHPacyl.pttpmmmpmpu	6.720e+43	5.88	5.88	3.522e+39	0.00711
16796	triHPacyl.mppppptmpmpu	4.484e+43	5.64	5.64	3.500e+39	0.00706
16797	triHPacyl.pptmmtmpmpu	7.667e+43	5.96	5.96	3.491e+39	0.00705
16798	triHPacyl.mmpmpppmpmpu	2.267e+43	5.23	5.23	3.486e+39	0.00704
16799	triHPacyl.tmpmtpmpmpu	2.044e+43	5.18	5.18	3.449e+39	0.00696
16800	triHPacyl.tptpmpmpmpu	5.096e+43	5.72	5.72	3.445e+39	0.00695
16801	triHPacyl.tmtmtpmpmpu	7.054e+43	5.92	5.92	3.424e+39	0.00691
16802	triHPacyl.mppppptmpmpu	1.141e+44	6.22	6.22	3.386e+39	0.00683
16803	triHPacyl.ptpmtmpmpu	1.719e+44	6.46	6.46	3.361e+39	0.00678
16804	triHPacyl.pppmmmpmpu	8.555e+42	4.68	4.68	3.352e+39	0.00676
16805	triHPacyl.tppppppmpmpu	5.493e+43	5.79	5.79	3.302e+39	0.00666
16806	triHPacyl.tmmptmpmpu	1.028e+44	6.18	6.18	3.251e+39	0.00656
16807	triHPacyl.tmmmtmpmpu	6.940e+43	5.94	5.94	3.251e+39	0.00656
16808	triHPacyl.ptmmpmpmpmpu	4.778e+43	5.72	5.72	3.233e+39	0.00653
16809	triHPacyl.tptmmpmpmpu	2.688e+43	5.38	5.38	3.229e+39	0.00652
16810	triHPacyl.pmpmtpmpmpu	1.437e+43	5.01	5.01	3.222e+39	0.0065
16811	triHPacyl.tmtpmtmpmpu	1.973e+44	6.57	6.57	3.212e+39	0.00648
16812	triHPacyl.ptttmtmpmpu	1.099e+44	6.23	6.23	3.159e+39	0.00638
16813	triHPacyl.mmmmtmpmpu	5.362e+43	5.81	5.81	3.131e+39	0.00632
16814	triHPacyl.tmtmtpmpmpu	7.963e+43	6.05	6.05	3.106e+39	0.00627
16815	triHPacyl.ppptmtpmpmpu	7.453e+43	6.01	6.01	3.105e+39	0.00627
16816	triHPacyl.tmmptmpmpu	2.906e+43	5.46	5.46	3.042e+39	0.00614
16817	triHPacyl.tmtmmtmpmpu	1.516e+44	6.45	6.45	3.034e+39	0.00612
16818	triHPacyl.ptttppmpmpu	1.044e+44	6.23	6.23	3.012e+39	0.00608
16819	triHPacyl.mmpptmpmpmpu	7.024e+43	6.00	6.00	3.001e+39	0.00606
16820	triHPacyl.ptpmpmpmpmpu	1.685e+43	5.15	5.15	2.981e+39	0.00602
16821	triHPacyl.pptmpmpmpmpu	1.207e+43	4.95	4.95	2.972e+39	0.006
16822	triHPacyl.tttptmpmpmpu	3.513e+43	5.59	5.59	2.970e+39	0.006
16823	triHPacyl.tmpmmpmpmpu	4.683e+43	5.76	5.76	2.958e+39	0.00597

16824	triHPacyl.tptpmtmpmu	3.569e+43	5.60	5.60	2.958e+39	0.00597
16825	triHPacyl.pmntpmpmpu	3.303e+43	5.56	5.56	2.952e+39	0.00596
16826	triHPacyl.pppmpttmmu	5.629e+43	5.88	5.88	2.938e+39	0.00593
16827	triHPacyl.tmmmmmmppu	2.310e+43	5.35	5.35	2.937e+39	0.00593
16828	triHPacyl.tmmppptpmu	4.232e+43	5.71	5.71	2.930e+39	0.00591
16829	triHPacyl.mptmptpppu	1.427e+43	5.06	5.06	2.923e+39	0.0059
16830	triHPacyl.mmpptpmpmu	6.139e+43	5.93	5.93	2.918e+39	0.00589
16831	triHPacyl.pppmmpmpmu	1.521e+43	5.11	5.11	2.898e+39	0.00585
16832	triHPacyl.pmtmptmnmu	5.335e+44	7.23	7.23	2.880e+39	0.00581
16833	triHPacyl.tttmtpppu	4.957e+43	5.82	5.82	2.876e+39	0.00581
16834	triHPacyl.ptttmtmpmu	8.460e+43	6.14	6.14	2.863e+39	0.00578
16835	triHPacyl.pttmmmtmmu	1.116e+44	6.30	6.30	2.861e+39	0.00577
16836	triHPacyl.mmpppptppu	9.727e+43	6.22	6.22	2.861e+39	0.00577
16837	triHPacyl.tpmmmtpmpu	3.244e+43	5.57	5.57	2.856e+39	0.00576
16838	triHPacyl.ptmmmmmpmu	4.126e+43	5.71	5.71	2.855e+39	0.00576
16839	triHPacyl.tptmptpmu	6.568e+44	7.36	7.36	2.851e+39	0.00575
16840	triHPacyl.mmmmmtppu	5.470e+43	5.88	5.88	2.849e+39	0.00575
16841	triHPacyl.pttmptmpu	5.536e+43	5.89	5.89	2.848e+39	0.00575
16842	triHPacyl.pmttppppu	1.201e+44	6.35	6.35	2.826e+39	0.0057
16843	triHPacyl.pppmptppu	5.815e+43	5.92	5.92	2.815e+39	0.00568
16844	triHPacyl.pttmmmtmpu	4.329e+43	5.75	5.75	2.809e+39	0.00567
16845	triHPacyl.tttmmmmppu	1.375e+44	6.44	6.44	2.799e+39	0.00565
16846	triHPacyl.mmpptpmpmu	5.030e+43	5.84	5.84	2.783e+39	0.00562
16847	triHPacyl.pttpmtmnmu	4.346e+43	5.76	5.76	2.772e+39	0.0056
16848	triHPacyl.tpmmmmpmpu	2.900e+43	5.52	5.52	2.748e+39	0.00555
16849	triHPacyl.tmmmpptppu	1.345e+43	5.07	5.07	2.738e+39	0.00553
16850	triHPacyl.pptpptppu	3.087e+43	5.57	5.57	2.706e+39	0.00546
16851	triHPacyl.tmmmpmpppu	3.506e+43	5.65	5.65	2.704e+39	0.00546
16852	triHPacyl.pttmptppmu	7.621e+43	6.11	6.11	2.701e+39	0.00545
16853	triHPacyl.pppmmpmmu	1.381e+43	5.10	5.10	2.681e+39	0.00541
16854	triHPacyl.pptmppppu	2.265e+43	5.39	5.39	2.673e+39	0.00539
16855	triHPacyl.ptpmmpmpu	1.505e+43	5.15	5.15	2.644e+39	0.00534
16856	triHPacyl.tptpptpmu	7.468e+43	6.11	6.11	2.641e+39	0.00533
16857	triHPacyl.ppppmtmmu	3.241e+43	5.61	5.61	2.637e+39	0.00532
16858	triHPacyl.pptmmpppu	2.371e+43	5.44	5.44	2.590e+39	0.00523
16859	triHPacyl.pmtmppppu	3.506e+43	5.67	5.67	2.583e+39	0.00521
16860	triHPacyl.pmtmpmnmnu	4.884e+44	7.26	7.26	2.527e+39	0.0051
16861	triHPacyl.ppptpmpmpu	5.509e+43	5.96	5.96	2.526e+39	0.0051
16862	triHPacyl.ptmmmmppmu	3.435e+43	5.67	5.67	2.526e+39	0.0051
16863	triHPacyl.pttmptmnmu	8.118e+43	6.19	6.19	2.524e+39	0.00509
16864	triHPacyl.mmpptppmpu	6.894e+43	6.09	6.09	2.520e+39	0.00509
16865	triHPacyl.pppmptppu	3.612e+43	5.71	5.71	2.512e+39	0.00507
16866	triHPacyl.tptmmpmpmu	2.891e+44	6.95	6.95	2.509e+39	0.00506
16867	triHPacyl.pmpptppmu	3.657e+43	5.72	5.72	2.506e+39	0.00506
16868	triHPacyl.pttmppppu	7.697e+43	6.17	6.17	2.474e+39	0.00499
16869	triHPacyl.tptmmmpmu	5.175e+44	7.30	7.30	2.470e+39	0.00499
16870	triHPacyl.pmtppmtmpu	1.809e+43	5.31	5.31	2.469e+39	0.00498
16871	triHPacyl.ptptpmpmpu	1.357e+44	6.51	6.51	2.464e+39	0.00497
16872	triHPacyl.mppppmpmpu	5.278e+44	7.33	7.33	2.426e+39	0.0049
16873	triHPacyl.tmtmptmnu	2.237e+43	5.44	5.44	2.420e+39	0.00488
16874	triHPacyl.mmtmptmpu	1.778e+44	6.68	6.68	2.420e+39	0.00488
16875	triHPacyl.ptmppmmpmu	4.190e+43	5.82	5.82	2.413e+39	0.00487
16876	triHPacyl.tmtppptmpu	5.322e+44	7.34	7.34	2.403e+39	0.00485
16877	triHPacyl.tttmmtmpu	8.229e+43	6.23	6.23	2.402e+39	0.00485
16878	triHPacyl.ppttptmpu	9.034e+43	6.28	6.28	2.397e+39	0.00484
16879	triHPacyl.ptttmtmnmu	1.500e+44	6.59	6.59	2.385e+39	0.00481
16880	triHPacyl.ptmtptmpmu	4.574e+43	5.88	5.88	2.385e+39	0.00481
16881	triHPacyl.tptmmmpmu	9.079e+43	6.29	6.29	2.375e+39	0.00479
16882	triHPacyl.ppttmtpppu	5.244e+43	5.97	5.97	2.359e+39	0.00476
16883	triHPacyl.ptpmpmpmpu	1.829e+43	5.34	5.34	2.357e+39	0.00476
16884	triHPacyl.mmtmmppppu	4.989e+43	5.94	5.94	2.353e+39	0.00475
16885	triHPacyl.tmtppppppu	8.513e+43	6.26	6.26	2.345e+39	0.00473
16886	triHPacyl.mmpmpptppu	4.541e+43	5.89	5.89	2.320e+39	0.00468
16887	triHPacyl.pttmptpmu	6.343e+43	6.10	6.10	2.292e+39	0.00463
16888	triHPacyl.mpppmtppmu	2.202e+43	5.47	5.47	2.268e+39	0.00458
16889	triHPacyl.pppmptmpmu	1.123e+43	5.07	5.07	2.261e+39	0.00456
16890	triHPacyl.pmpmpmtmpu	9.577e+42	4.98	4.98	2.251e+39	0.00454
16891	triHPacyl.tmpmmtmpmu	3.245e+43	5.71	5.71	2.243e+39	0.00453
16892	triHPacyl.pmpmmpmpmu	3.282e+43	5.72	5.72	2.241e+39	0.00452
16893	triHPacyl.ptmptmmpu	4.362e+43	5.89	5.89	2.239e+39	0.00452
16894	triHPacyl.ptmpptmpu	6.411e+43	6.12	6.12	2.236e+39	0.00451
16895	triHPacyl.tmpmmpmpu	1.360e+44	6.57	6.57	2.233e+39	0.00451

16896	triHPacyl.mmmppmmpmu	6.255e+43	6.11	6.11	2.231e+39	0.0045
16897	triHPacyl.ppmtmttppmu	3.926e+44	7.20	7.20	2.227e+39	0.00449
16898	triHPacyl.ptppmtmmmu	2.815e+43	5.63	5.63	2.227e+39	0.00449
16899	triHPacyl.tpppmtmmmu	2.762e+44	6.99	6.99	2.224e+39	0.00449
16900	triHPacyl.tpppmtmmpu	1.441e+44	6.61	6.61	2.209e+39	0.00446
16901	triHPacyl.pmmppmppmu	3.802e+43	5.81	5.81	2.208e+39	0.00446
16902	triHPacyl.tmtmptppmu	1.183e+44	6.50	6.50	2.194e+39	0.00443
16903	triHPacyl.pptpmppmu	3.083e+43	5.70	5.70	2.181e+39	0.0044
16904	triHPacyl.ptmtmtpppu	6.160e+43	6.11	6.11	2.169e+39	0.00438
16905	triHPacyl.mmtpmppppu	8.303e+43	6.29	6.29	2.168e+39	0.00438
16906	triHPacyl.tptmmtppmu	1.283e+44	6.55	6.55	2.154e+39	0.00435
16907	triHPacyl.tpmmpmmpu	1.403e+43	5.24	5.24	2.154e+39	0.00435
16908	triHPacyl.tmtpmppmu	3.421e+43	5.77	5.77	2.143e+39	0.00433
16909	triHPacyl.pmpmtmmpmu	6.710e+43	6.19	6.19	2.094e+39	0.00423
16910	triHPacyl.pmpppmtmmu	3.940e+43	5.87	5.87	2.091e+39	0.00422
16911	triHPacyl.mtmmpmtmmu	3.887e+43	5.86	5.86	2.088e+39	0.00421
16912	triHPacyl.ttmmtmmpu	5.100e+43	6.03	6.03	2.082e+39	0.0042
16913	triHPacyl.pmmtptppmu	8.870e+43	6.36	6.36	2.063e+39	0.00416
16914	triHPacyl.mmmmtppmu	3.700e+43	5.84	5.84	2.058e+39	0.00415
16915	triHPacyl.ppptptmppu	6.384e+43	6.17	6.17	2.049e+39	0.00413
16916	triHPacyl.ppmmttppmu	4.336e+43	5.94	5.94	2.048e+39	0.00413
16917	triHPacyl.mmpppmpppu	1.597e+44	6.72	6.72	2.047e+39	0.00413
16918	triHPacyl.pmtppmmpmu	3.035e+43	5.73	5.73	2.046e+39	0.00413
16919	triHPacyl.mptmptmmpu	1.389e+44	6.64	6.64	2.031e+39	0.0041
16920	triHPacyl.ppttpmtmmu	5.734e+43	6.11	6.11	2.030e+39	0.0041
16921	triHPacyl.tttmmmtppu	5.959e+43	6.13	6.13	2.028e+39	0.00409
16922	triHPacyl.ppmmmpppu	1.360e+43	5.25	5.25	2.026e+39	0.00409
16923	triHPacyl.pptppppppu	2.340e+43	5.58	5.58	2.014e+39	0.00407
16924	triHPacyl.tmpppptppmu	3.374e+43	5.80	5.80	1.997e+39	0.00403
16925	triHPacyl.pttmtmmpu	1.494e+44	6.70	6.70	1.966e+39	0.00397
16926	triHPacyl.ptppppppmu	9.145e+43	6.41	6.41	1.962e+39	0.00396
16927	triHPacyl.tmtmmtppu	1.311e+44	6.63	6.63	1.952e+39	0.00394
16928	triHPacyl.mmtmmmtmmpu	1.341e+44	6.64	6.64	1.937e+39	0.00391
16929	triHPacyl.pttpmmpmmpu	2.197e+43	5.58	5.58	1.906e+39	0.00385
16930	triHPacyl.mmpmptmmpu	4.385e+44	7.36	7.36	1.905e+39	0.00384
16931	triHPacyl.pttpptmmpu	1.971e+44	6.88	6.88	1.904e+39	0.00384
16932	triHPacyl.pptpmtmmpu	5.660e+43	6.14	6.14	1.891e+39	0.00382
16933	triHPacyl.pmmppmtmmu	3.371e+43	5.84	5.84	1.885e+39	0.00381
16934	triHPacyl.tttppmpppu	8.133e+43	6.36	6.36	1.885e+39	0.0038
16935	triHPacyl.ptpmppmmpu	4.806e+43	6.05	6.05	1.880e+39	0.00379
16936	triHPacyl.ppmmmmtmmpu	1.947e+43	5.51	5.51	1.872e+39	0.00378
16937	triHPacyl.tttppmmpmmpu	2.183e+43	5.58	5.58	1.865e+39	0.00376
16938	triHPacyl.ptppppptppu	1.448e+44	6.71	6.71	1.862e+39	0.00376
16939	triHPacyl.tmtmmtmmpu	3.209e+44	7.19	7.19	1.860e+39	0.00375
16940	triHPacyl.tmtppptmmpu	1.091e+44	6.55	6.55	1.850e+39	0.00373
16941	triHPacyl.pmttptmmpu	2.429e+44	7.03	7.03	1.840e+39	0.00371
16942	triHPacyl.mttmptpppu	2.894e+43	5.76	5.76	1.831e+39	0.0037
16943	triHPacyl.tmtmmtmmpu	3.744e+43	5.92	5.92	1.828e+39	0.00369
16944	triHPacyl.mmtmpmtmmpu	2.092e+44	6.95	6.95	1.820e+39	0.00367
16945	triHPacyl.pppmpttppmu	2.518e+44	7.06	7.06	1.819e+39	0.00367
16946	triHPacyl.tptmmmmmpu	4.643e+44	7.43	7.43	1.803e+39	0.00364
16947	triHPacyl.ppmmpmmpmmpu	1.612e+43	5.42	5.42	1.801e+39	0.00364
16948	triHPacyl.tmmmmmpmmpu	6.274e+43	6.24	6.24	1.800e+39	0.00363
16949	triHPacyl.mmtmmtmmpu	1.907e+44	6.90	6.90	1.799e+39	0.00363
16950	triHPacyl.ttpmtmmpu	6.343e+43	6.25	6.25	1.787e+39	0.00361
16951	triHPacyl.tmtmmmmppu	3.952e+44	7.34	7.34	1.781e+39	0.0036
16952	triHPacyl.ppptpttppmu	5.462e+44	7.53	7.53	1.777e+39	0.00359
16953	triHPacyl.ptttptmmpu	1.432e+44	6.74	6.74	1.770e+39	0.00357
16954	triHPacyl.tptmmtmmpu	1.215e+44	6.64	6.64	1.770e+39	0.00357
16955	triHPacyl.pmttptmmpu	1.214e+44	6.64	6.64	1.766e+39	0.00357
16956	triHPacyl.ptttmtpppu	8.896e+43	6.46	6.46	1.743e+39	0.00352
16957	triHPacyl.pmmtptmmpu	3.127e+43	5.84	5.84	1.741e+39	0.00351
16958	triHPacyl.pttppmtmmpu	8.412e+43	6.43	6.43	1.728e+39	0.00349
16959	triHPacyl.ptppmmtmmpu	6.774e+43	6.31	6.31	1.722e+39	0.00347
16960	triHPacyl.mptppptmmpu	2.281e+43	5.66	5.66	1.717e+39	0.00347
16961	triHPacyl.tppmtppmmpu	9.987e+43	6.55	6.55	1.695e+39	0.00342
16962	triHPacyl.tmmpmmtmmpu	5.948e+43	6.24	6.24	1.680e+39	0.00339
16963	triHPacyl.ptptmtpmmpu	5.697e+43	6.22	6.22	1.669e+39	0.00337
16964	triHPacyl.mppmmpmmpu	3.747e+43	5.97	5.97	1.666e+39	0.00336
16965	triHPacyl.pmmtpppppu	6.755e+43	6.33	6.33	1.656e+39	0.00334
16966	triHPacyl.mmpmptmmpu	2.442e+43	5.73	5.73	1.647e+39	0.00332
16967	triHPacyl.tmmpmtmmpu	5.107e+43	6.17	6.17	1.643e+39	0.00332

16968	triHPacyl.tmpmmtpppu	2.936e+43	5.84	5.84	1.641e+39	0.00331
16969	triHPacyl.tmpmmtppmu	2.112e+44	7.02	7.02	1.636e+39	0.0033
16970	triHPacyl.tmpmmtppmu	1.836e+43	5.56	5.56	1.635e+39	0.0033
16971	triHPacyl.ppmtmtppu	2.876e+44	7.21	7.21	1.610e+39	0.00325
16972	triHPacyl.tttmmppmu	5.139e+43	6.19	6.19	1.599e+39	0.00323
16973	triHPacyl.tmmmmppmu	3.226e+44	7.28	7.28	1.593e+39	0.00322
16974	triHPacyl.tpttmmppmu	3.286e+44	7.30	7.30	1.589e+39	0.00321
16975	triHPacyl.ptmmtmmmu	8.687e+43	6.50	6.50	1.587e+39	0.0032
16976	triHPacyl.ttttmmppmu	1.052e+44	6.62	6.62	1.582e+39	0.00319
16977	triHPacyl.pptmmppmu	1.876e+43	5.59	5.59	1.580e+39	0.00319
16978	triHPacyl.ptmppppmu	9.170e+43	6.55	6.55	1.563e+39	0.00315
16979	triHPacyl.mmpmmtmmu	4.140e+43	6.07	6.07	1.562e+39	0.00315
16980	triHPacyl.tmmtmtmmu	1.409e+44	6.80	6.80	1.557e+39	0.00314
16981	triHPacyl.pmmtppmmu	1.243e+43	5.36	5.36	1.555e+39	0.00314
16982	triHPacyl.mmmmtmmpu	1.519e+43	5.48	5.48	1.537e+39	0.0031
16983	triHPacyl.tttppmtpmu	1.198e+44	6.72	6.72	1.534e+39	0.0031
16984	triHPacyl.pttppmmpu	1.214e+44	6.72	6.72	1.532e+39	0.00309
16985	triHPacyl.mptmptmpu	1.906e+43	5.62	5.62	1.530e+39	0.00309
16986	triHPacyl.tmmpptmmu	1.254e+44	6.75	6.75	1.523e+39	0.00307
16987	triHPacyl.ptmptmmpu	3.341e+43	5.96	5.96	1.516e+39	0.00306
16988	triHPacyl.ttppmmpmu	3.080e+43	5.91	5.91	1.515e+39	0.00306
16989	triHPacyl.mppmtpmpu	8.262e+43	6.51	6.51	1.495e+39	0.00302
16990	triHPacyl.ptmtmmmpu	1.231e+44	6.75	6.75	1.494e+39	0.00301
16991	triHPacyl.pmmtptmpmu	1.535e+43	5.51	5.51	1.492e+39	0.00301
16992	triHPacyl.tttmmmtmmu	9.623e+43	6.60	6.60	1.491e+39	0.00301
16993	triHPacyl.mmmmmmtmmu	1.126e+44	6.70	6.70	1.483e+39	0.00299
16994	triHPacyl.ptmmmmmpu	5.571e+43	6.28	6.28	1.482e+39	0.00299
16995	triHPacyl.mmtmptmpu	2.684e+44	7.22	7.22	1.474e+39	0.00297
16996	triHPacyl.tmmtmtmpu	7.244e+43	6.44	6.44	1.464e+39	0.00296
16997	triHPacyl.mtppmmpmu	2.853e+43	5.89	5.89	1.463e+39	0.00295
16998	triHPacyl.pmppmtmpu	8.676e+43	6.55	6.55	1.460e+39	0.00295
16999	triHPacyl.tmmtmtpmu	2.079e+43	5.70	5.70	1.459e+39	0.00294
17000	triHPacyl.mptpppppu	1.729e+43	5.59	5.59	1.453e+39	0.00293
17001	triHPacyl.ttmtmtmpu	2.063e+44	7.07	7.07	1.448e+39	0.00292
17002	triHPacyl.pttpptmpu	1.038e+44	6.67	6.67	1.445e+39	0.00292
17003	triHPacyl.tmtmmmmmu	9.222e+43	6.60	6.60	1.432e+39	0.00289
17004	triHPacyl.mmmmmpppmu	7.211e+43	6.46	6.46	1.424e+39	0.00287
17005	triHPacyl.pppttppu	3.415e+44	7.39	7.39	1.415e+39	0.00286
17006	triHPacyl.tmtmtpmmu	6.426e+44	7.77	7.77	1.413e+39	0.00285
17007	triHPacyl.tmmmpmpmu	4.547e+43	6.19	6.19	1.404e+39	0.00283
17008	triHPacyl.ptmtmtmmu	8.619e+43	6.58	6.58	1.395e+39	0.00282
17009	triHPacyl.tptmtpmpu	1.238e+44	6.80	6.80	1.372e+39	0.00277
17010	triHPacyl.pppmmtmpu	7.181e+43	6.48	6.48	1.362e+39	0.00275
17011	triHPacyl.mmtmppppmu	9.079e+43	6.63	6.63	1.340e+39	0.0027
17012	triHPacyl.tmtmtpppu	1.580e+44	6.97	6.97	1.332e+39	0.00269
17013	triHPacyl.tptmtmpu	1.903e+44	7.08	7.08	1.329e+39	0.00268
17014	triHPacyl.ppppptppmu	1.363e+44	6.88	6.88	1.317e+39	0.00266
17015	triHPacyl.tppmtpmpu	4.983e+43	6.29	6.29	1.311e+39	0.00265
17016	triHPacyl.tmmmpmmpu	3.128e+43	6.01	6.01	1.310e+39	0.00264
17017	triHPacyl.ttmmpmtpu	1.160e+44	6.79	6.79	1.309e+39	0.00264
17018	triHPacyl.tmpmtpmpu	3.819e+43	6.13	6.13	1.308e+39	0.00264
17019	triHPacyl.tmmmpmmpu	3.289e+43	6.04	6.04	1.307e+39	0.00264
17020	triHPacyl.tmpmmmtmpu	5.067e+43	6.30	6.30	1.302e+39	0.00263
17021	triHPacyl.pttmmmpmu	8.387e+43	6.60	6.60	1.301e+39	0.00263
17022	triHPacyl.ppttptmmu	7.737e+43	6.55	6.55	1.299e+39	0.00262
17023	triHPacyl.tmppptmpmu	3.013e+43	5.99	5.99	1.297e+39	0.00262
17024	triHPacyl.tpmmpmmpu	6.010e+43	6.41	6.41	1.295e+39	0.00261
17025	triHPacyl.mmpmmpmpmu	3.388e+43	6.06	6.06	1.294e+39	0.00261
17026	triHPacyl.mmtppptmpu	1.003e+45	8.09	8.09	1.275e+39	0.00257
17027	triHPacyl.pttmtmpmu	7.540e+43	6.56	6.56	1.261e+39	0.00254
17028	triHPacyl.ptptmtmpu	3.535e+43	6.11	6.11	1.260e+39	0.00254
17029	triHPacyl.mtppmtpmu	6.452e+43	6.47	6.47	1.259e+39	0.00254
17030	triHPacyl.pttmmmpmu	1.318e+44	6.89	6.89	1.257e+39	0.00254
17031	triHPacyl.tmtmppppmu	4.345e+43	6.23	6.23	1.253e+39	0.00253
17032	triHPacyl.tmmtmtpppu	7.107e+43	6.53	6.53	1.252e+39	0.00253
17033	triHPacyl.ppptppmpu	1.460e+44	6.96	6.96	1.250e+39	0.00252
17034	triHPacyl.mmpmmpmmpu	5.363e+43	6.36	6.36	1.245e+39	0.00251
17035	triHPacyl.mmpmmpmmpu	5.351e+43	6.36	6.36	1.244e+39	0.00251
17036	triHPacyl.mtmmpmtpmu	3.923e+43	6.18	6.18	1.241e+39	0.0025
17037	triHPacyl.pmpmtpmpu	9.124e+43	6.68	6.68	1.231e+39	0.00249
17038	triHPacyl.pttmmpppu	3.880e+43	6.18	6.18	1.227e+39	0.00248
17039	triHPacyl.pmtmmtmpu	1.016e+44	6.75	6.75	1.224e+39	0.00247

17040	triHPacyl.pppmpptpmu	1.692e+44	7.06	7.06	1.217e+39	0.00246
17041	triHPacyl.tptnmtmpmu	3.438e+44	7.49	7.49	1.209e+39	0.00244
17042	triHPacyl.mmmmpmmpmu	2.844e+43	6.00	6.00	1.206e+39	0.00243
17043	triHPacyl.mmmmmmpppu	3.295e+43	6.09	6.09	1.203e+39	0.00243
17044	triHPacyl.tmtmpptmpu	1.257e+44	6.89	6.89	1.198e+39	0.00242
17045	triHPacyl.tppmmpmmu	7.336e+43	6.57	6.57	1.193e+39	0.00241
17046	triHPacyl.ttmmpmtmpu	1.612e+43	5.67	5.67	1.190e+39	0.0024
17047	triHPacyl.ttmmttmu	8.557e+43	6.68	6.68	1.169e+39	0.00236
17048	triHPacyl.mmtmptmmu	1.719e+44	7.09	7.09	1.169e+39	0.00236
17049	triHPacyl.tppmmmmu	1.011e+44	6.78	6.78	1.168e+39	0.00236
17050	triHPacyl.ttmmtmmu	1.663e+44	7.08	7.08	1.165e+39	0.00235
17051	triHPacyl.tttmmmpu	1.663e+44	7.08	7.08	1.157e+39	0.00234
17052	triHPacyl.tppmmmpu	5.981e+43	6.47	6.47	1.157e+39	0.00233
17053	triHPacyl.mpmptmpu	4.092e+43	6.24	6.24	1.156e+39	0.00233
17054	triHPacyl.ttmmttppu	1.424e+44	6.99	6.99	1.149e+39	0.00232
17055	triHPacyl.mtmtptmmu	7.050e+43	6.57	6.57	1.148e+39	0.00232
17056	triHPacyl.mmtmptmmu	6.424e+44	7.89	7.89	1.147e+39	0.00232
17057	triHPacyl.pmtmptmpu	6.055e+43	6.48	6.48	1.144e+39	0.00231
17058	triHPacyl.tmmpttppu	5.431e+43	6.42	6.42	1.144e+39	0.00231
17059	triHPacyl.ptmtttmpu	1.920e+44	7.17	7.17	1.142e+39	0.0023
17060	triHPacyl.tpppmtppu	9.039e+43	6.73	6.73	1.140e+39	0.0023
17061	triHPacyl.mptppmpu	1.825e+43	5.78	5.78	1.127e+39	0.00227
17062	triHPacyl.pmpmmmpu	1.712e+43	5.75	5.75	1.103e+39	0.00223
17063	triHPacyl.tmpptmmu	5.182e+43	6.42	6.42	1.093e+39	0.00221
17064	triHPacyl.tmtmmmpu	1.976e+44	7.22	7.22	1.089e+39	0.0022
17065	triHPacyl.mmtmtppu	1.112e+44	6.88	6.88	1.086e+39	0.00219
17066	triHPacyl.mpmptmpu	1.459e+43	5.67	5.67	1.086e+39	0.00219
17067	triHPacyl.mmpmpptmu	2.472e+44	7.36	7.36	1.081e+39	0.00218
17068	triHPacyl.tptmmmpu	2.193e+43	5.92	5.92	1.071e+39	0.00216
17069	triHPacyl.tpptmmmpu	5.243e+43	6.44	6.44	1.069e+39	0.00216
17070	triHPacyl.tpptmtmpu	8.873e+43	6.75	6.75	1.068e+39	0.00216
17071	triHPacyl.mptmptmpu	7.487e+43	6.66	6.66	1.060e+39	0.00214
17072	triHPacyl.tmmptmmu	2.021e+44	7.25	7.25	1.060e+39	0.00214
17073	triHPacyl.tpptpmpu	2.472e+44	7.37	7.37	1.059e+39	0.00214
17074	triHPacyl.pppmpmpu	3.144e+43	6.14	6.14	1.051e+39	0.00212
17075	triHPacyl.tpttppmpu	1.122e+44	6.91	6.91	1.043e+39	0.00211
17076	triHPacyl.mmtmptmpu	2.605e+44	7.41	7.41	1.041e+39	0.0021
17077	triHPacyl.tptnmtmpu	3.074e+43	6.14	6.14	1.039e+39	0.0021
17078	triHPacyl.ppmtnmmpu	4.693e+43	6.39	6.39	1.036e+39	0.00209
17079	triHPacyl.ptmmpptmpu	5.383e+43	6.47	6.47	1.035e+39	0.00209
17080	triHPacyl.ptptpmpu	1.833e+44	7.21	7.21	1.023e+39	0.00207
17081	triHPacyl.pppmpptmpu	4.967e+43	6.43	6.43	1.022e+39	0.00206
17082	triHPacyl.ptmtptmpu	1.815e+44	7.21	7.21	1.020e+39	0.00206
17083	triHPacyl.tmmppptmpu	4.174e+43	6.33	6.33	1.019e+39	0.00206
17084	triHPacyl.tptmptmpu	8.384e+43	6.75	6.75	1.011e+39	0.00204
17085	triHPacyl.ptpmmmmpu	2.318e+43	5.99	5.99	1.004e+39	0.00203
17086	triHPacyl.ptppmmmpu	3.021e+43	6.15	6.15	1.000e+39	0.00202
17087	triHPacyl.mtmtptppu	5.686e+43	6.53	6.53	9.951e+38	0.00201
17088	triHPacyl.pppmpptmpu	5.918e+43	6.56	6.56	9.922e+38	0.002
17089	triHPacyl.pppmpptmpu	2.770e+44	7.48	7.48	9.870e+38	0.00199
17090	triHPacyl.pmmppppppu	3.776e+43	6.30	6.30	9.771e+38	0.00197
17091	triHPacyl.mmmmmmmmpu	9.291e+43	6.83	6.83	9.762e+38	0.00197
17092	triHPacyl.pttpmtmpu	5.255e+43	6.50	6.50	9.727e+38	0.00196
17093	triHPacyl.ppmmmmmmpu	1.752e+43	5.84	5.84	9.702e+38	0.00196
17094	triHPacyl.tpptmmtmpu	4.704e+44	7.81	7.81	9.658e+38	0.00195
17095	triHPacyl.tmttmppu	1.275e+44	7.03	7.03	9.621e+38	0.00194
17096	triHPacyl.pttppmpu	5.939e+43	6.58	6.58	9.517e+38	0.00192
17097	triHPacyl.ppmtnmmpu	3.351e+43	6.24	6.24	9.496e+38	0.00192
17098	triHPacyl.pptmpppppu	7.094e+43	6.69	6.69	9.420e+38	0.0019
17099	triHPacyl.tmmppmmppu	3.066e+43	6.20	6.20	9.343e+38	0.00189
17100	triHPacyl.pppmpptmpu	1.234e+44	7.04	7.04	9.245e+38	0.00187
17101	triHPacyl.pttppppmu	7.539e+43	6.74	6.74	9.235e+38	0.00186
17102	triHPacyl.ttttmtmpu	1.519e+44	7.16	7.16	9.173e+38	0.00185
17103	triHPacyl.tmtmptmpu	3.585e+44	7.68	7.68	9.166e+38	0.00185
17104	triHPacyl.tmpmptppu	9.259e+43	6.87	6.87	9.105e+38	0.00184
17105	triHPacyl.tmpmmmtppu	4.782e+43	6.48	6.48	9.071e+38	0.00183
17106	triHPacyl.mtmtptmpu	3.328e+43	6.27	6.27	9.021e+38	0.00182
17107	triHPacyl.pmtmtppu	1.731e+44	7.25	7.25	9.001e+38	0.00182
17108	triHPacyl.pmtppptmpu	6.674e+43	6.69	6.69	8.983e+38	0.00181
17109	triHPacyl.mppmpptmpu	7.201e+43	6.74	6.74	8.919e+38	0.0018
17110	triHPacyl.pppptttmpu	2.614e+44	7.50	7.50	8.916e+38	0.0018
17111	triHPacyl.mmtmptmpu	2.941e+44	7.58	7.58	8.914e+38	0.0018

17112	triHPacyl.mpmtptmpu	1.882e+44	7.31	7.31	8.871e+38	0.00179
17113	triHPacyl.tmpnmtmpu	6.280e+43	6.66	6.66	8.867e+38	0.00179
17114	triHPacyl.pmpptmpu	3.613e+43	6.34	6.34	8.714e+38	0.00176
17115	triHPacyl.mmtptmpu	2.222e+44	7.42	7.42	8.698e+38	0.00176
17116	triHPacyl.pppmmpu	1.588e+43	5.85	5.85	8.688e+38	0.00175
17117	triHPacyl.mmpmpu	1.681e+44	7.26	7.26	8.660e+38	0.00175
17118	triHPacyl.tppmmpu	2.355e+43	6.09	6.09	8.646e+38	0.00174
17119	triHPacyl.tppptmpu	1.478e+44	7.18	7.18	8.623e+38	0.00174
17120	triHPacyl.pptppmpu	1.721e+44	7.28	7.28	8.615e+38	0.00174
17121	triHPacyl.tpptmtmpu	5.836e+44	8.01	8.01	8.563e+38	0.00173
17122	triHPacyl.ttmptmpu	5.673e+43	6.62	6.62	8.527e+38	0.00172
17123	triHPacyl.ptppmpu	7.104e+43	6.75	6.75	8.527e+38	0.00172
17124	triHPacyl.tttmmtmpu	1.049e+44	6.99	6.99	8.518e+38	0.00172
17125	triHPacyl.mppppmpu	6.123e+43	6.67	6.67	8.467e+38	0.00171
17126	triHPacyl.mmtmpmpu	2.234e+43	6.07	6.07	8.453e+38	0.00171
17127	triHPacyl.mmtmpmtmpu	1.279e+45	8.49	8.49	8.428e+38	0.0017
17128	triHPacyl.tmtptmpu	1.388e+44	7.16	7.16	8.412e+38	0.0017
17129	triHPacyl.mmpptmpu	2.337e+44	7.47	7.47	8.405e+38	0.0017
17130	triHPacyl.mpmtptmpu	3.648e+43	6.37	6.37	8.377e+38	0.00169
17131	triHPacyl.ptttmmpu	1.792e+44	7.32	7.32	8.376e+38	0.00169
17132	triHPacyl.ptppppmpu	1.194e+44	7.08	7.08	8.313e+38	0.00168
17133	triHPacyl.ppptptmpu	1.393e+44	7.17	7.17	8.266e+38	0.00167
17134	triHPacyl.tttptmpu	6.841e+43	6.75	6.75	8.242e+38	0.00166
17135	triHPacyl.ttptmpu	7.506e+43	6.81	6.81	8.225e+38	0.00166
17136	triHPacyl.pmtptmpu	3.413e+44	7.71	7.71	8.210e+38	0.00166
17137	triHPacyl.pptmtmpu	4.994e+43	6.57	6.57	8.153e+38	0.00165
17138	triHPacyl.ptttmtmpu	1.308e+44	7.15	7.15	8.109e+38	0.00164
17139	triHPacyl.ptttmmpu	1.353e+44	7.17	7.17	8.027e+38	0.00162
17140	triHPacyl.mtmptmpu	2.004e+43	6.04	6.04	8.023e+38	0.00162
17141	triHPacyl.mmpptmpu	3.648e+43	6.40	6.40	7.930e+38	0.0016
17142	triHPacyl.pmtptmpu	4.090e+43	6.47	6.47	7.926e+38	0.0016
17143	triHPacyl.mmtmtmpu	1.001e+44	7.00	7.00	7.921e+38	0.0016
17144	triHPacyl.tmpmpmpu	2.317e+43	6.13	6.13	7.897e+38	0.00159
17145	triHPacyl.mptppmpu	1.925e+43	6.02	6.02	7.893e+38	0.00159
17146	triHPacyl.pttmmpmpu	7.022e+43	6.79	6.79	7.892e+38	0.00159
17147	triHPacyl.tmtptmpu	3.861e+43	6.44	6.44	7.866e+38	0.00159
17148	triHPacyl.tmtmmpu	3.652e+44	7.78	7.78	7.841e+38	0.00158
17149	triHPacyl.tptppmpu	3.877e+43	6.44	6.44	7.836e+38	0.00158
17150	triHPacyl.tppptmpu	3.182e+43	6.33	6.33	7.822e+38	0.00158
17151	triHPacyl.ptpmtmpu	3.746e+43	6.43	6.43	7.784e+38	0.00157
17152	triHPacyl.tttptmpu	1.918e+44	7.41	7.41	7.716e+38	0.00156
17153	triHPacyl.mmpmtmpu	1.196e+44	7.13	7.13	7.702e+38	0.00155
17154	triHPacyl.tppppmpu	5.461e+43	6.66	6.66	7.695e+38	0.00155
17155	triHPacyl.ptppmpmpu	5.627e+43	6.68	6.68	7.650e+38	0.00154
17156	triHPacyl.pmpmtmpu	4.671e+43	6.57	6.57	7.650e+38	0.00154
17157	triHPacyl.pmtptmpu	1.173e+44	7.12	7.12	7.637e+38	0.00154
17158	triHPacyl.pmtptmpu	2.107e+44	7.47	7.47	7.599e+38	0.00153
17159	triHPacyl.ptmtmpu	5.773e+43	6.70	6.70	7.540e+38	0.00152
17160	triHPacyl.tmtptmpu	2.829e+44	7.65	7.65	7.517e+38	0.00152
17161	triHPacyl.mppmtmpu	9.447e+43	7.00	7.00	7.503e+38	0.00151
17162	triHPacyl.pptmpu	7.386e+43	6.86	6.86	7.461e+38	0.00151
17163	triHPacyl.pttmmpu	8.540e+43	6.94	6.94	7.453e+38	0.0015
17164	triHPacyl.tptmtmpu	1.062e+44	7.08	7.08	7.423e+38	0.0015
17165	triHPacyl.tttmtmpu	7.342e+43	6.86	6.86	7.421e+38	0.0015
17166	triHPacyl.ptmptmpu	1.420e+44	7.25	7.25	7.404e+38	0.00149
17167	triHPacyl.mptppmpu	2.291e+43	6.17	6.17	7.391e+38	0.00149
17168	triHPacyl.tmmmtmpu	4.236e+43	6.53	6.53	7.380e+38	0.00149
17169	triHPacyl.pptmtmpu	2.202e+44	7.52	7.52	7.369e+38	0.00149
17170	triHPacyl.tpptmtmpu	7.555e+44	8.25	8.25	7.361e+38	0.00149
17171	triHPacyl.tttmtmpu	7.054e+43	6.84	6.84	7.328e+38	0.00148
17172	triHPacyl.ptmptmpu	6.744e+43	6.82	6.82	7.311e+38	0.00148
17173	triHPacyl.tmtmpu	2.028e+44	7.47	7.47	7.303e+38	0.00147
17174	triHPacyl.mppmtmpu	6.423e+43	6.79	6.79	7.272e+38	0.00147
17175	triHPacyl.tttmtmpu	1.782e+44	7.40	7.40	7.245e+38	0.00146
17176	triHPacyl.tpptmtmpu	3.477e+44	7.80	7.80	7.213e+38	0.00146
17177	triHPacyl.pmmmpmpu	1.712e+44	7.38	7.38	7.212e+38	0.00146
17178	triHPacyl.mmmmpmpu	4.369e+43	6.57	6.57	7.123e+38	0.00144
17179	triHPacyl.pttptmpu	9.515e+43	7.04	7.04	7.088e+38	0.00143
17180	triHPacyl.mppptmpu	5.362e+43	6.70	6.70	7.087e+38	0.00143
17181	triHPacyl.ppptptmpu	1.839e+44	7.44	7.44	7.032e+38	0.00142
17182	triHPacyl.tppptmpu	3.617e+43	6.47	6.47	7.030e+38	0.00142
17183	triHPacyl.mppmmmpu	1.117e+43	5.77	5.77	7.029e+38	0.00142

17184	triHPacyl.tttmpmmpu	5.047e+43	6.67	6.67	6.976e+38	0.00141
17185	triHPacyl.tttptppmu	5.281e+43	6.70	6.70	6.899e+38	0.00139
17186	triHPacyl.mptppppmu	4.319e+43	6.59	6.59	6.848e+38	0.00138
17187	triHPacyl.pptmpmmpu	3.374e+43	6.44	6.44	6.834e+38	0.00138
17188	triHPacyl.pppmpmtmu	1.173e+44	7.19	7.19	6.826e+38	0.00138
17189	triHPacyl.tttpmmtmu	7.732e+43	6.94	6.94	6.759e+38	0.00136
17190	triHPacyl.mmmmmmtmu	1.181e+44	7.20	7.20	6.717e+38	0.00136
17191	triHPacyl.pmtptppmu	7.838e+43	6.96	6.96	6.698e+38	0.00135
17192	triHPacyl.ptttmmmtmu	1.783e+44	7.45	7.45	6.686e+38	0.00135
17193	triHPacyl.mmptptmpu	2.217e+44	7.58	7.58	6.668e+38	0.00135
17194	triHPacyl.mmpptptmu	2.236e+44	7.59	7.59	6.662e+38	0.00134
17195	triHPacyl.tmtmtmpmu	1.808e+43	6.09	6.09	6.649e+38	0.00134
17196	triHPacyl.pmtppppmu	1.488e+44	7.35	7.35	6.637e+38	0.00134
17197	triHPacyl.tmpmpmtmu	1.223e+44	7.24	7.24	6.532e+38	0.00132
17198	triHPacyl.tmtmtmtmu	5.614e+44	8.15	8.15	6.520e+38	0.00132
17199	triHPacyl.tptmtmtmu	4.474e+44	8.02	8.02	6.478e+38	0.00131
17200	triHPacyl.pttmpmpmu	4.199e+43	6.61	6.61	6.411e+38	0.00129
17201	triHPacyl.mmpmtmpmu	1.585e+43	6.03	6.03	6.389e+38	0.00129
17202	triHPacyl.tppppmpmu	2.687e+43	6.35	6.35	6.366e+38	0.00128
17203	triHPacyl.tmtpttpmu	4.373e+44	8.01	8.01	6.347e+38	0.00128
17204	triHPacyl.pmtmptmpu	5.471e+43	6.78	6.78	6.290e+38	0.00127
17205	triHPacyl.tptptmpmu	4.798e+43	6.70	6.70	6.287e+38	0.00127
17206	triHPacyl.ttmmmmmpu	4.783e+43	6.70	6.70	6.280e+38	0.00127
17207	triHPacyl.ptppppppu	1.143e+44	7.22	7.22	6.264e+38	0.00126
17208	triHPacyl.pmtmpmpmu	1.178e+44	7.24	7.24	6.263e+38	0.00126
17209	triHPacyl.mptmptppu	2.657e+43	6.36	6.36	6.222e+38	0.00126
17210	triHPacyl.tpppptppu	6.725e+44	8.28	8.28	6.208e+38	0.00125
17211	triHPacyl.mmpptmtmu	1.600e+44	7.43	7.43	6.204e+38	0.00125
17212	triHPacyl.mmtmptmpu	7.437e+43	6.97	6.97	6.193e+38	0.00125
17213	triHPacyl.mtppppppu	2.482e+43	6.32	6.32	6.172e+38	0.00125
17214	triHPacyl.ttmtmtmpu	5.985e+43	6.85	6.85	6.154e+38	0.00124
17215	triHPacyl.ptppmtmpu	4.223e+43	6.64	6.64	6.125e+38	0.00124
17216	triHPacyl.tmtppppmu	1.918e+43	6.17	6.17	6.100e+38	0.00123
17217	triHPacyl.tpptmmtmu	4.257e+44	8.02	8.02	6.076e+38	0.00123
17218	triHPacyl.tttmptppu	6.060e+43	6.86	6.86	6.069e+38	0.00122
17219	triHPacyl.tmtptmtpu	1.989e+44	7.57	7.57	6.066e+38	0.00122
17220	triHPacyl.ptmmmtppu	1.092e+44	7.21	7.21	6.062e+38	0.00122
17221	triHPacyl.mppmpmpmu	7.186e+43	6.97	6.97	6.055e+38	0.00122
17222	triHPacyl.tmpptmpmu	2.368e+43	6.31	6.31	5.993e+38	0.00121
17223	triHPacyl.mtmmptmtmu	5.135e+43	6.77	6.77	5.985e+38	0.00121
17224	triHPacyl.ppptmtppu	2.736e+44	7.77	7.77	5.955e+38	0.0012
17225	triHPacyl.pmpmmtmpu	2.422e+44	7.71	7.71	5.898e+38	0.00119
17226	triHPacyl.mppppmpmu	1.456e+44	7.40	7.40	5.880e+38	0.00119
17227	triHPacyl.ttpmmmpmu	1.725e+43	6.13	6.13	5.856e+38	0.00118
17228	triHPacyl.pptmmmpmu	1.379e+43	6.00	6.00	5.847e+38	0.00118
17229	triHPacyl.mtppptppu	2.284e+43	6.30	6.30	5.833e+38	0.00118
17230	triHPacyl.tttmtpppu	9.253e+43	7.14	7.14	5.801e+38	0.00117
17231	triHPacyl.pptptppu	1.411e+44	7.39	7.39	5.795e+38	0.00117
17232	triHPacyl.tptmtmtmu	1.671e+44	7.50	7.50	5.775e+38	0.00117
17233	triHPacyl.mppmpmmpmu	1.253e+43	5.95	5.95	5.774e+38	0.00117
17234	triHPacyl.pttpmmmtmu	5.840e+43	6.87	6.87	5.767e+38	0.00116
17235	triHPacyl.mppppppppu	1.211e+44	7.31	7.31	5.722e+38	0.00115
17236	triHPacyl.mmpmmtmtmu	5.207e+43	6.81	6.81	5.718e+38	0.00115
17237	triHPacyl.tpptmmmpu	5.848e+43	6.88	6.88	5.715e+38	0.00115
17238	triHPacyl.pmtmptppu	1.460e+44	7.42	7.42	5.711e+38	0.00115
17239	triHPacyl.ptptmmmpmu	1.702e+44	7.52	7.52	5.689e+38	0.00115
17240	triHPacyl.tpmmpmtmpu	2.684e+43	6.42	6.42	5.645e+38	0.00114
17241	triHPacyl.pttptppu	9.978e+43	7.21	7.21	5.623e+38	0.00113
17242	triHPacyl.ptmtmmmpmu	1.231e+44	7.33	7.33	5.621e+38	0.00113
17243	triHPacyl.mppppppmpu	2.287e+44	7.70	7.70	5.619e+38	0.00113
17244	triHPacyl.pmtmptmpu	5.159e+44	8.19	8.19	5.604e+38	0.00113
17245	triHPacyl.pptmmpppu	4.586e+43	6.75	6.75	5.580e+38	0.00113
17246	triHPacyl.pmttppppmu	1.450e+44	7.43	7.43	5.574e+38	0.00113
17247	triHPacyl.tmpmmmmmpu	3.254e+43	6.54	6.54	5.574e+38	0.00112
17248	triHPacyl.tmtmtmtmu	5.814e+44	8.26	8.26	5.571e+38	0.00112
17249	triHPacyl.tpmmpptppu	8.336e+43	7.11	7.11	5.550e+38	0.00112
17250	triHPacyl.tmpmmtppu	6.043e+43	6.92	6.92	5.541e+38	0.00112
17251	triHPacyl.ptmmpptmpu	2.583e+44	7.78	7.78	5.537e+38	0.00112
17252	triHPacyl.pmtmptmpu	3.540e+44	7.97	7.97	5.517e+38	0.00111
17253	triHPacyl.tmtmmpmpu	4.039e+43	6.68	6.68	5.514e+38	0.00111
17254	triHPacyl.tmtmmmpmu	3.144e+44	7.90	7.90	5.490e+38	0.00111
17255	triHPacyl.pmptmtmtmu	1.396e+44	7.42	7.42	5.471e+38	0.0011

17256	triHPacyl.tmttmmpmpu	3.360e+44	7.95	7.95	5.469e+38	0.0011
17257	triHPacyl.tpmmpmpmpu	3.975e+43	6.68	6.68	5.447e+38	0.0011
17258	triHPacyl.ptpmpppppu	5.887e+43	6.91	6.91	5.423e+38	0.00109
17259	triHPacyl.ppptptpppu	6.597e+43	6.98	6.98	5.401e+38	0.00109
17260	triHPacyl.tmmtmtppu	3.698e+44	8.02	8.02	5.351e+38	0.00108
17261	triHPacyl.ttptmtmpmu	4.145e+44	8.08	8.08	5.350e+38	0.00108
17262	triHPacyl.ppptmmmpu	9.755e+43	7.22	7.22	5.324e+38	0.00107
17263	triHPacyl.ptppmpmpu	5.261e+43	6.86	6.86	5.296e+38	0.00107
17264	triHPacyl.mmmppppmmu	1.286e+43	6.02	6.02	5.291e+38	0.00107
17265	triHPacyl.tmtmptmpu	9.341e+43	7.20	7.20	5.284e+38	0.00107
17266	triHPacyl.ppptptmmu	2.770e+44	7.85	7.85	5.263e+38	0.00106
17267	triHPacyl.ptptmmpmpu	9.286e+43	7.20	7.20	5.262e+38	0.00106
17268	triHPacyl.ppttmtmpu	1.201e+44	7.36	7.36	5.260e+38	0.00106
17269	triHPacyl.tttmmmpmpu	8.930e+43	7.18	7.18	5.254e+38	0.00106
17270	triHPacyl.mmpptptmpu	1.617e+44	7.53	7.53	5.253e+38	0.00106
17271	triHPacyl.tttptmtmpu	1.669e+44	7.56	7.56	5.227e+38	0.00105
17272	triHPacyl.ppmmmmtppu	2.770e+43	6.49	6.49	5.211e+38	0.00105
17273	triHPacyl.pmpptmpmu	7.930e+42	5.74	5.74	5.208e+38	0.00105
17274	triHPacyl.tpptmtmpu	7.239e+44	8.43	8.43	5.203e+38	0.00105
17275	triHPacyl.pptmmtmmu	1.654e+44	7.55	7.55	5.190e+38	0.00105
17276	triHPacyl.ppptptmpu	1.851e+44	7.62	7.62	5.172e+38	0.00104
17277	triHPacyl.tmtmmtmpu	1.126e+44	7.33	7.33	5.143e+38	0.00104
17278	triHPacyl.ttpmmmpmpu	4.299e+43	6.76	6.76	5.129e+38	0.00104
17279	triHPacyl.pppptmmpu	1.160e+44	7.35	7.35	5.128e+38	0.00103
17280	triHPacyl.pmmtptmmu	5.879e+43	6.95	6.95	5.084e+38	0.00103
17281	triHPacyl.ppttptmpu	1.813e+44	7.62	7.62	5.059e+38	0.00102
17282	triHPacyl.pmttptppu	1.813e+44	7.63	7.63	5.028e+38	0.00101
17283	triHPacyl.mmpmmmmmpu	5.643e+43	6.93	6.93	5.028e+38	0.00101
17284	triHPacyl.ppppmmtppu	2.149e+44	7.73	7.73	5.013e+38	0.00101
17285	triHPacyl.ptttptmpu	1.253e+44	7.41	7.41	5.002e+38	0.00101
17286	triHPacyl.tmtmtppmu	2.581e+44	7.84	7.84	4.993e+38	0.00101
17287	triHPacyl.tttptpppu	6.299e+43	7.01	7.01	4.965e+38	0.001
17288	triHPacyl.ppmptmpmpu	1.027e+43	5.93	5.93	4.933e+38	0.000996
17289	triHPacyl.ttpmmtmpu	9.691e+43	7.27	7.27	4.896e+38	0.000988
17290	triHPacyl.ttptmmmpu	8.624e+43	7.20	7.20	4.890e+38	0.000987
17291	triHPacyl.pptmmmpmpu	4.724e+43	6.84	6.84	4.890e+38	0.000987
17292	triHPacyl.ppmptmpmpu	4.818e+43	6.86	6.86	4.868e+38	0.000982
17293	triHPacyl.pmtmptmpu	8.001e+43	7.16	7.16	4.844e+38	0.000978
17294	triHPacyl.mtpppmmmpu	3.309e+43	6.64	6.64	4.826e+38	0.000974
17295	triHPacyl.ttpmttppu	4.745e+44	8.23	8.23	4.788e+38	0.000966
17296	triHPacyl.ptmpmmmpu	5.861e+43	6.98	6.98	4.782e+38	0.000965
17297	triHPacyl.mmpptmpmpu	4.329e+43	6.81	6.81	4.774e+38	0.000963
17298	triHPacyl.ttmmmpmpu	1.061e+44	7.34	7.34	4.766e+38	0.000962
17299	triHPacyl.ttpmmtppu	3.226e+44	8.01	8.01	4.724e+38	0.000953
17300	triHPacyl.ptppptmpu	1.241e+44	7.44	7.44	4.718e+38	0.000952
17301	triHPacyl.pmtptmmpu	9.779e+43	7.30	7.30	4.710e+38	0.000951
17302	triHPacyl.mtppmpmpu	4.533e+43	6.85	6.85	4.676e+38	0.000944
17303	triHPacyl.tmmmmmtmpu	1.372e+44	7.51	7.51	4.672e+38	0.000943
17304	triHPacyl.tppmmtmpu	5.046e+44	8.28	8.28	4.657e+38	0.00094
17305	triHPacyl.pmpmmmpmpu	1.138e+43	6.02	6.02	4.651e+38	0.000939
17306	triHPacyl.mptmppmpmpu	1.215e+44	7.44	7.44	4.648e+38	0.000938
17307	triHPacyl.ppptppmpmpu	1.273e+44	7.46	7.46	4.646e+38	0.000938
17308	triHPacyl.tmtmtmmmpu	4.719e+44	8.25	8.25	4.634e+38	0.000935
17309	triHPacyl.ptppptppu	1.801e+44	7.67	7.67	4.630e+38	0.000934
17310	triHPacyl.pmpmmtmpu	5.870e+43	7.01	7.01	4.620e+38	0.000933
17311	triHPacyl.mppppmmmpu	3.985e+43	6.78	6.78	4.620e+38	0.000932
17312	triHPacyl.ptttmtmpu	1.249e+44	7.46	7.46	4.617e+38	0.000932
17313	triHPacyl.ptptptmpu	2.424e+44	7.86	7.86	4.579e+38	0.000924
17314	triHPacyl.mmmppptmpu	2.593e+43	6.53	6.53	4.563e+38	0.000921
17315	triHPacyl.mppppmmmpu	7.163e+43	7.14	7.14	4.535e+38	0.000915
17316	triHPacyl.ppmmtmpmpu	4.494e+43	6.86	6.86	4.518e+38	0.000912
17317	triHPacyl.pptmmtmpu	3.796e+43	6.76	6.76	4.512e+38	0.000911
17318	triHPacyl.pppmmpmpu	4.820e+43	6.90	6.90	4.510e+38	0.00091
17319	triHPacyl.tmpmptmpu	9.353e+43	7.30	7.30	4.476e+38	0.000903
17320	triHPacyl.pmtppmmmpu	7.545e+43	7.18	7.18	4.450e+38	0.000898
17321	triHPacyl.ptpmmtmpu	5.710e+43	7.01	7.01	4.433e+38	0.000895
17322	triHPacyl.tppmptmpu	1.341e+44	7.53	7.53	4.388e+38	0.000886
17323	triHPacyl.tmpmmtmpu	4.342e+43	6.86	6.86	4.347e+38	0.000877
17324	triHPacyl.tptmptppu	1.411e+44	7.57	7.57	4.338e+38	0.000876
17325	triHPacyl.tptmmtmpu	6.388e+43	7.10	7.10	4.289e+38	0.000866
17326	triHPacyl.pmtppmtmpu	1.157e+44	7.46	7.46	4.276e+38	0.000863
17327	triHPacyl.tttmtmpmpu	1.626e+44	7.66	7.66	4.261e+38	0.00086

17328	triHPacyl.tttppmmppu	7.191e+43	7.18	7.18	4.254e+38	0.000859
17329	triHPacyl.pppmptppu	1.678e+43	6.31	6.31	4.218e+38	0.000851
17330	triHPacyl.tpmttppu	7.693e+43	7.22	7.22	4.197e+38	0.000847
17331	triHPacyl.pppmptppu	1.241e+44	7.51	7.51	4.165e+38	0.000841
17332	triHPacyl.tmtmtmpu	5.152e+44	8.36	8.36	4.163e+38	0.00084
17333	triHPacyl.ptttptmpu	2.762e+44	7.99	7.99	4.160e+38	0.00084
17334	triHPacyl.ptmtmtmmu	1.984e+44	7.80	7.80	4.155e+38	0.000839
17335	triHPacyl.pmttptmmu	1.582e+45	9.04	9.04	4.100e+38	0.000828
17336	triHPacyl.ptpttppu	6.700e+43	7.16	7.16	4.088e+38	0.000825
17337	triHPacyl.ptpttppu	1.028e+44	7.41	7.41	4.082e+38	0.000824
17338	triHPacyl.ptpttppu	4.021e+44	8.23	8.23	4.079e+38	0.000823
17339	triHPacyl.ptmmpmpu	5.117e+43	7.00	7.00	4.065e+38	0.00082
17340	triHPacyl.pmpmtpmmu	4.415e+43	6.91	6.91	4.059e+38	0.000819
17341	triHPacyl.mttptppmu	2.446e+43	6.56	6.56	4.047e+38	0.000817
17342	triHPacyl.tppmtpu	1.482e+44	7.64	7.64	4.043e+38	0.000816
17343	triHPacyl.mmtmtmpu	1.684e+43	6.34	6.34	4.042e+38	0.000816
17344	triHPacyl.tmtmtmmu	4.422e+43	6.92	6.92	4.039e+38	0.000815
17345	triHPacyl.tppppmpu	5.537e+43	7.05	7.05	4.029e+38	0.000813
17346	triHPacyl.ppttptmpu	6.101e+43	7.11	7.11	4.023e+38	0.000812
17347	triHPacyl.pmpmtpmmu	6.100e+43	7.11	7.11	4.015e+38	0.00081
17348	triHPacyl.tmtmmpmpu	1.672e+44	7.72	7.72	3.992e+38	0.000806
17349	triHPacyl.mmtptppmu	1.720e+44	7.73	7.73	3.991e+38	0.000806
17350	triHPacyl.ppttppmmu	3.095e+44	8.09	8.09	3.981e+38	0.000803
17351	triHPacyl.tmpptmmu	2.095e+44	7.86	7.86	3.972e+38	0.000802
17352	triHPacyl.pttppmmu	2.390e+44	7.93	7.93	3.963e+38	0.0008
17353	triHPacyl.tptptmpu	7.869e+44	8.65	8.65	3.963e+38	0.0008
17354	triHPacyl.ppttptmpu	6.965e+43	7.20	7.20	3.955e+38	0.000798
17355	triHPacyl.tmpmtpu	7.243e+43	7.23	7.23	3.922e+38	0.000792
17356	triHPacyl.pmpmtpu	1.696e+44	7.74	7.74	3.908e+38	0.000789
17357	triHPacyl.pmpmtpu	7.943e+44	8.67	8.67	3.850e+38	0.000777
17358	triHPacyl.mmpptppmu	2.981e+44	8.08	8.08	3.850e+38	0.000777
17359	triHPacyl.ptpmmppu	3.157e+43	6.75	6.75	3.849e+38	0.000777
17360	triHPacyl.mmtmpmmu	2.019e+44	7.85	7.85	3.829e+38	0.000773
17361	triHPacyl.pmpmtpu	9.582e+43	7.41	7.41	3.821e+38	0.000771
17362	triHPacyl.pppmtpu	1.162e+43	6.15	6.15	3.815e+38	0.00077
17363	triHPacyl.ptptmtpu	7.670e+43	7.29	7.29	3.758e+38	0.000759
17364	triHPacyl.ptptmtpu	1.161e+44	7.54	7.54	3.736e+38	0.000754
17365	triHPacyl.ptmtmtpu	6.697e+43	7.22	7.22	3.704e+38	0.000748
17366	triHPacyl.pmttptppu	7.587e+43	7.29	7.29	3.699e+38	0.000747
17367	triHPacyl.tttmptmpu	8.725e+43	7.38	7.38	3.696e+38	0.000746
17368	triHPacyl.pmpmtpu	1.374e+44	7.65	7.65	3.679e+38	0.000742
17369	triHPacyl.pptmtpmu	4.244e+43	6.95	6.95	3.655e+38	0.000738
17370	triHPacyl.mmtmtpu	7.940e+43	7.33	7.33	3.654e+38	0.000737
17371	triHPacyl.mtmmtmpu	3.622e+43	6.86	6.86	3.633e+38	0.000733
17372	triHPacyl.tpmtmmpu	5.935e+43	7.16	7.16	3.627e+38	0.000732
17373	triHPacyl.mpttptmpu	5.576e+43	7.12	7.12	3.624e+38	0.000731
17374	triHPacyl.mppmtmpu	8.574e+43	7.38	7.38	3.614e+38	0.000729
17375	triHPacyl.tptmtmpu	2.447e+44	8.01	8.01	3.594e+38	0.000725
17376	triHPacyl.pmpmtpu	1.406e+44	7.68	7.68	3.575e+38	0.000722
17377	triHPacyl.mptmtpu	2.304e+43	6.60	6.60	3.574e+38	0.000721
17378	triHPacyl.ptppmmu	4.510e+43	7.01	7.01	3.550e+38	0.000717
17379	triHPacyl.tmtmtmpu	5.065e+44	8.45	8.45	3.549e+38	0.000716
17380	triHPacyl.mttmtpmu	1.311e+44	7.64	7.64	3.538e+38	0.000714
17381	triHPacyl.tttmtpu	9.779e+43	7.47	7.47	3.536e+38	0.000714
17382	triHPacyl.pmtptmpu	1.819e+43	6.47	6.47	3.508e+38	0.000708
17383	triHPacyl.pmtmtpu	1.223e+44	7.61	7.61	3.497e+38	0.000706
17384	triHPacyl.ptmtmmpu	1.438e+44	7.71	7.71	3.488e+38	0.000704
17385	triHPacyl.pmtptmpu	1.479e+44	7.73	7.73	3.473e+38	0.000701
17386	triHPacyl.tppmmtpu	3.219e+44	8.19	8.19	3.452e+38	0.000697
17387	triHPacyl.pmtmtpu	2.577e+43	6.70	6.70	3.411e+38	0.000689
17388	triHPacyl.mttmtpu	4.345e+43	7.01	7.01	3.401e+38	0.000686
17389	triHPacyl.mtpmtpu	4.911e+43	7.09	7.09	3.374e+38	0.000681
17390	triHPacyl.ptmmpmmu	1.137e+44	7.59	7.59	3.369e+38	0.00068
17391	triHPacyl.tppptmpu	1.125e+45	8.96	8.96	3.360e+38	0.000678
17392	triHPacyl.ptmtpmmpu	2.433e+44	8.05	8.05	3.351e+38	0.000676
17393	triHPacyl.tmtpppmmu	1.291e+44	7.67	7.67	3.314e+38	0.000669
17394	triHPacyl.pptmtpu	8.313e+43	7.41	7.41	3.312e+38	0.000669
17395	triHPacyl.ptppmtpu	7.194e+43	7.34	7.34	3.255e+38	0.000657
17396	triHPacyl.pptmtpmmpu	3.522e+44	8.28	8.28	3.253e+38	0.000656
17397	triHPacyl.tmtppppu	9.753e+43	7.52	7.52	3.251e+38	0.000656
17398	triHPacyl.tmpmtpmmpu	2.852e+43	6.79	6.79	3.245e+38	0.000655
17399	triHPacyl.mtmmtmpu	1.633e+43	6.46	6.46	3.225e+38	0.000651

17400	triHPacyl.ptmtptmpmu	1.596e+44	7.82	7.82	3.220e+38	0.00065
17401	triHPacyl.mptpmtmpmu	2.763e+43	6.77	6.77	3.219e+38	0.00065
17402	triHPacyl.ptptptpmu	2.387e+44	8.07	8.07	3.161e+38	0.000638
17403	triHPacyl.mmtpmtmpmu	2.811e+43	6.79	6.79	3.160e+38	0.000638
17404	triHPacyl.pmmmpmpmmu	6.739e+43	7.32	7.32	3.151e+38	0.000636
17405	triHPacyl.ttpmmtppu	5.986e+43	7.25	7.25	3.135e+38	0.000633
17406	triHPacyl.tmtmttppu	4.472e+44	8.45	8.45	3.131e+38	0.000632
17407	triHPacyl.pmtmppmpu	7.571e+43	7.40	7.40	3.104e+38	0.000626
17408	triHPacyl.ptpmmmtmpu	5.387e+43	7.19	7.19	3.093e+38	0.000624
17409	triHPacyl.mppmptmmu	3.120e+43	6.87	6.87	3.081e+38	0.000622
17410	triHPacyl.pppptppmpu	1.544e+44	7.83	7.83	3.077e+38	0.000621
17411	triHPacyl.tmtmmmtmpu	3.943e+44	8.39	8.39	3.072e+38	0.00062
17412	triHPacyl.ppttpttpmu	1.434e+44	7.78	7.78	3.057e+38	0.000617
17413	triHPacyl.ppmtpppmpu	4.792e+43	7.13	7.13	3.053e+38	0.000616
17414	triHPacyl.mmppttpmu	2.641e+44	8.15	8.15	3.040e+38	0.000614
17415	triHPacyl.ptptmpmmu	3.896e+44	8.39	8.39	3.021e+38	0.00061
17416	triHPacyl.pmpmtmmu	4.673e+44	8.50	8.50	3.018e+38	0.000609
17417	triHPacyl.pmmtpmpmu	1.218e+43	6.32	6.32	3.014e+38	0.000608
17418	triHPacyl.mmtmtmpu	3.169e+44	8.27	8.27	2.998e+38	0.000605
17419	triHPacyl.pttptpmpu	1.006e+44	7.59	7.59	2.987e+38	0.000603
17420	triHPacyl.mtppmpmpu	3.078e+43	6.88	6.88	2.975e+38	0.0006
17421	triHPacyl.tpttppmpu	2.585e+44	8.16	8.16	2.949e+38	0.000595
17422	triHPacyl.tppmmmtmmu	4.404e+44	8.48	8.48	2.944e+38	0.000594
17423	triHPacyl.tttppmpmpu	1.682e+44	7.91	7.91	2.928e+38	0.000591
17424	triHPacyl.tpttmtppu	2.404e+44	8.12	8.12	2.913e+38	0.000588
17425	triHPacyl.pttpmmmpu	7.161e+43	7.40	7.40	2.898e+38	0.000585
17426	triHPacyl.mmtmpmmmpu	3.762e+44	8.40	8.40	2.865e+38	0.000578
17427	triHPacyl.ppmmtmpu	6.727e+43	7.38	7.38	2.828e+38	0.000571
17428	triHPacyl.tmppppmpu	4.066e+43	7.08	7.08	2.825e+38	0.00057
17429	triHPacyl.pppppmmmpu	8.572e+43	7.53	7.53	2.822e+38	0.00057
17430	triHPacyl.mttmpmpu	5.098e+43	7.22	7.22	2.820e+38	0.000569
17431	triHPacyl.mtmmptppu	3.220e+43	6.94	6.94	2.819e+38	0.000569
17432	triHPacyl.mmpppptppu	3.294e+43	6.96	6.96	2.801e+38	0.000565
17433	triHPacyl.tmpmptmpu	8.539e+43	7.53	7.53	2.788e+38	0.000563
17434	triHPacyl.mtppmtppu	2.290e+43	6.75	6.75	2.779e+38	0.000561
17435	triHPacyl.ptmtptppu	3.459e+44	8.37	8.37	2.778e+38	0.000561
17436	triHPacyl.tmmppppmpu	3.452e+43	6.99	6.99	2.777e+38	0.000561
17437	triHPacyl.ptptppppu	5.617e+43	7.28	7.28	2.772e+38	0.000559
17438	triHPacyl.mmpptppu	1.338e+44	7.80	7.80	2.767e+38	0.000558
17439	triHPacyl.pmtpmtmpu	7.838e+43	7.49	7.49	2.760e+38	0.000557
17440	triHPacyl.tmppmmppu	7.921e+43	7.49	7.49	2.750e+38	0.000555
17441	triHPacyl.pmmmpmpmpu	1.392e+43	6.46	6.46	2.737e+38	0.000552
17442	triHPacyl.tmtpptmpu	3.206e+44	8.33	8.33	2.734e+38	0.000552
17443	triHPacyl.tmttptppu	2.076e+44	8.07	8.07	2.733e+38	0.000552
17444	triHPacyl.tppmmtmmu	8.402e+44	8.91	8.91	2.711e+38	0.000547
17445	triHPacyl.mtppptppu	3.727e+43	7.05	7.05	2.709e+38	0.000547
17446	triHPacyl.pmpmtmpu	1.482e+44	7.88	7.88	2.708e+38	0.000547
17447	triHPacyl.pppmptppu	7.661e+43	7.49	7.49	2.681e+38	0.000541
17448	triHPacyl.ttpmptmpu	8.258e+43	7.54	7.54	2.677e+38	0.00054
17449	triHPacyl.ptptppmpu	6.004e+43	7.35	7.35	2.674e+38	0.00054
17450	triHPacyl.pptpptppu	1.166e+44	7.74	7.74	2.666e+38	0.000538
17451	triHPacyl.tppmmppmu	6.921e+44	8.81	8.81	2.660e+38	0.000537
17452	triHPacyl.ptmpptmpu	2.639e+43	6.86	6.86	2.651e+38	0.000535
17453	triHPacyl.tpttppmpu	1.367e+44	7.84	7.84	2.647e+38	0.000534
17454	triHPacyl.tptmppmpu	5.192e+43	7.27	7.27	2.646e+38	0.000534
17455	triHPacyl.mtpppmmmpu	4.853e+43	7.23	7.23	2.639e+38	0.000533
17456	triHPacyl.tmmtnmmpu	2.347e+43	6.79	6.79	2.634e+38	0.000532
17457	triHPacyl.tmmptmpu	6.937e+43	7.45	7.45	2.608e+38	0.000526
17458	triHPacyl.ttttmpppu	6.505e+43	7.41	7.41	2.605e+38	0.000526
17459	triHPacyl.mmtmpmmmpu	3.073e+44	8.34	8.34	2.597e+38	0.000524
17460	triHPacyl.ptpmpmpmpu	5.223e+43	7.28	7.28	2.580e+38	0.000521
17461	triHPacyl.tmpmptmpu	7.553e+43	7.51	7.51	2.557e+38	0.000516
17462	triHPacyl.pmmmpmpmu	3.142e+43	6.99	6.99	2.540e+38	0.000513
17463	triHPacyl.tptpptppu	5.581e+43	7.33	7.33	2.538e+38	0.000512
17464	triHPacyl.mmpmmtmpu	2.916e+43	6.95	6.95	2.530e+38	0.000511
17465	triHPacyl.pppmptmmu	1.794e+43	6.66	6.66	2.527e+38	0.00051
17466	triHPacyl.tmpmmpmpu	2.096e+44	8.13	8.13	2.505e+38	0.000506
17467	triHPacyl.ttpmmmpmpu	1.224e+44	7.81	7.81	2.498e+38	0.000504
17468	triHPacyl.mtmmmmmpu	6.945e+43	7.47	7.47	2.494e+38	0.000503
17469	triHPacyl.pmtmptmpu	5.116e+43	7.29	7.29	2.486e+38	0.000502
17470	triHPacyl.mppppptppu	1.182e+44	7.80	7.80	2.478e+38	0.0005
17471	triHPacyl.ptmtptmpu	7.210e+43	7.50	7.50	2.475e+38	0.000499

17472	triHPacyl.ptmpptppu	1.117e+44	7.76	7.76	2.473e+38	0.000499
17473	triHPacyl.ttmpttmmu	1.222e+44	7.82	7.82	2.468e+38	0.000498
17474	triHPacyl.ttmptmppy	8.726e+43	7.62	7.62	2.464e+38	0.000497
17475	triHPacyl.ttttmmtmpu	1.610e+44	7.99	7.99	2.452e+38	0.000495
17476	triHPacyl.mmtmmpmmu	1.669e+45	9.38	9.38	2.439e+38	0.000492
17477	triHPacyl.tmmptmmmu	2.040e+44	8.13	8.13	2.434e+38	0.000491
17478	triHPacyl.mptmptpmu	4.291e+43	7.20	7.20	2.427e+38	0.00049
17479	triHPacyl.pmmptpmu	1.165e+44	7.80	7.80	2.427e+38	0.00049
17480	triHPacyl.mmtmptppu	3.476e+44	8.45	8.45	2.416e+38	0.000488
17481	triHPacyl.tpmmttmmu	1.079e+44	7.76	7.76	2.389e+38	0.000482
17482	triHPacyl.tpptpmppy	2.957e+44	8.36	8.36	2.388e+38	0.000482
17483	triHPacyl.tmtmmmpmu	2.799e+44	8.33	8.33	2.373e+38	0.000479
17484	triHPacyl.tptmnmmpu	5.321e+43	7.35	7.35	2.372e+38	0.000479
17485	triHPacyl.tmpppttmmu	9.128e+43	7.67	7.67	2.369e+38	0.000478
17486	triHPacyl.tmtmtmmmu	8.522e+44	9.01	9.01	2.341e+38	0.000473
17487	triHPacyl.mptmpmpu	1.700e+43	6.68	6.68	2.318e+38	0.000468
17488	triHPacyl.tmpmpmpu	6.772e+43	7.51	7.51	2.299e+38	0.000464
17489	triHPacyl.mmtmtmtpu	6.990e+43	7.53	7.53	2.286e+38	0.000461
17490	triHPacyl.ptpmttmpu	7.857e+43	7.60	7.60	2.283e+38	0.000461
17491	triHPacyl.pmpmtmtpu	8.618e+43	7.66	7.66	2.282e+38	0.000461
17492	triHPacyl.ptmtpttmmu	6.414e+43	7.48	7.48	2.281e+38	0.00046
17493	triHPacyl.ttmmtmtpu	1.729e+44	8.07	8.07	2.277e+38	0.00046
17494	triHPacyl.ptptpppu	3.026e+43	7.03	7.03	2.277e+38	0.00046
17495	triHPacyl.mtmtmptmpu	4.384e+43	7.25	7.25	2.274e+38	0.000459
17496	triHPacyl.mmpptmmpu	9.759e+43	7.73	7.73	2.267e+38	0.000458
17497	triHPacyl.pptmmtppu	7.227e+43	7.56	7.56	2.248e+38	0.000454
17498	triHPacyl.pptppmmmu	5.186e+43	7.36	7.36	2.243e+38	0.000453
17499	triHPacyl.ptmtmtmmu	9.861e+43	7.75	7.75	2.242e+38	0.000452
17500	triHPacyl.tpttmpppu	1.363e+44	7.94	7.94	2.241e+38	0.000452
17501	triHPacyl.tmmmpmpu	4.320e+43	7.26	7.26	2.231e+38	0.00045
17502	triHPacyl.ptptmtmmpu	5.505e+43	7.41	7.41	2.184e+38	0.000441
17503	triHPacyl.ptppptmmpu	1.556e+44	8.04	8.04	2.178e+38	0.00044
17504	triHPacyl.mmtmtmmpu	4.873e+44	8.72	8.72	2.176e+38	0.000439
17505	triHPacyl.ttmptmtpu	8.993e+43	7.72	7.72	2.138e+38	0.000432
17506	triHPacyl.tppmmmpu	5.551e+43	7.43	7.43	2.135e+38	0.000431
17507	triHPacyl.tptmptppu	1.294e+44	7.94	7.94	2.135e+38	0.000431
17508	triHPacyl.mmpmtpppu	3.895e+43	7.22	7.22	2.135e+38	0.000431
17509	triHPacyl.mtppmtmmpu	5.489e+43	7.43	7.43	2.132e+38	0.00043
17510	triHPacyl.mmpptppu	1.882e+44	8.16	8.16	2.123e+38	0.000429
17511	triHPacyl.tmtptmmpu	1.137e+44	7.87	7.87	2.112e+38	0.000426
17512	triHPacyl.mptppmpu	2.480e+43	6.97	6.97	2.091e+38	0.000422
17513	triHPacyl.ptmtppmmu	5.725e+43	7.47	7.47	2.083e+38	0.00042
17514	triHPacyl.tmtmptmpu	4.482e+43	7.32	7.32	2.082e+38	0.00042
17515	triHPacyl.ptmtpttppu	5.947e+43	7.49	7.49	2.077e+38	0.000419
17516	triHPacyl.pppmpmpu	5.975e+43	7.50	7.50	2.048e+38	0.000413
17517	triHPacyl.tmtmpmpu	9.934e+43	7.81	7.81	2.031e+38	0.00041
17518	triHPacyl.ptmptmmpu	2.080e+44	8.25	8.25	2.021e+38	0.000408
17519	triHPacyl.pptmmpmpu	2.892e+43	7.08	7.08	2.008e+38	0.000405
17520	triHPacyl.pmtmptmmpu	1.704e+44	8.14	8.14	2.007e+38	0.000405
17521	triHPacyl.tmmptmmpu	9.245e+43	7.77	7.77	2.006e+38	0.000405
17522	triHPacyl.tptmptmpu	3.490e+44	8.57	8.57	2.004e+38	0.000405
17523	triHPacyl.tptmmtmmpu	5.127e+44	8.80	8.80	1.997e+38	0.000403
17524	triHPacyl.ptmtmtpmmpu	8.540e+43	7.73	7.73	1.997e+38	0.000403
17525	triHPacyl.tmtmppmpu	9.800e+43	7.82	7.82	1.984e+38	0.000401
17526	triHPacyl.tttmmmpmmpu	5.441e+43	7.47	7.47	1.972e+38	0.000398
17527	triHPacyl.pptmmtmmpu	2.886e+43	7.09	7.09	1.961e+38	0.000396
17528	triHPacyl.mttpttmpu	9.864e+43	7.83	7.83	1.956e+38	0.000395
17529	triHPacyl.pmtmmtmmpu	5.988e+44	8.91	8.91	1.950e+38	0.000394
17530	triHPacyl.tmmptmmpu	5.519e+43	7.49	7.49	1.941e+38	0.000392
17531	triHPacyl.tppmtmmpu	8.857e+44	9.15	9.15	1.922e+38	0.000388
17532	triHPacyl.tpmmtmmpu	4.798e+43	7.41	7.41	1.919e+38	0.000387
17533	triHPacyl.pppmtmmpu	1.002e+44	7.85	7.85	1.908e+38	0.000385
17534	triHPacyl.pmtmmpmmpu	2.802e+44	8.47	8.47	1.900e+38	0.000383
17535	triHPacyl.pptmttmmu	1.106e+44	7.91	7.91	1.899e+38	0.000383
17536	triHPacyl.mmtmmtmmpu	5.973e+44	8.92	8.92	1.892e+38	0.000382
17537	triHPacyl.mpmpttmpu	5.534e+44	8.88	8.88	1.881e+38	0.00038
17538	triHPacyl.pmmptmmpu	1.055e+43	6.52	6.52	1.877e+38	0.000379
17539	triHPacyl.ttmpttppu	2.237e+44	8.34	8.34	1.868e+38	0.000377
17540	triHPacyl.mppmptmmpu	7.351e+43	7.68	7.68	1.865e+38	0.000376
17541	triHPacyl.mptmmtmmpu	6.379e+43	7.60	7.60	1.860e+38	0.000375
17542	triHPacyl.ptmmpmpu	6.387e+43	7.60	7.60	1.849e+38	0.000373
17543	triHPacyl.pmmpttppu	1.370e+44	8.06	8.06	1.840e+38	0.000371

17544	triHPacyl.tpmtmtmpu	6.106e+43	7.58	7.58	1.838e+38	0.000371
17545	triHPacyl.tmtmpppmu	5.091e+44	8.85	8.85	1.826e+38	0.000369
17546	triHPacyl.tmtmtmtmmu	2.277e+44	8.37	8.37	1.824e+38	0.000368
17547	triHPacyl.tptmtmtppu	2.195e+44	8.35	8.35	1.818e+38	0.000367
17548	triHPacyl.mtmtmmtmmu	9.711e+43	7.87	7.87	1.810e+38	0.000365
17549	triHPacyl.pmpmmpmmu	8.354e+43	7.78	7.78	1.804e+38	0.000364
17550	triHPacyl.ppttptmpu	7.951e+43	7.75	7.75	1.801e+38	0.000364
17551	triHPacyl.triHPacyl.pptmmtmmu	8.761e+43	7.81	7.81	1.798e+38	0.000363
17552	triHPacyl.ptmppmtmmu	1.313e+44	8.05	8.05	1.795e+38	0.000362
17553	triHPacyl.pmtmmtmmu	7.398e+43	7.71	7.71	1.791e+38	0.000362
17554	triHPacyl.mttppmtmpu	1.443e+44	8.11	8.11	1.790e+38	0.000361
17555	triHPacyl.pmtpttppu	3.339e+44	8.61	8.61	1.789e+38	0.000361
17556	triHPacyl.tptpmtmpu	2.043e+44	8.32	8.32	1.787e+38	0.000361
17557	triHPacyl.tmtmmtmpu	5.730e+44	8.93	8.93	1.786e+38	0.00036
17558	triHPacyl.tttmptmpu	1.457e+44	8.12	8.12	1.784e+38	0.00036
17559	triHPacyl.ttptmtmpu	2.765e+43	7.13	7.13	1.778e+38	0.000359
17560	triHPacyl.tmtpttmmu	2.916e+44	8.53	8.53	1.777e+38	0.000359
17561	triHPacyl.tmtmptppu	3.153e+43	7.21	7.21	1.777e+38	0.000359
17562	triHPacyl.pmtptmmpu	3.530e+44	8.65	8.65	1.776e+38	0.000359
17563	triHPacyl.mmtpttppu	1.921e+44	8.28	8.28	1.775e+38	0.000358
17564	triHPacyl.pmtptmtpu	2.815e+44	8.51	8.51	1.767e+38	0.000357
17565	triHPacyl.ptmpttppu	9.709e+43	7.88	7.88	1.766e+38	0.000357
17566	triHPacyl.pmtmmtmpu	3.980e+44	8.72	8.72	1.766e+38	0.000356
17567	triHPacyl.ppttptmpu	5.435e+44	8.91	8.91	1.757e+38	0.000355
17568	triHPacyl.mmtptmmpu	5.082e+44	8.87	8.87	1.752e+38	0.000354
17569	triHPacyl.tttmmtmmu	4.906e+43	7.48	7.48	1.751e+38	0.000353
17570	triHPacyl.pmtmtmpu	4.106e+43	7.37	7.37	1.748e+38	0.000353
17571	triHPacyl.mpttptmpu	1.262e+44	8.04	8.04	1.744e+38	0.000352
17572	triHPacyl.pmttppmmu	4.683e+44	8.83	8.83	1.743e+38	0.000352
17573	triHPacyl.ttmmtmmpu	1.025e+44	7.92	7.92	1.734e+38	0.00035
17574	triHPacyl.ttptmmpmpu	6.873e+43	7.69	7.69	1.731e+38	0.000349
17575	triHPacyl.mmpmpmmpu	2.348e+44	8.42	8.42	1.724e+38	0.000348
17576	triHPacyl.pmmmpmmpu	2.003e+43	6.95	6.95	1.721e+38	0.000347
17577	triHPacyl.ptmtmmtmpu	2.180e+44	8.38	8.38	1.720e+38	0.000347
17578	triHPacyl.pttmmpmpu	1.337e+44	8.09	8.09	1.717e+38	0.000347
17579	triHPacyl.mmtmmtmpu	8.759e+43	7.84	7.84	1.715e+38	0.000346
17580	triHPacyl.ptmtpmmpu	4.416e+43	7.43	7.43	1.714e+38	0.000346
17581	triHPacyl.tmtmtmmpu	4.548e+44	8.82	8.82	1.713e+38	0.000346
17582	triHPacyl.tttmptppu	1.192e+44	8.02	8.02	1.710e+38	0.000345
17583	triHPacyl.tptmmpmpu	4.085e+44	8.76	8.76	1.708e+38	0.000345
17584	triHPacyl.pttptmmpu	1.171e+44	8.01	8.01	1.704e+38	0.000344
17585	triHPacyl.pttptmmpu	6.366e+43	7.66	7.66	1.681e+38	0.000339
17586	triHPacyl.tpmmtmmpu	5.656e+43	7.59	7.59	1.680e+38	0.000339
17587	triHPacyl.tptptmmpu	8.217e+43	7.81	7.81	1.674e+38	0.000338
17588	triHPacyl.ptmmtmmpu	7.475e+43	7.76	7.76	1.673e+38	0.000338
17589	triHPacyl.ptptmmpu	2.918e+43	7.20	7.20	1.657e+38	0.000334
17590	triHPacyl.mttppmtmpu	7.672e+43	7.78	7.78	1.653e+38	0.000334
17591	triHPacyl.ppttppmpu	1.875e+44	8.31	8.31	1.644e+38	0.000332
17592	triHPacyl.ptmtpmmpu	1.274e+44	8.09	8.09	1.640e+38	0.000331
17593	triHPacyl.tptmmtmmu	5.071e+44	8.91	8.91	1.637e+38	0.00033
17594	triHPacyl.mmtmmpmpu	1.057e+44	7.98	7.98	1.626e+38	0.000328
17595	triHPacyl.mpttptmpu	7.140e+43	7.75	7.75	1.618e+38	0.000327
17596	triHPacyl.pmtmtmpu	4.767e+43	7.51	7.51	1.614e+38	0.000326
17597	triHPacyl.pmpmtmpu	2.310e+43	7.08	7.08	1.614e+38	0.000326
17598	triHPacyl.tttppmtmpu	4.770e+44	8.88	8.88	1.611e+38	0.000325
17599	triHPacyl.tmtptmpu	1.622e+44	8.24	8.24	1.601e+38	0.000323
17600	triHPacyl.mmtmmtmpu	4.386e+44	8.85	8.85	1.579e+38	0.000319
17601	triHPacyl.pmtmmtmpu	8.704e+43	7.88	7.88	1.574e+38	0.000318
17602	triHPacyl.mmtmmpmpu	3.497e+44	8.71	8.71	1.571e+38	0.000317
17603	triHPacyl.ptmptmtpu	1.090e+44	8.02	8.02	1.566e+38	0.000316
17604	triHPacyl.mmtmmpmpu	1.001e+44	7.97	7.97	1.566e+38	0.000316
17605	triHPacyl.ptptmtpu	2.010e+44	8.39	8.39	1.551e+38	0.000313
17606	triHPacyl.tptmptmpu	4.099e+43	7.44	7.44	1.546e+38	0.000312
17607	triHPacyl.tmtmmtppu	1.838e+44	8.34	8.34	1.538e+38	0.00031
17608	triHPacyl.tmpmptppu	1.164e+44	8.07	8.07	1.537e+38	0.00031
17609	triHPacyl.tmpmptppu	5.092e+43	7.58	7.58	1.534e+38	0.00031
17610	triHPacyl.mmpmmtmpu	7.317e+43	7.80	7.80	1.529e+38	0.000309
17611	triHPacyl.mptmmtmpu	1.134e+44	8.06	8.06	1.523e+38	0.000307
17612	triHPacyl.ptppmpppu	2.116e+44	8.44	8.44	1.515e+38	0.000306
17613	triHPacyl.pptmmpmpu	2.490e+43	7.16	7.16	1.506e+38	0.000304
17614	triHPacyl.pmtmmpmpu	5.662e+43	7.65	7.65	1.505e+38	0.000304
17615	triHPacyl.pmtmmpmpu	7.257e+43	7.80	7.80	1.503e+38	0.000303

17616	triHPacyl.pmttptmmpu	7.381e+44	9.19	9.19	1.490e+38	0.000301
17617	triHPacyl.mtppmpmpmu	4.285e+43	7.49	7.49	1.489e+38	0.000301
17618	triHPacyl.ppptmtpppu	1.003e+44	8.00	8.00	1.489e+38	0.0003
17619	triHPacyl.mtptmtpmmu	2.363e+43	7.14	7.14	1.487e+38	0.0003
17620	triHPacyl.pmmtmpmpu	9.661e+43	7.98	7.98	1.485e+38	0.0003
17621	triHPacyl.mmptptmmpu	4.986e+44	8.96	8.96	1.478e+38	0.000298
17622	triHPacyl.pptpmmtmpu	7.904e+43	7.87	7.87	1.460e+38	0.000295
17623	triHPacyl.pptpmmpmu	6.093e+43	7.72	7.72	1.459e+38	0.000295
17624	triHPacyl.ppmtmpmpu	4.227e+43	7.50	7.50	1.448e+38	0.000292
17625	triHPacyl.tmtmtmpmu	1.368e+44	8.21	8.21	1.439e+38	0.00029
17626	triHPacyl.mppppptmmpu	6.115e+43	7.73	7.73	1.437e+38	0.00029
17627	triHPacyl.mppmpptppu	1.751e+43	6.98	6.98	1.434e+38	0.000289
17628	triHPacyl.mtptmmpmu	7.268e+43	7.83	7.83	1.431e+38	0.000289
17629	triHPacyl.ttptmtpmmu	1.489e+44	8.26	8.26	1.426e+38	0.000288
17630	triHPacyl.mtptmtpmu	2.127e+44	8.48	8.48	1.413e+38	0.000285
17631	triHPacyl.tttmpttmmu	2.163e+44	8.49	8.49	1.412e+38	0.000285
17632	triHPacyl.mttmpmpmpu	1.052e+44	8.06	8.06	1.411e+38	0.000285
17633	triHPacyl.pttpptmmpu	1.180e+44	8.13	8.13	1.408e+38	0.000284
17634	triHPacyl.tmppmtpppu	7.070e+43	7.83	7.83	1.407e+38	0.000284
17635	triHPacyl.ptmpmtmmpu	5.426e+43	7.67	7.67	1.406e+38	0.000284
17636	triHPacyl.tmttptmmpu	6.066e+44	9.11	9.11	1.404e+38	0.000283
17637	triHPacyl.mtttpptppu	7.878e+43	7.90	7.90	1.394e+38	0.000281
17638	triHPacyl.mmpptppppu	9.944e+43	8.04	8.04	1.392e+38	0.000281
17639	triHPacyl.ptmmmtppu	1.531e+44	8.29	8.29	1.392e+38	0.000281
17640	triHPacyl.ptmpptppu	2.339e+44	8.55	8.55	1.392e+38	0.000281
17641	triHPacyl.mmtptmmpu	4.137e+44	8.89	8.89	1.385e+38	0.000279
17642	triHPacyl.mptmpmmpu	1.978e+43	7.08	7.08	1.382e+38	0.000279
17643	triHPacyl.pmttptppu	2.508e+44	8.59	8.59	1.379e+38	0.000278
17644	triHPacyl.mtppmmpmu	2.275e+43	7.16	7.16	1.376e+38	0.000278
17645	triHPacyl.ptmpmtmmpu	9.441e+43	8.01	8.01	1.376e+38	0.000278
17646	triHPacyl.tmtmptppu	1.430e+44	8.26	8.26	1.374e+38	0.000277
17647	triHPacyl.mppppptmmpu	6.861e+43	7.83	7.83	1.367e+38	0.000276
17648	triHPacyl.mttmpmmpu	2.910e+44	8.69	8.69	1.363e+38	0.000275
17649	triHPacyl.ttppmmpmu	4.930e+43	7.63	7.63	1.360e+38	0.000275
17650	triHPacyl.tmppptppu	1.023e+44	8.07	8.07	1.351e+38	0.000273
17651	triHPacyl.tmppmpmpu	6.619e+43	7.81	7.81	1.347e+38	0.000272
17652	triHPacyl.ptmtmmpu	6.726e+43	7.82	7.82	1.343e+38	0.000271
17653	triHPacyl.tpptpppu	1.708e+44	8.38	8.38	1.342e+38	0.000271
17654	triHPacyl.ttmmpmmpu	7.044e+43	7.85	7.85	1.337e+38	0.00027
17655	triHPacyl.ttmtmtpu	2.101e+44	8.51	8.51	1.337e+38	0.00027
17656	triHPacyl.tmpmtmpu	4.128e+43	7.54	7.54	1.331e+38	0.000269
17657	triHPacyl.ttmmpmpu	2.671e+43	7.29	7.29	1.316e+38	0.000266
17658	triHPacyl.pptmtpmpu	6.598e+43	7.83	7.83	1.310e+38	0.000264
17659	triHPacyl.pttppmpu	6.491e+43	7.82	7.82	1.307e+38	0.000264
17660	triHPacyl.mmtmtmmpu	3.020e+44	8.74	8.74	1.306e+38	0.000264
17661	triHPacyl.ppmtmtpu	2.521e+44	8.63	8.63	1.306e+38	0.000264
17662	triHPacyl.tpptppmpu	1.536e+44	8.33	8.33	1.304e+38	0.000263
17663	triHPacyl.tttmpmpu	5.324e+43	7.70	7.70	1.303e+38	0.000263
17664	triHPacyl.mppppmpu	3.854e+43	7.51	7.51	1.301e+38	0.000263
17665	triHPacyl.mppptppmu	8.423e+43	7.98	7.98	1.301e+38	0.000262
17666	triHPacyl.pttppmpu	7.102e+43	7.88	7.88	1.296e+38	0.000262
17667	triHPacyl.mtmtmmpu	1.730e+44	8.41	8.41	1.290e+38	0.00026
17668	triHPacyl.mmtmtpu	1.594e+44	8.37	8.37	1.283e+38	0.000259
17669	triHPacyl.mppmmpu	4.245e+43	7.58	7.58	1.268e+38	0.000256
17670	triHPacyl.tmmmpmmpu	5.762e+43	7.77	7.77	1.267e+38	0.000256
17671	triHPacyl.tttmmmpu	2.685e+44	8.68	8.68	1.266e+38	0.000255
17672	triHPacyl.pmpptmmpu	5.792e+44	9.15	9.15	1.261e+38	0.000254
17673	triHPacyl.mppmmtmmpu	2.924e+44	8.74	8.74	1.257e+38	0.000254
17674	triHPacyl.pttmtmpu	2.836e+44	8.72	8.72	1.252e+38	0.000253
17675	triHPacyl.mmpmtpmpu	3.868e+43	7.54	7.54	1.251e+38	0.000252
17676	triHPacyl.mppppmmpu	1.971e+44	8.51	8.51	1.247e+38	0.000252
17677	triHPacyl.tttmtmpu	8.999e+43	8.05	8.05	1.240e+38	0.00025
17678	triHPacyl.pmpmmpu	2.961e+44	8.76	8.76	1.239e+38	0.00025
17679	triHPacyl.tppmtpppu	3.756e+43	7.52	7.52	1.239e+38	0.00025
17680	triHPacyl.ppmtmmpu	5.174e+43	7.72	7.72	1.238e+38	0.00025
17681	triHPacyl.pppppmpu	2.199e+43	7.21	7.21	1.238e+38	0.00025
17682	triHPacyl.mppmtpu	6.278e+43	7.83	7.83	1.237e+38	0.00025
17683	triHPacyl.tpptmpu	2.113e+44	8.56	8.56	1.233e+38	0.000249
17684	triHPacyl.tmppmmpu	5.197e+44	9.09	9.09	1.231e+38	0.000249
17685	triHPacyl.mpppmpu	2.994e+43	7.39	7.39	1.229e+38	0.000248
17686	triHPacyl.ttppmtppu	2.072e+44	8.55	8.55	1.229e+38	0.000248
17687	triHPacyl.ptmtmmpu	2.638e+44	8.69	8.69	1.227e+38	0.000248

17688	triHPacyl.ttppmptmmu	1.694e+44	8.43	8.43	1.225e+38	0.000247
17689	triHPacyl.ptmtmmmmmpu	2.092e+44	8.56	8.56	1.218e+38	0.000246
17690	triHPacyl.mmtmmmtppu	1.792e+44	8.47	8.47	1.215e+38	0.000245
17691	triHPacyl.mtmmpmpmpu	2.427e+43	7.28	7.28	1.212e+38	0.000245
17692	triHPacyl.ptttmmmtmmu	1.513e+44	8.37	8.37	1.208e+38	0.000244
17693	triHPacyl.tmpppmmmmu	5.937e+43	7.82	7.82	1.200e+38	0.000242
17694	triHPacyl.mmpmmmpmpu	9.237e+43	8.08	8.08	1.191e+38	0.00024
17695	triHPacyl.mtpppmtmmu	8.233e+43	8.02	8.02	1.189e+38	0.00024
17696	triHPacyl.ptttmmmpmmu	7.744e+43	7.98	7.98	1.185e+38	0.000239
17697	triHPacyl.mmtmmmtmmu	8.950e+44	9.44	9.44	1.180e+38	0.000238
17698	triHPacyl.mpttptpmmu	9.795e+43	8.13	8.13	1.173e+38	0.000237
17699	triHPacyl.ppttptmppu	2.329e+44	8.65	8.65	1.168e+38	0.000236
17700	triHPacyl.tttppmmmpu	8.567e+43	8.05	8.05	1.167e+38	0.000236
17701	triHPacyl.ppptmtmmmu	9.325e+43	8.10	8.10	1.166e+38	0.000235
17702	triHPacyl.tppppmtmmu	1.324e+45	9.69	9.69	1.163e+38	0.000235
17703	triHPacyl.pmttppmmpu	3.570e+44	8.91	8.91	1.162e+38	0.000234
17704	triHPacyl.tpttmmmmmpu	6.532e+44	9.27	9.27	1.157e+38	0.000234
17705	triHPacyl.ttmptmtpu	2.101e+44	8.59	8.59	1.154e+38	0.000233
17706	triHPacyl.pptppppmpu	2.072e+43	7.21	7.21	1.154e+38	0.000233
17707	triHPacyl.mppmmmpmmu	1.681e+43	7.09	7.09	1.150e+38	0.000232
17708	triHPacyl.pptpmmtpmu	1.158e+44	8.24	8.24	1.148e+38	0.000232
17709	triHPacyl.mmtppmmmpu	1.508e+45	9.77	9.77	1.146e+38	0.000231
17710	triHPacyl.ptpmpmpmmu	4.055e+43	7.62	7.62	1.145e+38	0.000231
17711	triHPacyl.tppmtmmmu	1.466e+44	8.38	8.38	1.143e+38	0.000231
17712	triHPacyl.tmtptmtpu	9.023e+44	9.47	9.47	1.139e+38	0.00023
17713	triHPacyl.tptmptmtpu	7.975e+43	8.03	8.03	1.132e+38	0.000229
17714	triHPacyl.ttppmmpmpu	1.097e+44	8.22	8.22	1.131e+38	0.000228
17715	triHPacyl.mmtmppppmpu	1.185e+44	8.27	8.27	1.124e+38	0.000227
17716	triHPacyl.mtpppmtmmu	2.853e+44	8.80	8.80	1.118e+38	0.000226
17717	triHPacyl.pmmtpmmmmu	4.524e+43	7.70	7.70	1.111e+38	0.000224
17718	triHPacyl.ptmptmtpu	2.036e+44	8.60	8.60	1.108e+38	0.000224
17719	triHPacyl.tpttptpmmu	2.346e+44	8.69	8.69	1.094e+38	0.000221
17720	triHPacyl.tmpmpmmpu	8.552e+43	8.10	8.10	1.081e+38	0.000218
17721	triHPacyl.mtppptmppu	7.245e+43	8.00	8.00	1.081e+38	0.000218
17722	triHPacyl.tttppmtmpu	2.334e+44	8.70	8.70	1.073e+38	0.000217
17723	triHPacyl.tmpmmtpmpu	8.834e+43	8.13	8.13	1.061e+38	0.000214
17724	triHPacyl.ptppptpppu	9.383e+43	8.16	8.16	1.060e+38	0.000214
17725	triHPacyl.ttmtmmtpmu	2.183e+44	8.67	8.67	1.059e+38	0.000214
17726	triHPacyl.mtppmtmpmu	3.259e+43	7.53	7.53	1.058e+38	0.000213
17727	triHPacyl.ttptmmtpu	1.057e+44	8.24	8.24	1.055e+38	0.000213
17728	triHPacyl.pptmmpmmu	2.167e+44	8.67	8.67	1.054e+38	0.000213
17729	triHPacyl.tttmtpppu	1.407e+44	8.41	8.41	1.051e+38	0.000212
17730	triHPacyl.mttmptpmmu	6.340e+43	7.94	7.94	1.037e+38	0.000209
17731	triHPacyl.ptttptppmu	1.184e+44	8.32	8.32	1.036e+38	0.000209
17732	triHPacyl.tmmmmmpu	6.941e+43	8.00	8.00	1.036e+38	0.000209
17733	triHPacyl.tppmptmpu	6.965e+43	8.00	8.00	1.035e+38	0.000209
17734	triHPacyl.mpttptppu	3.838e+43	7.65	7.65	1.033e+38	0.000208
17735	triHPacyl.pmmppptppu	4.205e+43	7.70	7.70	1.031e+38	0.000208
17736	triHPacyl.pppmpmpmmu	5.870e+42	6.53	6.53	1.031e+38	0.000208
17737	triHPacyl.ptptptmtpu	9.205e+43	8.17	8.17	1.031e+38	0.000208
17738	triHPacyl.pppmptmpu	2.983e+43	7.50	7.50	1.028e+38	0.000207
17739	triHPacyl.tpmtptmppu	7.210e+43	8.03	8.03	1.024e+38	0.000207
17740	triHPacyl.tttppptppu	9.930e+43	8.22	8.22	1.016e+38	0.000205
17741	triHPacyl.pppmmtpmmu	5.083e+43	7.83	7.83	1.013e+38	0.000204
17742	triHPacyl.pppmmmmmu	1.177e+43	6.95	6.95	1.012e+38	0.000204
17743	triHPacyl.tttmptmpu	1.520e+44	8.48	8.48	1.008e+38	0.000203
17744	triHPacyl.tpppmtmpu	9.237e+43	8.18	8.18	1.008e+38	0.000203
17745	triHPacyl.ttpppmtmpu	1.444e+44	8.45	8.45	1.002e+38	0.000202
17746	triHPacyl.tpptmmmmmpu	1.561e+44	8.51	8.51	9.933e+37	0.0002
17747	triHPacyl.pmttppmpmmu	1.218e+44	8.36	8.36	9.918e+37	0.0002
17748	triHPacyl.mmpptppppmu	1.186e+44	8.34	8.34	9.917e+37	0.0002
17749	triHPacyl.mtmmmmppu	2.941e+44	8.89	8.89	9.897e+37	0.0002
17750	triHPacyl.mptmmtpmpu	5.407e+43	7.88	7.88	9.885e+37	0.0002
17751	triHPacyl.tmptmtpmmu	3.905e+44	9.06	9.06	9.868e+37	0.000199
17752	triHPacyl.mptmmpmpmu	4.942e+43	7.83	7.83	9.847e+37	0.000199
17753	triHPacyl.mptmptmmpu	7.649e+43	8.09	8.09	9.845e+37	0.000199
17754	triHPacyl.ttppppppmu	5.272e+43	7.87	7.87	9.813e+37	0.000198
17755	triHPacyl.pmpptpmpu	2.640e+43	7.46	7.46	9.770e+37	0.000197
17756	triHPacyl.ttmtmmmtmmu	1.679e+44	8.56	8.56	9.740e+37	0.000197
17757	triHPacyl.tptmptmmpu	1.870e+44	8.63	8.63	9.737e+37	0.000197
17758	triHPacyl.tppmppppmu	1.870e+43	7.25	7.25	9.717e+37	0.000196
17759	triHPacyl.tpptmmmmmu	1.249e+44	8.39	8.39	9.714e+37	0.000196

17760	triHPacyl.ttptmttppu	6.337e+43	7.98	7.98	9.694e+37	0.000196
17761	triHPacyl.ttttmttppu	2.820e+44	8.88	8.88	9.594e+37	0.000194
17762	triHPacyl.mtmmmpmmu	8.065e+44	9.51	9.51	9.567e+37	0.000193
17763	triHPacyl.tpttmppmmu	1.642e+44	8.56	8.56	9.563e+37	0.000193
17764	triHPacyl.pmtmtppmmu	3.856e+43	7.70	7.70	9.436e+37	0.00019
17765	triHPacyl.pmpmmmmmpu	1.660e+44	8.58	8.58	9.376e+37	0.000189
17766	triHPacyl.pttptmmpmu	9.178e+43	8.23	8.23	9.282e+37	0.000187
17767	triHPacyl.ttmmpmtmmu	2.070e+44	8.72	8.72	9.238e+37	0.000186
17768	triHPacyl.mmpmmtmmu	5.054e+43	7.88	7.88	9.218e+37	0.000186
17769	triHPacyl.pttpttmmu	1.837e+44	8.65	8.65	9.205e+37	0.000186
17770	triHPacyl.ppmttppmu	4.753e+43	7.85	7.85	9.134e+37	0.000184
17771	triHPacyl.tmtmtmppu	1.930e+44	8.68	8.68	9.102e+37	0.000184
17772	triHPacyl.mptpmppmmu	7.105e+43	8.09	8.09	9.080e+37	0.000183
17773	triHPacyl.ptmmmtppmu	6.490e+44	9.41	9.41	9.056e+37	0.000183
17774	triHPacyl.tttmpmtppu	7.894e+43	8.16	8.16	9.036e+37	0.000182
17775	triHPacyl.ppttmppppu	6.509e+43	8.04	8.04	9.031e+37	0.000182
17776	triHPacyl.mpmtppmpmu	1.057e+44	8.33	8.33	9.019e+37	0.000182
17777	triHPacyl.pttmmppmu	1.099e+44	8.36	8.36	8.995e+37	0.000182
17778	triHPacyl.tppmpppmu	3.640e+43	7.70	7.70	8.993e+37	0.000182
17779	triHPacyl.ttptmtmmpu	4.054e+43	7.76	7.76	8.973e+37	0.000181
17780	triHPacyl.tptmttppmu	2.028e+44	8.73	8.73	8.924e+37	0.00018
17781	triHPacyl.tmpmtppmu	2.746e+44	8.91	8.91	8.886e+37	0.000179
17782	triHPacyl.tmppmmtppu	3.496e+44	9.05	9.05	8.857e+37	0.000179
17783	triHPacyl.pppmmmtppu	4.130e+43	7.78	7.78	8.839e+37	0.000178
17784	triHPacyl.ptmppmmmpu	3.803e+44	9.11	9.11	8.830e+37	0.000178
17785	triHPacyl.tptmtppmu	2.616e+44	8.88	8.88	8.825e+37	0.000178
17786	triHPacyl.ttmmmmmmpu	1.340e+44	8.49	8.49	8.810e+37	0.000178
17787	triHPacyl.ttpmmmpppu	7.080e+43	8.11	8.11	8.784e+37	0.000177
17788	triHPacyl.tmmtppppu	8.143e+43	8.19	8.19	8.756e+37	0.000177
17789	triHPacyl.mpmtppmmmpu	5.195e+43	7.93	7.93	8.737e+37	0.000176
17790	triHPacyl.pptpmpmpu	4.261e+43	7.82	7.82	8.591e+37	0.000173
17791	triHPacyl.tpmttppmu	7.731e+43	8.17	8.17	8.585e+37	0.000173
17792	triHPacyl.tmpmmmpmmu	5.709e+43	8.00	8.00	8.491e+37	0.000171
17793	triHPacyl.tttmtmmtmmu	1.080e+44	8.38	8.38	8.482e+37	0.000171
17794	triHPacyl.ttptmmpmu	6.221e+43	8.05	8.05	8.440e+37	0.00017
17795	triHPacyl.mppppptppmu	7.548e+43	8.17	8.17	8.404e+37	0.00017
17796	triHPacyl.ptptptppmu	3.165e+44	9.03	9.03	8.394e+37	0.000169
17797	triHPacyl.mttmmtppmu	1.094e+44	8.39	8.39	8.383e+37	0.000169
17798	triHPacyl.ttmpppptpmu	7.152e+43	8.14	8.14	8.362e+37	0.000169
17799	triHPacyl.tppmmpmpmu	4.383e+43	7.85	7.85	8.348e+37	0.000168
17800	triHPacyl.ptptmmmmmpu	2.864e+44	8.97	8.97	8.333e+37	0.000168
17801	triHPacyl.pmpmtmmpmu	5.565e+43	8.00	8.00	8.306e+37	0.000168
17802	triHPacyl.mmtmmtmmpu	3.689e+43	7.75	7.75	8.283e+37	0.000167
17803	triHPacyl.tmtppmtmmu	2.691e+44	8.94	8.94	8.266e+37	0.000167
17804	triHPacyl.pmmmpmtppmu	4.017e+43	7.81	7.81	8.238e+37	0.000166
17805	triHPacyl.pppmtmmpmu	9.203e+43	8.30	8.30	8.213e+37	0.000166
17806	triHPacyl.mptmptppmu	2.010e+43	7.40	7.40	8.200e+37	0.000165
17807	triHPacyl.pppmmmtmmu	1.564e+43	7.25	7.25	8.185e+37	0.000165
17808	triHPacyl.tttmptppu	1.363e+44	8.54	8.54	8.166e+37	0.000165
17809	triHPacyl.tmpmtmppmu	2.727e+44	8.96	8.96	8.083e+37	0.000163
17810	triHPacyl.tmpmtmpppu	8.060e+43	8.24	8.24	7.958e+37	0.000161
17811	triHPacyl.ttmmmmpppmu	5.462e+43	8.01	8.01	7.955e+37	0.000161
17812	triHPacyl.ptptppmmmu	1.169e+44	8.47	8.47	7.930e+37	0.00016
17813	triHPacyl.tttmmtmmu	1.383e+44	8.57	8.57	7.924e+37	0.00016
17814	triHPacyl.mtppmpmpmu	2.748e+44	8.98	8.98	7.921e+37	0.00016
17815	triHPacyl.ppppmppppu	9.409e+43	8.34	8.34	7.873e+37	0.000159
17816	triHPacyl.tptpmmtppu	1.601e+44	8.66	8.66	7.823e+37	0.000158
17817	triHPacyl.tmmmpmtppu	1.530e+43	7.26	7.26	7.814e+37	0.000158
17818	triHPacyl.mttppmtmmu	1.337e+44	8.56	8.56	7.771e+37	0.000157
17819	triHPacyl.pppmmpmmpmu	1.428e+43	7.23	7.23	7.763e+37	0.000157
17820	triHPacyl.pptmptmmmu	3.722e+44	9.17	9.17	7.729e+37	0.000156
17821	triHPacyl.tppmtmmpmu	1.399e+44	8.59	8.59	7.692e+37	0.000155
17822	triHPacyl.mmmmmppppu	2.276e+43	7.51	7.51	7.682e+37	0.000155
17823	triHPacyl.pmtmmtppmu	9.407e+43	8.36	8.36	7.675e+37	0.000155
17824	triHPacyl.mpmtppmmpmu	4.128e+43	7.87	7.87	7.671e+37	0.000155
17825	triHPacyl.pppmpttmmu	5.355e+43	8.03	8.03	7.607e+37	0.000154
17826	triHPacyl.mptmmpmmpmu	4.788e+44	9.33	9.33	7.599e+37	0.000153
17827	triHPacyl.ttttmtppmu	1.183e+44	8.51	8.51	7.499e+37	0.000151
17828	triHPacyl.pmmtpmmpmu	3.585e+43	7.80	7.80	7.498e+37	0.000151
17829	triHPacyl.ttppmtmmpmu	1.567e+44	8.68	8.68	7.488e+37	0.000151
17830	triHPacyl.mmttptppmu	1.325e+45	9.95	9.95	7.458e+37	0.000151
17831	triHPacyl.tppppmmpmu	8.427e+43	8.31	8.31	7.438e+37	0.00015

17832	triHPacyl.mpptmtppmu	1.230e+44	8.54	8.54	7.381e+37	0.000149
17833	triHPacyl.tmttpttpmu	3.882e+44	9.23	9.23	7.375e+37	0.000149
17834	triHPacyl.mmmmtmtppmu	8.302e+43	8.31	8.31	7.374e+37	0.000149
17835	triHPacyl.mptmtmtppmu	1.456e+44	8.64	8.64	7.345e+37	0.000148
17836	triHPacyl.tmttptppmu	2.284e+44	8.92	8.92	7.316e+37	0.000148
17837	triHPacyl.ttpppmppmu	1.257e+44	8.56	8.56	7.259e+37	0.000147
17838	triHPacyl.ptmtptppu	8.682e+43	8.34	8.34	7.241e+37	0.000146
17839	triHPacyl.tpttmmppmu	8.849e+43	8.36	8.36	7.192e+37	0.000145
17840	triHPacyl.mptpmtmmu	2.485e+43	7.61	7.61	7.159e+37	0.000145
17841	triHPacyl.tptmtmmpu	6.124e+43	8.15	8.15	7.135e+37	0.000144
17842	triHPacyl.mmmmtmtppu	8.525e+43	8.34	8.34	7.116e+37	0.000144
17843	triHPacyl.ttptmtmpu	2.374e+44	8.96	8.96	7.056e+37	0.000142
17844	triHPacyl.mpptmtmpu	8.798e+43	8.37	8.37	7.009e+37	0.000141
17845	triHPacyl.tttptppmu	4.468e+43	7.98	7.98	6.906e+37	0.000139
17846	triHPacyl.mppmptmmu	4.098e+43	7.93	7.93	6.874e+37	0.000139
17847	triHPacyl.tmtptmpu	5.136e+43	8.06	8.06	6.856e+37	0.000138
17848	triHPacyl.tpmmtmpu	4.010e+43	7.92	7.92	6.840e+37	0.000138
17849	triHPacyl.tmttptmmu	8.361e+44	9.73	9.73	6.804e+37	0.000137
17850	triHPacyl.mpptptmpu	8.393e+43	8.36	8.36	6.800e+37	0.000137
17851	triHPacyl.tmpptmpu	1.804e+44	8.82	8.82	6.796e+37	0.000137
17852	triHPacyl.ptpmmtpu	9.133e+43	8.41	8.41	6.791e+37	0.000137
17853	triHPacyl.ttptmtmpu	2.784e+44	9.08	9.08	6.790e+37	0.000137
17854	triHPacyl.pptmptppu	5.371e+43	8.10	8.10	6.761e+37	0.000136
17855	triHPacyl.mmtmmmmmu	7.014e+44	9.63	9.63	6.754e+37	0.000136
17856	triHPacyl.ptmtptmpu	2.256e+44	8.96	8.96	6.721e+37	0.000136
17857	triHPacyl.mttmptmpu	3.480e+43	7.85	7.85	6.705e+37	0.000135
17858	triHPacyl.ttmmtpppu	4.375e+43	7.99	7.99	6.615e+37	0.000134
17859	triHPacyl.ptmpmtmpu	3.985e+44	9.31	9.31	6.584e+37	0.000133
17860	triHPacyl.mptppppmu	1.233e+44	8.61	8.61	6.581e+37	0.000133
17861	triHPacyl.pmmppptmpu	4.070e+43	7.95	7.95	6.557e+37	0.000132
17862	triHPacyl.tttpttpu	2.369e+44	9.00	9.00	6.531e+37	0.000132
17863	triHPacyl.ttptmtmpu	1.304e+44	8.65	8.65	6.525e+37	0.000132
17864	triHPacyl.mpppmmppu	8.552e+43	8.40	8.40	6.511e+37	0.000131
17865	triHPacyl.pppmmtpmu	3.263e+43	7.82	7.82	6.508e+37	0.000131
17866	triHPacyl.pmpmtmmu	1.560e+44	8.76	8.76	6.497e+37	0.000131
17867	triHPacyl.tptmtmpu	1.191e+44	8.60	8.60	6.494e+37	0.000131
17868	triHPacyl.mtpmmpmpu	4.170e+43	7.97	7.97	6.477e+37	0.000131
17869	triHPacyl.mppmmtppu	7.667e+43	8.34	8.34	6.451e+37	0.00013
17870	triHPacyl.mtmmmpmpu	2.200e+43	7.60	7.60	6.439e+37	0.00013
17871	triHPacyl.mmttmmtmmu	4.189e+44	9.35	9.35	6.427e+37	0.00013
17872	triHPacyl.pttpmtmpu	1.183e+44	8.60	8.60	6.401e+37	0.000129
17873	triHPacyl.mptmpmpmpu	3.437e+43	7.87	7.87	6.396e+37	0.000129
17874	triHPacyl.ttptmtpppu	3.825e+43	7.93	7.93	6.356e+37	0.000128
17875	triHPacyl.mptmpppmu	5.566e+43	8.16	8.16	6.327e+37	0.000128
17876	triHPacyl.tmmmpmtppu	8.669e+43	8.43	8.43	6.263e+37	0.000126
17877	triHPacyl.mttmmmtppu	1.632e+44	8.81	8.81	6.262e+37	0.000126
17878	triHPacyl.ptmmtpmpu	3.914e+43	7.96	7.96	6.236e+37	0.000126
17879	triHPacyl.tpmtmmpmu	4.906e+43	8.09	8.09	6.225e+37	0.000126
17880	triHPacyl.ptptmtppmu	1.783e+44	8.86	8.86	6.219e+37	0.000126
17881	triHPacyl.ttmptmtmmu	1.065e+44	8.56	8.56	6.217e+37	0.000125
17882	triHPacyl.tmpmmmmmpu	1.270e+44	8.66	8.66	6.205e+37	0.000125
17883	triHPacyl.ptmppptmpu	2.483e+43	7.69	7.69	6.191e+37	0.000125
17884	triHPacyl.pppmptmmu	3.151e+43	7.84	7.84	6.141e+37	0.000124
17885	triHPacyl.mppmmtmpu	3.383e+44	9.26	9.26	6.119e+37	0.000124
17886	triHPacyl.pttppmmmu	2.855e+44	9.16	9.16	6.103e+37	0.000123
17887	triHPacyl.ttmmpmtmpu	9.844e+43	8.52	8.52	6.092e+37	0.000123
17888	triHPacyl.pmttptmpu	7.498e+43	8.37	8.37	5.995e+37	0.000121
17889	triHPacyl.tmttptmpu	6.072e+44	9.62	9.62	5.987e+37	0.000121
17890	triHPacyl.mpmtpptppu	2.749e+44	9.15	9.15	5.961e+37	0.00012
17891	triHPacyl.mtmtptppmu	5.808e+43	8.22	8.22	5.948e+37	0.00012
17892	triHPacyl.tpmmttmmu	6.402e+43	8.28	8.28	5.933e+37	0.00012
17893	triHPacyl.mpttppmmu	1.621e+44	8.84	8.84	5.908e+37	0.000119
17894	triHPacyl.pppppmpmpu	4.529e+43	8.08	8.08	5.881e+37	0.000119
17895	triHPacyl.mptmtpppmu	4.687e+43	8.10	8.10	5.859e+37	0.000118
17896	triHPacyl.ppppmmmpu	7.737e+43	8.40	8.40	5.858e+37	0.000118
17897	triHPacyl.pttppmmmpu	3.466e+44	9.30	9.30	5.823e+37	0.000118
17898	triHPacyl.tmtmptmpu	1.400e+44	8.76	8.76	5.806e+37	0.000117
17899	triHPacyl.ttmppmtpu	1.021e+44	8.57	8.57	5.794e+37	0.000117
17900	triHPacyl.ppmmtmpu	1.675e+44	8.87	8.87	5.780e+37	0.000117
17901	triHPacyl.tppppmtppu	6.381e+44	9.67	9.67	5.768e+37	0.000116
17902	triHPacyl.mmtmmmmmpu	2.004e+45	10.36	10.36	5.692e+37	0.000115
17903	triHPacyl.tpmmmmmmpu	3.045e+43	7.86	7.86	5.679e+37	0.000115

17904	triHPacyl.tppppppmpu	1.952e+44	8.97	8.97	5.659e+37	0.000114
17905	triHPacyl.ttmtmmmmu	6.704e+43	8.34	8.34	5.634e+37	0.000114
17906	triHPacyl.ttpmmpppu	5.775e+43	8.25	8.25	5.613e+37	0.000113
17907	triHPacyl.pmpmtppmu	1.745e+44	8.91	8.91	5.598e+37	0.000113
17908	triHPacyl.mmttmpppu	1.423e+44	8.79	8.79	5.580e+37	0.000113
17909	triHPacyl.pmpmmmpmu	1.316e+43	7.38	7.38	5.572e+37	0.000112
17910	triHPacyl.tppppmtmpu	1.334e+45	10.13	10.13	5.571e+37	0.000112
17911	triHPacyl.tmmtpmpu	1.026e+44	8.60	8.60	5.540e+37	0.000112
17912	triHPacyl.mppptmmpu	4.807e+43	8.15	8.15	5.530e+37	0.000112
17913	triHPacyl.pptmtpmu	2.793e+44	9.20	9.20	5.512e+37	0.000111
17914	triHPacyl.mptmppppmu	3.118e+43	7.90	7.90	5.472e+37	0.00011
17915	triHPacyl.tmpmmppmu	6.485e+43	8.34	8.34	5.437e+37	0.00011
17916	triHPacyl.pmtmtpmpu	1.034e+44	8.62	8.62	5.420e+37	0.000109
17917	triHPacyl.pppmtmpmu	2.150e+44	9.06	9.06	5.413e+37	0.000109
17918	triHPacyl.tmtmtpmu	9.533e+44	9.95	9.95	5.404e+37	0.000109
17919	triHPacyl.tpppmmmmu	1.680e+44	8.91	8.91	5.403e+37	0.000109
17920	triHPacyl.pmmmtmpu	7.608e+43	8.44	8.44	5.392e+37	0.000109
17921	triHPacyl.tpppptpmu	1.107e+44	8.67	8.67	5.343e+37	0.000108
17922	triHPacyl.tttmtmmu	2.717e+44	9.21	9.21	5.326e+37	0.000108
17923	triHPacyl.tppmtppu	2.142e+44	9.07	9.07	5.325e+37	0.000107
17924	triHPacyl.pmpmtmpu	1.372e+44	8.80	8.80	5.316e+37	0.000107
17925	triHPacyl.pmmptmmu	7.485e+43	8.44	8.44	5.295e+37	0.000107
17926	triHPacyl.pppmmppmu	3.167e+43	7.93	7.93	5.289e+37	0.000107
17927	triHPacyl.tppppmpu	1.336e+44	8.79	8.79	5.261e+37	0.000106
17928	triHPacyl.pptppppu	1.018e+44	8.63	8.63	5.252e+37	0.000106
17929	triHPacyl.mtmmmpmu	3.193e+44	9.31	9.31	5.245e+37	0.000106
17930	triHPacyl.tttptmmu	7.722e+43	8.47	8.47	5.241e+37	0.000106
17931	triHPacyl.mptmtpmpu	3.100e+43	7.93	7.93	5.174e+37	0.000104
17932	triHPacyl.pptmmtmpu	3.236e+43	7.96	7.96	5.165e+37	0.000104
17933	triHPacyl.pmpptmpu	1.608e+43	7.54	7.54	5.149e+37	0.000104
17934	triHPacyl.ttmmtpmu	2.772e+44	9.24	9.24	5.124e+37	0.000103
17935	triHPacyl.tppmmppmu	2.726e+43	7.86	7.86	5.086e+37	0.000103
17936	triHPacyl.ptmpmpmpu	6.962e+43	8.42	8.42	5.085e+37	0.000103
17937	triHPacyl.tmtmmmpu	1.490e+44	8.88	8.88	5.040e+37	0.000102
17938	triHPacyl.tmpmtpmpu	5.504e+43	8.29	8.29	5.018e+37	0.000101
17939	triHPacyl.mpmtpmpmu	6.348e+43	8.38	8.38	5.012e+37	0.000101
17940	triHPacyl.tmmtpmpmu	2.887e+43	7.91	7.91	4.997e+37	0.000101
17941	triHPacyl.mmpptmpmu	7.095e+43	8.45	8.45	4.936e+37	9.96e-05
17942	triHPacyl.mttptmpmu	1.282e+44	8.81	8.81	4.919e+37	9.93e-05
17943	triHPacyl.ppttpppu	1.233e+44	8.79	8.79	4.906e+37	9.9e-05
17944	triHPacyl.ptmpmtmpu	8.515e+43	8.57	8.57	4.881e+37	9.85e-05
17945	triHPacyl.tttmmmpmu	6.936e+43	8.45	8.45	4.858e+37	9.81e-05
17946	triHPacyl.tppmmppmu	1.087e+44	8.72	8.72	4.845e+37	9.78e-05
17947	triHPacyl.tpmmtmpmu	9.733e+43	8.65	8.65	4.828e+37	9.75e-05
17948	triHPacyl.pptmtpmpu	4.464e+43	8.19	8.19	4.808e+37	9.7e-05
17949	triHPacyl.pppmtpmpu	2.565e+43	7.86	7.86	4.805e+37	9.7e-05
17950	triHPacyl.mtmtptmpu	8.084e+43	8.55	8.55	4.790e+37	9.67e-05
17951	triHPacyl.tmpmpmtmpu	1.105e+44	8.74	8.74	4.778e+37	9.64e-05
17952	triHPacyl.ttmptmpu	1.075e+44	8.73	8.73	4.728e+37	9.54e-05
17953	triHPacyl.tppmpmpu	7.386e+43	8.50	8.50	4.728e+37	9.54e-05
17954	triHPacyl.ptmpmpmpu	5.125e+44	9.66	9.66	4.710e+37	9.51e-05
17955	triHPacyl.pptmmtmpu	7.409e+43	8.51	8.51	4.677e+37	9.44e-05
17956	triHPacyl.tppmpmpu	7.813e+44	9.92	9.92	4.652e+37	9.39e-05
17957	triHPacyl.mmtmtpmpu	1.099e+45	10.12	10.12	4.635e+37	9.35e-05
17958	triHPacyl.mpppptpu	1.186e+44	8.80	8.80	4.633e+37	9.35e-05
17959	triHPacyl.tppppppmu	2.296e+44	9.19	9.19	4.629e+37	9.34e-05
17960	triHPacyl.mtmptmpu	6.823e+43	8.47	8.47	4.587e+37	9.26e-05
17961	triHPacyl.tppppmpmu	3.465e+43	8.07	8.07	4.564e+37	9.21e-05
17962	triHPacyl.ttmptmpu	1.201e+44	8.81	8.81	4.559e+37	9.2e-05
17963	triHPacyl.pppmtmpu	1.531e+44	8.96	8.96	4.553e+37	9.19e-05
17964	triHPacyl.mtmppppmu	4.340e+43	8.21	8.21	4.540e+37	9.16e-05
17965	triHPacyl.ttpmtmpu	1.266e+44	8.85	8.85	4.524e+37	9.13e-05
17966	triHPacyl.ttmtmtmpu	1.619e+44	9.00	9.00	4.520e+37	9.12e-05
17967	triHPacyl.tmpmtmpu	5.876e+44	9.77	9.77	4.503e+37	9.09e-05
17968	triHPacyl.tppmptmpu	1.266e+45	10.23	10.23	4.500e+37	9.08e-05
17969	triHPacyl.mmtmtpmpu	2.560e+44	9.28	9.28	4.455e+37	8.99e-05
17970	triHPacyl.tpmtmpmpu	9.884e+43	8.71	8.71	4.442e+37	8.97e-05
17971	triHPacyl.tttmtmpu	3.319e+44	9.44	9.44	4.438e+37	8.96e-05
17972	triHPacyl.pmpmtmpu	1.701e+43	7.67	7.67	4.428e+37	8.94e-05
17973	triHPacyl.ptmtmtpmu	1.005e+45	10.10	10.10	4.415e+37	8.91e-05
17974	triHPacyl.mptpmpmpu	1.067e+44	8.77	8.77	4.374e+37	8.83e-05
17975	triHPacyl.pmttptmpu	1.704e+44	9.05	9.05	4.338e+37	8.76e-05

17976	triHPacyl.ttmtmmmpu	1.675e+44	9.04	9.04	4.337e+37	8.75e-05
17977	triHPacyl.mmpmmmtmpu	8.150e+43	8.61	8.61	4.332e+37	8.74e-05
17978	triHPacyl.ttmtmpmmu	1.150e+44	8.83	8.83	4.272e+37	8.62e-05
17979	triHPacyl.ptmtmpmpu	4.892e+43	8.32	8.32	4.271e+37	8.62e-05
17980	triHPacyl.pptppmmmpu	5.218e+43	8.36	8.36	4.266e+37	8.61e-05
17981	triHPacyl.ptmpmmmpu	1.573e+44	9.02	9.02	4.247e+37	8.57e-05
17982	triHPacyl.tpmpmmmpu	2.602e+43	7.95	7.95	4.229e+37	8.54e-05
17983	triHPacyl.pptpmtmpu	4.413e+43	8.26	8.26	4.227e+37	8.53e-05
17984	triHPacyl.tttmmmmmpu	7.034e+43	8.54	8.54	4.224e+37	8.53e-05
17985	triHPacyl.tptppmpu	7.500e+43	8.58	8.58	4.195e+37	8.47e-05
17986	triHPacyl.ttmmpmtppu	2.599e+44	9.33	9.33	4.176e+37	8.43e-05
17987	triHPacyl.mpttpmpu	1.010e+44	8.76	8.76	4.173e+37	8.42e-05
17988	triHPacyl.ttpptmmu	1.046e+44	8.78	8.78	4.170e+37	8.42e-05
17989	triHPacyl.tmtptmpu	6.370e+44	9.86	9.86	4.158e+37	8.39e-05
17990	triHPacyl.ppptppmpu	6.076e+44	9.84	9.84	4.145e+37	8.37e-05
17991	triHPacyl.mppmppppu	1.814e+43	7.74	7.74	4.144e+37	8.36e-05
17992	triHPacyl.mtmmmtmpu	8.608e+43	8.67	8.67	4.142e+37	8.36e-05
17993	triHPacyl.mptpmmmpu	3.693e+43	8.17	8.17	4.127e+37	8.33e-05
17994	triHPacyl.mmmmtmpu	1.510e+44	9.01	9.01	4.106e+37	8.29e-05
17995	triHPacyl.mttppmpu	3.278e+43	8.10	8.10	4.098e+37	8.27e-05
17996	triHPacyl.tmtmtmpu	6.641e+44	9.90	9.90	4.081e+37	8.24e-05
17997	triHPacyl.mtppppmpu	2.494e+43	7.94	7.94	4.081e+37	8.24e-05
17998	triHPacyl.mptpmtmpu	1.151e+44	8.86	8.86	4.073e+37	8.22e-05
17999	triHPacyl.tmtmpmmu	3.221e+44	9.47	9.47	4.067e+37	8.21e-05
18000	triHPacyl.pmmmtmpu	3.502e+43	8.15	8.15	4.053e+37	8.18e-05
18001	triHPacyl.pmpmtmpu	1.451e+43	7.62	7.62	4.049e+37	8.17e-05
18002	triHPacyl.mmmmtmpu	3.574e+43	8.16	8.16	4.048e+37	8.17e-05
18003	triHPacyl.pptmtmpu	2.660e+44	9.36	9.36	4.048e+37	8.17e-05
18004	triHPacyl.pptmtmmu	1.069e+44	8.82	8.82	4.032e+37	8.14e-05
18005	triHPacyl.tpptptmpu	2.050e+45	10.58	10.58	4.029e+37	8.13e-05
18006	triHPacyl.mptmmmtmpu	6.694e+43	8.54	8.54	4.027e+37	8.13e-05
18007	triHPacyl.tmpmtmpu	1.213e+44	8.89	8.89	4.024e+37	8.12e-05
18008	triHPacyl.tptpmtppu	1.259e+44	8.92	8.92	3.992e+37	8.06e-05
18009	triHPacyl.ptmpmtmpu	1.455e+44	9.01	9.01	3.982e+37	8.04e-05
18010	triHPacyl.tptppmpu	1.514e+44	9.03	9.03	3.967e+37	8.01e-05
18011	triHPacyl.pttmtmpu	1.165e+44	8.88	8.88	3.945e+37	7.96e-05
18012	triHPacyl.pmpptpppu	3.077e+43	8.09	8.09	3.905e+37	7.88e-05
18013	triHPacyl.mppptmpu	5.976e+43	8.49	8.49	3.894e+37	7.86e-05
18014	triHPacyl.mtppptmpu	2.472e+43	7.97	7.97	3.877e+37	7.83e-05
18015	triHPacyl.pttppppmpu	6.934e+43	8.58	8.58	3.874e+37	7.82e-05
18016	triHPacyl.mttptmpu	1.417e+44	9.01	9.01	3.870e+37	7.81e-05
18017	triHPacyl.pptmmtpu	2.988e+44	9.46	9.46	3.846e+37	7.76e-05
18018	triHPacyl.pppmmtmpu	2.611e+44	9.38	9.38	3.846e+37	7.76e-05
18019	triHPacyl.tttmtmpu	6.946e+43	8.59	8.59	3.839e+37	7.75e-05
18020	triHPacyl.tmpptpppu	4.205e+43	8.29	8.29	3.830e+37	7.73e-05
18021	triHPacyl.mpmmtmpu	1.482e+43	7.67	7.67	3.830e+37	7.73e-05
18022	triHPacyl.mmpptmpu	4.248e+44	9.67	9.67	3.829e+37	7.73e-05
18023	triHPacyl.ttmtmpmpu	1.020e+44	8.83	8.83	3.790e+37	7.65e-05
18024	triHPacyl.ttpmmmmmpu	5.433e+43	8.45	8.45	3.783e+37	7.63e-05
18025	triHPacyl.ptmtppppu	9.358e+43	8.78	8.78	3.782e+37	7.63e-05
18026	triHPacyl.mmtmpmpu	2.194e+44	9.29	9.29	3.758e+37	7.58e-05
18027	triHPacyl.tttptmpu	8.030e+43	8.69	8.69	3.753e+37	7.57e-05
18028	triHPacyl.tmtptmpu	9.483e+43	8.79	8.79	3.741e+37	7.55e-05
18029	triHPacyl.pptmtmpu	3.339e+44	9.54	9.54	3.730e+37	7.53e-05
18030	triHPacyl.tpmpmtmpu	4.236e+43	8.31	8.31	3.714e+37	7.5e-05
18031	triHPacyl.tmtpmtppu	1.101e+44	8.89	8.89	3.695e+37	7.46e-05
18032	triHPacyl.pppmpmpu	9.769e+42	7.44	7.44	3.693e+37	7.45e-05
18033	triHPacyl.tptmmmmmpu	4.729e+43	8.39	8.39	3.627e+37	7.32e-05
18034	triHPacyl.mmmmtmpu	4.868e+43	8.41	8.41	3.615e+37	7.3e-05
18035	triHPacyl.pptmmmpu	8.468e+43	8.74	8.74	3.611e+37	7.29e-05
18036	triHPacyl.ptmtptmpu	2.633e+44	9.42	9.42	3.602e+37	7.27e-05
18037	triHPacyl.pptptppu	2.199e+44	9.32	9.32	3.597e+37	7.26e-05
18038	triHPacyl.tptmtmpu	2.752e+44	9.45	9.45	3.589e+37	7.24e-05
18039	triHPacyl.pptmtmmu	2.161e+44	9.31	9.31	3.585e+37	7.23e-05
18040	triHPacyl.ttpppmtmpu	2.025e+44	9.27	9.27	3.583e+37	7.23e-05
18041	triHPacyl.ptptptmpu	2.089e+44	9.29	9.29	3.578e+37	7.22e-05
18042	triHPacyl.tmtmtmpu	3.067e+44	9.52	9.52	3.556e+37	7.18e-05
18043	triHPacyl.mmpmtmpu	1.224e+44	8.98	8.98	3.534e+37	7.13e-05
18044	triHPacyl.mmtmmtpu	2.090e+44	9.30	9.30	3.526e+37	7.12e-05
18045	triHPacyl.pmpmtppu	1.701e+44	9.17	9.17	3.526e+37	7.12e-05
18046	triHPacyl.mppmtmpu	2.781e+43	8.10	8.10	3.518e+37	7.1e-05
18047	triHPacyl.mppmtmpu	2.070e+44	9.30	9.30	3.499e+37	7.06e-05

18048	triHPacyl.mtppppppmpu	4.844e+43	8.43	8.43	3.495e+37	7.05e-05
18049	triHPacyl.mmmppmmmmmu	8.434e+43	8.76	8.76	3.492e+37	7.05e-05
18050	triHPacyl.tttpmttmmu	2.656e+44	9.45	9.45	3.481e+37	7.03e-05
18051	triHPacyl.tttppmpppu	1.277e+44	9.02	9.02	3.404e+37	6.87e-05
18052	triHPacyl.pptpmtppu	8.356e+43	8.77	8.77	3.386e+37	6.83e-05
18053	triHPacyl.mmmmtppppu	1.117e+44	8.95	8.95	3.373e+37	6.81e-05
18054	triHPacyl.pptmtmtppu	1.513e+44	9.13	9.13	3.366e+37	6.79e-05
18055	triHPacyl.ppppmtppu	3.944e+43	8.33	8.33	3.358e+37	6.78e-05
18056	triHPacyl.ttmtmtppu	4.935e+44	9.84	9.84	3.332e+37	6.73e-05
18057	triHPacyl.mptmttppu	7.634e+43	8.73	8.73	3.326e+37	6.71e-05
18058	triHPacyl.pptppmmppu	8.844e+43	8.83	8.83	3.293e+37	6.65e-05
18059	triHPacyl.ptmmpmtppu	7.014e+43	8.69	8.69	3.286e+37	6.63e-05
18060	triHPacyl.mptmpttmmu	5.042e+43	8.49	8.49	3.268e+37	6.6e-05
18061	triHPacyl.mptpmttppu	4.508e+43	8.43	8.43	3.267e+37	6.59e-05
18062	triHPacyl.tmpmmtppu	5.947e+43	8.59	8.59	3.264e+37	6.59e-05
18063	triHPacyl.tttmpttmmu	1.836e+44	9.27	9.27	3.259e+37	6.58e-05
18064	triHPacyl.pmttptppu	9.394e+43	8.87	8.87	3.252e+37	6.56e-05
18065	triHPacyl.mptmttmmu	1.662e+44	9.21	9.21	3.237e+37	6.53e-05
18066	triHPacyl.ttttptppu	1.863e+44	9.28	9.28	3.212e+37	6.48e-05
18067	triHPacyl.ttpppmmpu	4.373e+43	8.42	8.42	3.210e+37	6.48e-05
18068	triHPacyl.pptmmpmpu	2.677e+43	8.13	8.13	3.208e+37	6.48e-05
18069	triHPacyl.tppttppu	8.808e+44	10.21	10.21	3.207e+37	6.47e-05
18070	triHPacyl.tpmttmmu	1.307e+44	9.07	9.07	3.205e+37	6.47e-05
18071	triHPacyl.pmmpmtppu	8.185e+43	8.80	8.80	3.202e+37	6.46e-05
18072	triHPacyl.mtttptmmpu	1.709e+44	9.24	9.24	3.200e+37	6.46e-05
18073	triHPacyl.pmpmtmmmpu	4.594e+44	9.83	9.83	3.196e+37	6.45e-05
18074	triHPacyl.mmpptppmpu	8.419e+43	8.82	8.82	3.188e+37	6.44e-05
18075	triHPacyl.ptpmpmtppu	1.182e+44	9.02	9.02	3.172e+37	6.4e-05
18076	triHPacyl.ptptmptmmu	4.254e+44	9.78	9.78	3.170e+37	6.4e-05
18077	triHPacyl.tttmmpmpu	9.648e+43	8.90	8.90	3.155e+37	6.37e-05
18078	triHPacyl.tmtpptppu	2.865e+44	9.55	9.55	3.154e+37	6.37e-05
18079	triHPacyl.tmmppttppu	5.279e+43	8.54	8.54	3.149e+37	6.35e-05
18080	triHPacyl.ttmtmtppu	9.092e+43	8.87	8.87	3.142e+37	6.34e-05
18081	triHPacyl.tmmpppppu	2.476e+43	8.10	8.10	3.124e+37	6.3e-05
18082	triHPacyl.pmppttppu	1.512e+43	7.81	7.81	3.114e+37	6.29e-05
18083	triHPacyl.tpppppppu	8.977e+43	8.87	8.87	3.103e+37	6.26e-05
18084	triHPacyl.tmpmtpppu	5.477e+43	8.58	8.58	3.097e+37	6.25e-05
18085	triHPacyl.pmpmpmpmu	4.146e+43	8.41	8.41	3.088e+37	6.23e-05
18086	triHPacyl.ptttptmmpu	3.352e+44	9.66	9.66	3.071e+37	6.2e-05
18087	triHPacyl.mtmmpptppu	6.470e+43	8.68	8.68	3.063e+37	6.18e-05
18088	triHPacyl.pptmtmmpu	1.831e+44	9.31	9.31	3.033e+37	6.12e-05
18089	triHPacyl.tpmppttppu	1.182e+44	9.05	9.05	3.029e+37	6.11e-05
18090	triHPacyl.mpmmtmmpu	1.482e+43	7.81	7.81	3.012e+37	6.08e-05
18091	triHPacyl.mptmpttppu	4.175e+43	8.43	8.43	3.008e+37	6.07e-05
18092	triHPacyl.tmpppmtmmu	1.051e+44	8.98	8.98	3.007e+37	6.07e-05
18093	triHPacyl.pmtmmmpmpu	9.454e+43	8.92	8.92	2.994e+37	6.04e-05
18094	triHPacyl.ttmtmtmmpu	9.541e+44	10.30	10.30	2.976e+37	6.01e-05
18095	triHPacyl.ttpptppmu	9.807e+43	8.95	8.95	2.966e+37	5.99e-05
18096	triHPacyl.ptptptmmpu	6.386e+44	10.07	10.07	2.965e+37	5.99e-05
18097	triHPacyl.ptptptppmu	1.807e+44	9.31	9.31	2.964e+37	5.98e-05
18098	triHPacyl.mptmmtpppu	1.067e+44	9.00	9.00	2.956e+37	5.97e-05
18099	triHPacyl.pmtmmmmmpu	1.453e+44	9.19	9.19	2.950e+37	5.95e-05
18100	triHPacyl.tmttptmmpu	3.683e+44	9.74	9.74	2.940e+37	5.93e-05
18101	triHPacyl.tptmmpmpu	4.071e+44	9.81	9.81	2.916e+37	5.89e-05
18102	triHPacyl.mptpmttppu	1.867e+44	9.34	9.34	2.915e+37	5.88e-05
18103	triHPacyl.ptmptmmpu	3.345e+43	8.33	8.33	2.868e+37	5.79e-05
18104	triHPacyl.mppmtmmpmu	2.256e+44	9.47	9.47	2.852e+37	5.76e-05
18105	triHPacyl.pppmtmtpu	3.502e+44	9.73	9.73	2.842e+37	5.74e-05
18106	triHPacyl.tmtppptppu	3.119e+44	9.67	9.67	2.833e+37	5.72e-05
18107	triHPacyl.ttmmpptppu	1.190e+45	10.47	10.47	2.819e+37	5.69e-05
18108	triHPacyl.tpmmtppmu	5.877e+43	8.68	8.68	2.782e+37	5.62e-05
18109	triHPacyl.ptmppmmpu	2.038e+44	9.43	9.43	2.773e+37	5.6e-05
18110	triHPacyl.mmpptppmmu	3.898e+44	9.81	9.81	2.765e+37	5.58e-05
18111	triHPacyl.mtppmtmmpu	2.840e+43	8.26	8.26	2.741e+37	5.53e-05
18112	triHPacyl.pppmmtppu	7.962e+43	8.87	8.87	2.740e+37	5.53e-05
18113	triHPacyl.pmpmtmmpu	5.637e+43	8.67	8.67	2.731e+37	5.51e-05
18114	triHPacyl.tptmptppu	1.592e+44	9.29	9.29	2.730e+37	5.51e-05
18115	triHPacyl.mtpppmtppu	8.797e+43	8.94	8.94	2.697e+37	5.44e-05
18116	triHPacyl.pmppttppu	1.011e+44	9.03	9.03	2.692e+37	5.43e-05
18117	triHPacyl.pmpptmtpu	5.629e+43	8.68	8.68	2.688e+37	5.42e-05
18118	triHPacyl.tmtpppmpu	6.217e+43	8.74	8.74	2.679e+37	5.41e-05
18119	triHPacyl.mmpmmmmmpu	6.078e+43	8.73	8.73	2.673e+37	5.39e-05

18120	triHPacyl.mptmmmpmpu	7.328e+43	8.84	8.84	2.657e+37	5.36e-05
18121	triHPacyl.tptpnmmpu	1.232e+44	9.15	9.15	2.651e+37	5.35e-05
18122	triHPacyl.ttptpnmmpu	2.442e+44	9.57	9.57	2.625e+37	5.3e-05
18123	triHPacyl.tmpptmtmpu	2.297e+44	9.53	9.53	2.611e+37	5.27e-05
18124	triHPacyl.pptppppmu	1.182e+44	9.14	9.14	2.610e+37	5.27e-05
18125	triHPacyl.mmtpmmmmu	3.612e+44	9.80	9.80	2.605e+37	5.26e-05
18126	triHPacyl.pmmtpmmpu	1.494e+43	7.91	7.91	2.599e+37	5.25e-05
18127	triHPacyl.mmttmmtmu	6.594e+44	10.17	10.17	2.593e+37	5.23e-05
18128	triHPacyl.tttppptpmu	4.663e+44	9.96	9.96	2.590e+37	5.23e-05
18129	triHPacyl.pmtppppmu	1.406e+44	9.25	9.25	2.589e+37	5.22e-05
18130	triHPacyl.tmpmtttmpu	1.090e+45	10.47	10.47	2.583e+37	5.21e-05
18131	triHPacyl.pmpmtmmmu	3.113e+44	9.72	9.72	2.579e+37	5.21e-05
18132	triHPacyl.ttmpmtppmu	3.859e+43	8.48	8.48	2.577e+37	5.2e-05
18133	triHPacyl.pmttppmpmu	1.339e+44	9.22	9.22	2.563e+37	5.17e-05
18134	triHPacyl.ttptpmmmu	1.600e+44	9.33	9.33	2.562e+37	5.17e-05
18135	triHPacyl.mmttmmtmpu	6.807e+45	11.57	11.57	2.552e+37	5.15e-05
18136	triHPacyl.tmmpmmmpu	1.172e+43	7.77	7.77	2.542e+37	5.13e-05
18137	triHPacyl.ttpmmmpmu	4.174e+43	8.54	8.54	2.524e+37	5.09e-05
18138	triHPacyl.ptmpmpmmu	1.034e+44	9.08	9.08	2.515e+37	5.08e-05
18139	triHPacyl.tmttppppmu	1.432e+44	9.27	9.27	2.513e+37	5.07e-05
18140	triHPacyl.tmpptmpmu	1.013e+44	9.07	9.07	2.512e+37	5.07e-05
18141	triHPacyl.mpmmptpmu	1.540e+43	7.95	7.95	2.501e+37	5.05e-05
18142	triHPacyl.tptpmtmpu	1.606e+44	9.35	9.35	2.498e+37	5.04e-05
18143	triHPacyl.pttptmmmu	2.865e+44	9.69	9.69	2.494e+37	5.03e-05
18144	triHPacyl.pmpmpmpmu	5.374e+43	8.69	8.69	2.491e+37	5.03e-05
18145	triHPacyl.tpmptmpmu	7.220e+43	8.87	8.87	2.488e+37	5.02e-05
18146	triHPacyl.tptpptppmu	9.057e+43	9.01	9.01	2.488e+37	5.02e-05
18147	triHPacyl.pmpmtttmpu	1.430e+44	9.28	9.28	2.480e+37	5.01e-05
18148	triHPacyl.tpmptmpmu	2.782e+43	8.31	8.31	2.471e+37	4.99e-05
18149	triHPacyl.tmpmpmmmu	7.165e+43	8.87	8.87	2.463e+37	4.97e-05
18150	triHPacyl.ptmtmmpmu	5.433e+43	8.71	8.71	2.462e+37	4.97e-05
18151	triHPacyl.tmpmpmtppu	1.238e+44	9.21	9.21	2.410e+37	4.86e-05
18152	triHPacyl.mppppmmmu	2.141e+44	9.54	9.54	2.402e+37	4.85e-05
18153	triHPacyl.mmpmmmtppu	8.242e+43	8.97	8.97	2.401e+37	4.85e-05
18154	triHPacyl.mmttmtppmu	1.736e+44	9.42	9.42	2.401e+37	4.85e-05
18155	triHPacyl.mttptmmtmu	5.323e+44	10.09	10.09	2.384e+37	4.81e-05
18156	triHPacyl.tmtppmtppu	1.437e+45	10.68	10.68	2.371e+37	4.79e-05
18157	triHPacyl.ttttmmpmu	9.054e+43	9.04	9.04	2.354e+37	4.75e-05
18158	triHPacyl.mpttpmmpmu	9.633e+43	9.08	9.08	2.352e+37	4.75e-05
18159	triHPacyl.pptmtmmmu	3.070e+44	9.77	9.77	2.342e+37	4.73e-05
18160	triHPacyl.tmpmtppmu	1.216e+44	9.22	9.22	2.320e+37	4.68e-05
18161	triHPacyl.pmtmmmtppu	1.669e+44	9.41	9.41	2.317e+37	4.68e-05
18162	triHPacyl.tmpmttppu	1.766e+44	9.45	9.45	2.317e+37	4.68e-05
18163	triHPacyl.mmttppppmu	5.659e+44	10.14	10.14	2.316e+37	4.67e-05
18164	triHPacyl.ttmtptmpmu	2.202e+44	9.58	9.58	2.298e+37	4.64e-05
18165	triHPacyl.pptpmtmpu	9.040e+43	9.06	9.06	2.288e+37	4.62e-05
18166	triHPacyl.tpmppmmmu	2.225e+43	8.22	8.22	2.275e+37	4.59e-05
18167	triHPacyl.tmpmmmtmpu	6.583e+43	8.87	8.87	2.266e+37	4.57e-05
18168	triHPacyl.mtpmpmmmu	3.842e+43	8.55	8.55	2.257e+37	4.56e-05
18169	triHPacyl.pmtmmmmmu	8.552e+43	9.03	9.03	2.244e+37	4.53e-05
18170	triHPacyl.mpmtpppmu	5.413e+43	8.77	8.77	2.215e+37	4.47e-05
18171	triHPacyl.mppppmpmu	1.198e+44	9.24	9.24	2.207e+37	4.45e-05
18172	triHPacyl.mppmtmpmu	5.708e+44	10.18	10.18	2.204e+37	4.45e-05
18173	triHPacyl.ttmtmtmpu	1.529e+44	9.39	9.39	2.191e+37	4.42e-05
18174	triHPacyl.tttptttmpu	3.457e+44	9.88	9.88	2.188e+37	4.42e-05
18175	triHPacyl.tmpmmmtmpu	6.734e+43	8.91	8.91	2.187e+37	4.41e-05
18176	triHPacyl.mttptmmtmu	1.620e+44	9.44	9.44	2.162e+37	4.36e-05
18177	triHPacyl.tttppmmmu	1.326e+44	9.32	9.32	2.158e+37	4.36e-05
18178	triHPacyl.mttpmmpmu	3.633e+43	8.55	8.55	2.155e+37	4.35e-05
18179	triHPacyl.ptmpptttmpu	1.796e+43	8.13	8.13	2.135e+37	4.31e-05
18180	triHPacyl.tptmpmtmpu	7.048e+44	10.33	10.33	2.118e+37	4.27e-05
18181	triHPacyl.tptmtmmpu	3.876e+44	9.97	9.97	2.109e+37	4.26e-05
18182	triHPacyl.pmpmtmppmu	2.586e+44	9.73	9.73	2.106e+37	4.25e-05
18183	triHPacyl.mmtmtmmpu	6.086e+44	10.24	10.24	2.095e+37	4.23e-05
18184	triHPacyl.tmmpptmpu	4.078e+43	8.64	8.64	2.087e+37	4.21e-05
18185	triHPacyl.pmtppmpmu	6.212e+43	8.89	8.89	2.083e+37	4.2e-05
18186	triHPacyl.pmpptmmpu	1.226e+44	9.29	9.29	2.080e+37	4.2e-05
18187	triHPacyl.mmttptmmpu	1.824e+45	10.91	10.91	2.069e+37	4.18e-05
18188	triHPacyl.mtmtptttmpu	1.668e+44	9.48	9.48	2.061e+37	4.16e-05
18189	triHPacyl.pmpptpmpu	6.279e+43	8.90	8.90	2.060e+37	4.16e-05
18190	triHPacyl.mtmmpmmmu	1.293e+44	9.33	9.33	2.057e+37	4.15e-05
18191	triHPacyl.mmmmtmpmu	5.239e+43	8.80	8.80	2.052e+37	4.14e-05

18192	triHPacyl.ptmppppppu	1.782e+43	8.15	8.15	2.052e+37	4.14e-05
18193	triHPacyl.pptmmmmmmu	1.660e+44	9.49	9.49	2.039e+37	4.12e-05
18194	triHPacyl.pmtppmtppu	5.782e+43	8.86	8.86	2.030e+37	4.1e-05
18195	triHPacyl.pmtmmtppu	1.974e+44	9.59	9.59	2.026e+37	4.09e-05
18196	triHPacyl.mpppmtppu	1.176e+44	9.29	9.29	2.024e+37	4.09e-05
18197	triHPacyl.tmptptmpu	5.215e+43	8.80	8.80	2.022e+37	4.08e-05
18198	triHPacyl.pppmmppmmu	4.976e+43	8.78	8.78	2.013e+37	4.06e-05
18199	triHPacyl.pppmtpppu	2.023e+43	8.24	8.24	2.011e+37	4.06e-05
18200	triHPacyl.ppptptmmu	1.042e+44	9.22	9.22	2.010e+37	4.06e-05
18201	triHPacyl.tmptmmtppu	4.827e+44	10.13	10.13	2.005e+37	4.05e-05
18202	triHPacyl.mpptmtppu	1.007e+44	9.20	9.20	2.002e+37	4.04e-05
18203	triHPacyl.tttppmtppu	1.697e+44	9.51	9.51	1.991e+37	4.02e-05
18204	triHPacyl.tmptmmmpu	1.427e+44	9.41	9.41	1.991e+37	4.02e-05
18205	triHPacyl.pmttppmmu	7.686e+43	9.04	9.04	1.983e+37	4e-05
18206	triHPacyl.mmtmmtpmmu	1.223e+44	9.32	9.32	1.978e+37	3.99e-05
18207	triHPacyl.pppmptppu	8.422e+42	7.73	7.73	1.967e+37	3.97e-05
18208	triHPacyl.tmtmptppu	1.760e+44	9.55	9.55	1.959e+37	3.95e-05
18209	triHPacyl.mmmppmmmpu	3.715e+43	8.62	8.62	1.956e+37	3.95e-05
18210	triHPacyl.ttttptmpu	2.074e+44	9.65	9.65	1.947e+37	3.93e-05
18211	triHPacyl.tttmptppu	5.731e+43	8.88	8.88	1.937e+37	3.91e-05
18212	triHPacyl.ttmtptmpu	2.406e+44	9.74	9.74	1.934e+37	3.9e-05
18213	triHPacyl.pptpmtmpu	9.717e+43	9.20	9.20	1.934e+37	3.9e-05
18214	triHPacyl.ttttppppu	1.243e+44	9.35	9.35	1.930e+37	3.9e-05
18215	triHPacyl.tpmmmtpmmu	3.136e+43	8.53	8.53	1.927e+37	3.89e-05
18216	triHPacyl.ppptpmmmmu	9.882e+43	9.21	9.21	1.918e+37	3.87e-05
18217	triHPacyl.tpppmtmpu	1.872e+44	9.59	9.59	1.918e+37	3.87e-05
18218	triHPacyl.ppmpttmmu	1.267e+44	9.36	9.36	1.916e+37	3.87e-05
18219	triHPacyl.tmtmtpmpu	1.976e+44	9.63	9.63	1.915e+37	3.87e-05
18220	triHPacyl.tttmptmpu	1.956e+44	9.62	9.62	1.911e+37	3.86e-05
18221	triHPacyl.tpmmmmpmmu	2.532e+43	8.40	8.40	1.911e+37	3.86e-05
18222	triHPacyl.mtmmtpmmu	1.117e+44	9.29	9.29	1.911e+37	3.86e-05
18223	triHPacyl.tptmptppu	2.622e+44	9.80	9.80	1.909e+37	3.85e-05
18224	triHPacyl.tttmptppu	1.405e+44	9.43	9.43	1.908e+37	3.85e-05
18225	triHPacyl.ttmtptmpu	8.311e+43	9.12	9.12	1.898e+37	3.83e-05
18226	triHPacyl.mtppmmmpu	1.100e+44	9.28	9.28	1.896e+37	3.83e-05
18227	triHPacyl.tmpmptppu	9.525e+43	9.21	9.21	1.863e+37	3.76e-05
18228	triHPacyl.mmmmtmmpu	6.483e+43	8.98	8.98	1.860e+37	3.75e-05
18229	triHPacyl.mtptpmtppu	9.082e+43	9.18	9.18	1.850e+37	3.73e-05
18230	triHPacyl.mptpmtppu	1.041e+44	9.27	9.27	1.842e+37	3.72e-05
18231	triHPacyl.ttmppmmppu	3.281e+43	8.58	8.58	1.833e+37	3.7e-05
18232	triHPacyl.mmtmtmpmpu	9.464e+44	10.59	10.59	1.829e+37	3.69e-05
18233	triHPacyl.ttmtmmppu	1.403e+44	9.45	9.45	1.823e+37	3.68e-05
18234	triHPacyl.ttppppmmu	7.633e+43	9.09	9.09	1.819e+37	3.67e-05
18235	triHPacyl.mptpmmppu	6.289e+43	8.98	8.98	1.809e+37	3.65e-05
18236	triHPacyl.pttpmmtppu	1.324e+44	9.43	9.43	1.783e+37	3.6e-05
18237	triHPacyl.mpmptppmpu	1.785e+44	9.62	9.62	1.767e+37	3.57e-05
18238	triHPacyl.mmtppmmmpu	5.620e+44	10.30	10.30	1.764e+37	3.56e-05
18239	triHPacyl.mpptpmpmpu	1.011e+44	9.28	9.28	1.756e+37	3.54e-05
18240	triHPacyl.ttttppmmu	2.250e+44	9.76	9.76	1.751e+37	3.53e-05
18241	triHPacyl.pmpmptppu	6.009e+43	8.97	8.97	1.741e+37	3.51e-05
18242	triHPacyl.mmttptmmu	8.007e+44	10.52	10.52	1.738e+37	3.51e-05
18243	triHPacyl.tmpmmmtmpu	7.311e+43	9.10	9.10	1.732e+37	3.49e-05
18244	triHPacyl.pppmmpmpu	2.336e+43	8.42	8.42	1.729e+37	3.49e-05
18245	triHPacyl.ttmppmmmpu	1.541e+44	9.54	9.54	1.721e+37	3.47e-05
18246	triHPacyl.ptmtmtppu	3.848e+44	10.09	10.09	1.718e+37	3.47e-05
18247	triHPacyl.pptpmtppu	1.995e+44	9.70	9.70	1.717e+37	3.47e-05
18248	triHPacyl.tpppmtmmu	3.175e+44	9.98	9.98	1.712e+37	3.46e-05
18249	triHPacyl.mppmptmpu	8.858e+43	9.22	9.22	1.711e+37	3.45e-05
18250	triHPacyl.tppmptmmu	4.765e+43	8.85	8.85	1.708e+37	3.45e-05
18251	triHPacyl.ptppmptmpu	1.757e+44	9.63	9.63	1.703e+37	3.44e-05
18252	triHPacyl.ptttmtppu	3.814e+44	10.09	10.09	1.696e+37	3.42e-05
18253	triHPacyl.tmtmptppu	4.828e+44	10.24	10.24	1.680e+37	3.39e-05
18254	triHPacyl.mmmppmtppu	4.828e+43	8.87	8.87	1.680e+37	3.39e-05
18255	triHPacyl.mmtmpmpmpu	6.150e+43	9.01	9.01	1.677e+37	3.38e-05
18256	triHPacyl.pmpmptppu	1.878e+43	8.31	8.31	1.674e+37	3.38e-05
18257	triHPacyl.tpmmtmtpu	4.018e+44	10.13	10.13	1.672e+37	3.38e-05
18258	triHPacyl.ttmtptmpu	1.291e+44	9.46	9.46	1.662e+37	3.35e-05
18259	triHPacyl.mtppmtppu	2.583e+44	9.87	9.87	1.661e+37	3.35e-05
18260	triHPacyl.ppmmtmmpu	9.775e+43	9.30	9.30	1.651e+37	3.33e-05
18261	triHPacyl.ttmtptmmu	7.650e+43	9.15	9.15	1.644e+37	3.32e-05
18262	triHPacyl.ttmppmtpu	2.921e+43	8.58	8.58	1.643e+37	3.32e-05
18263	triHPacyl.pppmmmtmpu	3.348e+44	10.04	10.04	1.637e+37	3.3e-05

18264	triHPacyl.tmmppmmpmu	2.793e+43	8.56	8.56	1.633e+37	3.3e-05
18265	triHPacyl.mptmmpmpmu	1.576e+44	9.59	9.59	1.631e+37	3.29e-05
18266	triHPacyl.tmpptpppu	7.596e+44	10.53	10.53	1.629e+37	3.29e-05
18267	triHPacyl.mpttppmpu	1.435e+44	9.54	9.54	1.624e+37	3.28e-05
18268	triHPacyl.pmptmmtmpu	2.976e+44	9.98	9.98	1.606e+37	3.24e-05
18269	triHPacyl.tmtptmmpu	1.052e+44	9.36	9.36	1.602e+37	3.23e-05
18270	triHPacyl.ptptmmtmmu	4.173e+44	10.18	10.18	1.601e+37	3.23e-05
18271	triHPacyl.pmptmtpppu	1.827e+44	9.69	9.69	1.596e+37	3.22e-05
18272	triHPacyl.tmtptmpmu	2.708e+44	9.93	9.93	1.581e+37	3.19e-05
18273	triHPacyl.mpptmpmpu	1.227e+44	9.46	9.46	1.563e+37	3.15e-05
18274	triHPacyl.mtmtmmtmmu	1.143e+44	9.42	9.42	1.561e+37	3.15e-05
18275	triHPacyl.mtmtmmtmpu	1.942e+44	9.74	9.74	1.554e+37	3.14e-05
18276	triHPacyl.ttptmtmpu	3.450e+44	10.09	10.09	1.549e+37	3.13e-05
18277	triHPacyl.tpmttpppu	9.512e+43	9.32	9.32	1.546e+37	3.12e-05
18278	triHPacyl.tptppmtmpu	2.245e+44	9.83	9.83	1.542e+37	3.11e-05
18279	triHPacyl.tmtmmtmpu	7.416e+44	10.55	10.55	1.530e+37	3.09e-05
18280	triHPacyl.mtmtmpmpmu	1.056e+44	9.39	9.39	1.522e+37	3.07e-05
18281	triHPacyl.mmmmpmtmpu	9.051e+43	9.30	9.30	1.518e+37	3.06e-05
18282	triHPacyl.pmtptmpu	5.596e+44	10.40	10.40	1.497e+37	3.02e-05
18283	triHPacyl.ppptmmpu	1.214e+44	9.49	9.49	1.490e+37	3.01e-05
18284	triHPacyl.tptmpmpu	9.789e+43	9.36	9.36	1.486e+37	3e-05
18285	triHPacyl.tttmtppmu	1.286e+44	9.53	9.53	1.466e+37	2.96e-05
18286	triHPacyl.tppmtmpu	4.317e+44	10.25	10.25	1.465e+37	2.96e-05
18287	triHPacyl.tppttppu	9.718e+44	10.74	10.74	1.459e+37	2.95e-05
18288	triHPacyl.ppptmpmpu	1.270e+44	9.53	9.53	1.447e+37	2.92e-05
18289	triHPacyl.mtmmmmmpmu	9.976e+43	9.39	9.39	1.445e+37	2.92e-05
18290	triHPacyl.ppmttpppu	5.320e+43	9.02	9.02	1.438e+37	2.9e-05
18291	triHPacyl.tmpptmpu	9.075e+43	9.34	9.34	1.413e+37	2.85e-05
18292	triHPacyl.mmttppppmu	6.406e+44	10.51	10.51	1.409e+37	2.84e-05
18293	triHPacyl.mtmtmpmpmu	1.165e+44	9.50	9.50	1.397e+37	2.82e-05
18294	triHPacyl.ttmppmtmmu	1.238e+44	9.54	9.54	1.396e+37	2.82e-05
18295	triHPacyl.tmtmmtmpu	9.947e+43	9.41	9.41	1.394e+37	2.81e-05
18296	triHPacyl.pmptmmtppu	3.562e+44	10.17	10.17	1.393e+37	2.81e-05
18297	triHPacyl.mppmtmpu	3.982e+44	10.24	10.24	1.392e+37	2.81e-05
18298	triHPacyl.tttmpmmpmu	1.992e+44	9.82	9.82	1.389e+37	2.8e-05
18299	triHPacyl.mmmmpmtppu	3.323e+43	8.76	8.76	1.386e+37	2.8e-05
18300	triHPacyl.ttttmmmpu	3.667e+44	10.19	10.19	1.383e+37	2.79e-05
18301	triHPacyl.mtptmtpu	2.739e+43	8.64	8.64	1.382e+37	2.79e-05
18302	triHPacyl.ppptmmpu	2.027e+44	9.84	9.84	1.381e+37	2.79e-05
18303	triHPacyl.tttmmpmpu	7.204e+43	9.22	9.22	1.378e+37	2.78e-05
18304	triHPacyl.tmtmpmpmu	4.002e+44	10.25	10.25	1.373e+37	2.77e-05
18305	triHPacyl.mmmmpmpu	6.271e+43	9.14	9.14	1.367e+37	2.76e-05
18306	triHPacyl.tmtptmpu	1.522e+44	9.68	9.68	1.361e+37	2.75e-05
18307	triHPacyl.mptptmmpu	8.305e+43	9.32	9.32	1.346e+37	2.72e-05
18308	triHPacyl.ttpptppu	3.560e+44	10.19	10.19	1.337e+37	2.7e-05
18309	triHPacyl.ttptmmpu	4.495e+43	8.96	8.96	1.332e+37	2.69e-05
18310	triHPacyl.tmtptmpu	9.031e+44	10.75	10.75	1.329e+37	2.68e-05
18311	triHPacyl.mptmptmpu	3.006e+43	8.72	8.72	1.327e+37	2.68e-05
18312	triHPacyl.pmtptmmpu	1.059e+44	9.48	9.48	1.322e+37	2.67e-05
18313	triHPacyl.mtmtmmpmu	6.798e+43	9.22	9.22	1.313e+37	2.65e-05
18314	triHPacyl.ttpmmpmpu	7.899e+43	9.31	9.31	1.310e+37	2.64e-05
18315	triHPacyl.ttttmmmmmpu	3.290e+44	10.16	10.16	1.301e+37	2.63e-05
18316	triHPacyl.mtptmmpu	1.111e+44	9.52	9.52	1.299e+37	2.62e-05
18317	triHPacyl.mtptmmpu	8.274e+43	9.34	9.34	1.297e+37	2.62e-05
18318	triHPacyl.tttptmmpu	9.522e+43	9.43	9.43	1.293e+37	2.61e-05
18319	triHPacyl.mmmmmmmmpu	3.808e+43	8.88	8.88	1.283e+37	2.59e-05
18320	triHPacyl.ttpppmmpu	1.443e+44	9.68	9.68	1.282e+37	2.59e-05
18321	triHPacyl.pptmmpmpu	7.466e+43	9.29	9.29	1.277e+37	2.58e-05
18322	triHPacyl.mppppmmpu	7.362e+43	9.28	9.28	1.275e+37	2.57e-05
18323	triHPacyl.pmptmmpu	6.145e+43	9.18	9.18	1.271e+37	2.57e-05
18324	triHPacyl.mptmtmmpu	1.939e+44	9.86	9.86	1.270e+37	2.56e-05
18325	triHPacyl.mpttptmmpu	1.046e+44	9.49	9.49	1.269e+37	2.56e-05
18326	triHPacyl.ptmmpmmpu	1.937e+44	9.86	9.86	1.261e+37	2.55e-05
18327	triHPacyl.ttttptmpu	2.311e+44	9.98	9.98	1.250e+37	2.52e-05
18328	triHPacyl.mtptmmpu	5.019e+43	9.07	9.07	1.237e+37	2.5e-05
18329	triHPacyl.mtmtmmmpu	4.162e+44	10.34	10.34	1.229e+37	2.48e-05
18330	triHPacyl.mtmtptppu	6.997e+43	9.28	9.28	1.225e+37	2.47e-05
18331	triHPacyl.mmtmmpmpu	1.603e+45	11.14	11.14	1.224e+37	2.47e-05
18332	triHPacyl.tpmtmtmpu	4.500e+44	10.39	10.39	1.221e+37	2.47e-05
18333	triHPacyl.ppptppppmu	1.971e+44	9.89	9.89	1.220e+37	2.46e-05
18334	triHPacyl.mppmmmpmpu	2.968e+43	8.77	8.77	1.219e+37	2.46e-05
18335	triHPacyl.mppmmmtmpu	1.881e+43	8.50	8.50	1.217e+37	2.46e-05

18336	triHPacyl.mppmptmmmu	2.163e+43	8.58	8.58	1.215e+37	2.45e-05
18337	triHPacyl.tpptttmpu	1.640e+45	11.16	11.16	1.209e+37	2.44e-05
18338	triHPacyl.mttmtpmpu	3.084e+43	8.79	8.79	1.208e+37	2.44e-05
18339	triHPacyl.pmtmpttpmu	1.106e+45	10.93	10.93	1.205e+37	2.43e-05
18340	triHPacyl.pmtmmtmpu	4.469e+43	9.02	9.02	1.204e+37	2.43e-05
18341	triHPacyl.ttpmptmpu	3.132e+43	8.81	8.81	1.199e+37	2.42e-05
18342	triHPacyl.pmpptmmmpu	5.432e+43	9.14	9.14	1.198e+37	2.42e-05
18343	triHPacyl.ttpmptmpu	3.493e+44	10.25	10.25	1.184e+37	2.39e-05
18344	triHPacyl.pmppttppu	1.259e+44	9.65	9.65	1.173e+37	2.37e-05
18345	triHPacyl.tmtptmpmpu	1.217e+44	9.63	9.63	1.173e+37	2.37e-05
18346	triHPacyl.mtpmpmpmpu	3.629e+43	8.91	8.91	1.163e+37	2.35e-05
18347	triHPacyl.tmtmtpmpu	8.004e+43	9.39	9.39	1.160e+37	2.34e-05
18348	triHPacyl.mpmpttmmu	8.958e+43	9.46	9.46	1.146e+37	2.31e-05
18349	triHPacyl.tmtmmpmpu	6.775e+43	9.30	9.30	1.145e+37	2.31e-05
18350	triHPacyl.tttmptmmu	4.438e+44	10.42	10.42	1.138e+37	2.3e-05
18351	triHPacyl.mmmptmpmpu	4.285e+43	9.03	9.03	1.130e+37	2.28e-05
18352	triHPacyl.mmtmpmpmpu	6.124e+44	10.62	10.62	1.129e+37	2.28e-05
18353	triHPacyl.tmmppmmmmu	6.941e+43	9.32	9.32	1.127e+37	2.27e-05
18354	triHPacyl.mppmtppmpu	3.594e+43	8.93	8.93	1.125e+37	2.27e-05
18355	triHPacyl.pmttptmpu	1.903e+44	9.93	9.93	1.117e+37	2.25e-05
18356	triHPacyl.mtppmmmmu	1.131e+44	9.62	9.62	1.117e+37	2.25e-05
18357	triHPacyl.tttmmtmpu	1.024e+44	9.56	9.56	1.114e+37	2.25e-05
18358	triHPacyl.tmtpttmmu	2.519e+44	10.10	10.10	1.112e+37	2.24e-05
18359	triHPacyl.mpttpmpmpu	5.246e+43	9.16	9.16	1.109e+37	2.24e-05
18360	triHPacyl.pptmmtmmu	1.392e+44	9.75	9.75	1.108e+37	2.24e-05
18361	triHPacyl.mpmptmpmpu	1.148e+44	9.63	9.63	1.107e+37	2.23e-05
18362	triHPacyl.tpptttmpu	2.616e+44	10.12	10.12	1.106e+37	2.23e-05
18363	triHPacyl.ttpttpppu	5.049e+43	9.14	9.14	1.101e+37	2.22e-05
18364	triHPacyl.ttpmpmpmpu	5.576e+43	9.21	9.21	1.095e+37	2.21e-05
18365	triHPacyl.pmpmtmpmpu	9.633e+43	9.53	9.53	1.094e+37	2.21e-05
18366	triHPacyl.mmttmppmpu	1.491e+44	9.80	9.80	1.085e+37	2.19e-05
18367	triHPacyl.tpptmpmpu	8.991e+43	9.50	9.50	1.082e+37	2.18e-05
18368	triHPacyl.mpppmtpppu	7.803e+44	10.79	10.79	1.082e+37	2.18e-05
18369	triHPacyl.mpttptmpu	1.453e+44	9.79	9.79	1.081e+37	2.18e-05
18370	triHPacyl.tmpmtmmmmu	2.771e+44	10.17	10.17	1.079e+37	2.18e-05
18371	triHPacyl.mtptmtpmpu	1.643e+44	9.86	9.86	1.071e+37	2.16e-05
18372	triHPacyl.pmttmtmmu	6.623e+44	10.70	10.70	1.068e+37	2.16e-05
18373	triHPacyl.mtttptmpu	1.187e+44	9.67	9.67	1.065e+37	2.15e-05
18374	triHPacyl.mtpmmmpmpu	2.702e+43	8.79	8.79	1.060e+37	2.14e-05
18375	triHPacyl.tmtmmpmpu	2.523e+44	10.13	10.13	1.057e+37	2.13e-05
18376	triHPacyl.mtttppmmmu	3.200e+44	10.27	10.27	1.055e+37	2.13e-05
18377	triHPacyl.mttmmtpppu	3.859e+43	9.01	9.01	1.052e+37	2.12e-05
18378	triHPacyl.ttmppmtmpu	2.512e+44	10.13	10.13	1.048e+37	2.12e-05
18379	triHPacyl.mptppmmmpu	8.485e+43	9.48	9.48	1.046e+37	2.11e-05
18380	triHPacyl.mtmtptmmu	4.471e+44	10.48	10.48	1.045e+37	2.11e-05
18381	triHPacyl.ppptmmmpu	9.546e+43	9.56	9.56	1.038e+37	2.1e-05
18382	triHPacyl.mpmptmpmpu	2.136e+44	10.04	10.04	1.037e+37	2.09e-05
18383	triHPacyl.tppmpmpmpu	3.087e+43	8.89	8.89	1.036e+37	2.09e-05
18384	triHPacyl.ttmppmpmpu	5.387e+43	9.22	9.22	1.034e+37	2.09e-05
18385	triHPacyl.pmpmpmtmpu	4.863e+44	10.53	10.53	1.032e+37	2.08e-05
18386	triHPacyl.tttmptmpu	1.189e+44	9.70	9.70	1.027e+37	2.07e-05
18387	triHPacyl.tptmptmmu	1.600e+44	9.87	9.87	1.026e+37	2.07e-05
18388	triHPacyl.mtptmtpmpu	3.171e+43	8.91	8.91	1.022e+37	2.06e-05
18389	triHPacyl.mppptmpmpu	7.404e+43	9.42	9.42	1.010e+37	2.04e-05
18390	triHPacyl.tpmppmtmpu	1.652e+43	8.54	8.54	1.001e+37	2.02e-05
18391	triHPacyl.ptttmtmpu	3.105e+44	10.29	10.29	9.957e+36	2.01e-05
18392	triHPacyl.mpmptmpmpu	3.417e+44	10.35	10.35	9.929e+36	2e-05
18393	triHPacyl.mtppmpmpu	4.959e+43	9.20	9.20	9.922e+36	2e-05
18394	triHPacyl.mtttptmpu	1.829e+44	9.97	9.97	9.921e+36	2e-05
18395	triHPacyl.ptptmtmpu	1.126e+44	9.69	9.69	9.907e+36	2e-05
18396	triHPacyl.tmtmtmpu	1.858e+44	9.99	9.99	9.880e+36	1.99e-05
18397	triHPacyl.tptpmtmpu	1.883e+44	10.00	10.00	9.698e+36	1.96e-05
18398	triHPacyl.pmmppmtmpu	9.548e+42	8.23	8.23	9.610e+36	1.94e-05
18399	triHPacyl.pptmpmpmpu	1.382e+44	9.83	9.83	9.480e+36	1.91e-05
18400	triHPacyl.mtptmpmpu	1.279e+44	9.79	9.79	9.460e+36	1.91e-05
18401	triHPacyl.mtpmmtmpu	1.567e+43	8.54	8.54	9.432e+36	1.9e-05
18402	triHPacyl.mtttppmmmpu	2.576e+44	10.21	10.21	9.370e+36	1.89e-05
18403	triHPacyl.pptmtpmpu	2.304e+44	10.15	10.15	9.313e+36	1.88e-05
18404	triHPacyl.tpmppmtmpu	2.579e+43	8.85	8.85	9.277e+36	1.87e-05
18405	triHPacyl.pmpptmpmpu	5.204e+43	9.27	9.27	9.264e+36	1.87e-05
18406	triHPacyl.mppptpppu	8.784e+43	9.58	9.58	9.258e+36	1.87e-05
18407	triHPacyl.tpmmtmpmpu	5.279e+43	9.28	9.28	9.242e+36	1.87e-05

18408	triHPacyl.ttmtmmpmmu	4.213e+43	9.14	9.14	9.201e+36	1.86e-05
18409	triHPacyl.ptmmpmpmmu	5.666e+43	9.32	9.32	9.162e+36	1.85e-05
18410	triHPacyl.mmttmmpmmu	4.417e+44	10.55	10.55	9.136e+36	1.84e-05
18411	triHPacyl.mmmmmmpmmu	1.131e+44	9.74	9.74	9.126e+36	1.84e-05
18412	triHPacyl.mptpmmtmpu	2.017e+44	10.08	10.08	9.097e+36	1.84e-05
18413	triHPacyl.ttppttppu	6.612e+43	9.42	9.42	9.051e+36	1.83e-05
18414	triHPacyl.mtmtmtmpmu	5.682e+43	9.33	9.33	9.035e+36	1.82e-05
18415	triHPacyl.pptpmmmmu	3.579e+43	9.06	9.06	9.027e+36	1.82e-05
18416	triHPacyl.mppmtmmpmu	1.050e+44	9.70	9.70	9.010e+36	1.82e-05
18417	triHPacyl.mpttmtmpmu	1.158e+44	9.77	9.77	8.912e+36	1.8e-05
18418	triHPacyl.pptmptmmpu	4.574e+43	9.21	9.21	8.906e+36	1.8e-05
18419	triHPacyl.tptmmpmmpu	3.857e+43	9.11	9.11	8.886e+36	1.79e-05
18420	triHPacyl.tmpptppmpu	3.076e+44	10.35	10.35	8.805e+36	1.78e-05
18421	triHPacyl.mtppmpmmu	2.069e+43	8.75	8.75	8.785e+36	1.77e-05
18422	triHPacyl.tpttptmpmu	1.655e+44	9.99	9.99	8.772e+36	1.77e-05
18423	triHPacyl.pmttppmmpu	8.523e+43	9.59	9.59	8.748e+36	1.77e-05
18424	triHPacyl.mppptppmu	8.992e+43	9.64	9.64	8.597e+36	1.74e-05
18425	triHPacyl.mttmmmmmu	1.993e+44	10.11	10.11	8.584e+36	1.73e-05
18426	triHPacyl.mmmmttppu	6.202e+44	10.79	10.79	8.565e+36	1.73e-05
18427	triHPacyl.tmpptmpu	2.167e+43	8.80	8.80	8.474e+36	1.71e-05
18428	triHPacyl.mtppmtmpu	2.026e+43	8.76	8.76	8.446e+36	1.7e-05
18429	triHPacyl.mtmtmmpu	2.514e+44	10.26	10.26	8.383e+36	1.69e-05
18430	triHPacyl.mpppmmpu	1.852e+44	10.08	10.08	8.380e+36	1.69e-05
18431	triHPacyl.tptpmtmmpu	1.166e+44	9.81	9.81	8.326e+36	1.68e-05
18432	triHPacyl.mttmmpppu	5.352e+43	9.35	9.35	8.265e+36	1.67e-05
18433	triHPacyl.ttmmpmmmu	1.708e+44	10.04	10.04	8.224e+36	1.66e-05
18434	triHPacyl.tpttptmmpu	3.143e+44	10.41	10.41	8.221e+36	1.66e-05
18435	triHPacyl.mppmtppmu	2.733e+43	8.96	8.96	8.167e+36	1.65e-05
18436	triHPacyl.tmtppmmmu	2.175e+44	10.19	10.19	8.150e+36	1.64e-05
18437	triHPacyl.pppmtppmu	1.001e+44	9.73	9.73	8.141e+36	1.64e-05
18438	triHPacyl.mtppmtmmpu	1.265e+44	9.87	9.87	8.105e+36	1.64e-05
18439	triHPacyl.mpppmtppu	1.720e+44	10.06	10.06	8.028e+36	1.62e-05
18440	triHPacyl.ttmmpmmpu	8.204e+43	9.62	9.62	8.025e+36	1.62e-05
18441	triHPacyl.mtmtmmpu	4.527e+43	9.27	9.27	7.953e+36	1.61e-05
18442	triHPacyl.mptpmmmmu	8.282e+43	9.64	9.64	7.910e+36	1.6e-05
18443	triHPacyl.mpppmmpu	3.459e+44	10.50	10.50	7.811e+36	1.58e-05
18444	triHPacyl.tpmtmtmmpu	1.329e+44	9.93	9.93	7.809e+36	1.58e-05
18445	triHPacyl.mppmtppmu	1.518e+44	10.01	10.01	7.720e+36	1.56e-05
18446	triHPacyl.ppttptmmpu	2.551e+44	10.33	10.33	7.675e+36	1.55e-05
18447	triHPacyl.tmmtppppu	8.517e+43	9.67	9.67	7.643e+36	1.54e-05
18448	triHPacyl.tmpptppmu	3.788e+44	10.57	10.57	7.588e+36	1.53e-05
18449	triHPacyl.mptpmmmmu	9.801e+43	9.77	9.77	7.539e+36	1.52e-05
18450	triHPacyl.tmpmtmmpu	2.210e+44	10.25	10.25	7.519e+36	1.52e-05
18451	triHPacyl.ttpptmmpu	2.046e+44	10.21	10.21	7.455e+36	1.5e-05
18452	triHPacyl.ttttptmmpu	3.372e+44	10.51	10.51	7.381e+36	1.49e-05
18453	triHPacyl.tptmptmmpu	4.860e+44	10.74	10.74	7.274e+36	1.47e-05
18454	triHPacyl.ptmmpmmmu	2.231e+44	10.28	10.28	7.241e+36	1.46e-05
18455	triHPacyl.tmppttppu	4.717e+44	10.73	10.73	7.192e+36	1.45e-05
18456	triHPacyl.mptmptmpu	1.101e+44	9.86	9.86	7.188e+36	1.45e-05
18457	triHPacyl.mptmtmmpu	2.736e+44	10.41	10.41	7.162e+36	1.45e-05
18458	triHPacyl.mtppmtmpu	5.527e+43	9.46	9.46	7.109e+36	1.43e-05
18459	triHPacyl.mtppmmpmu	3.591e+43	9.20	9.20	7.103e+36	1.43e-05
18460	triHPacyl.tpmttppu	3.246e+44	10.52	10.52	7.098e+36	1.43e-05
18461	triHPacyl.ttmptppmu	5.777e+43	9.49	9.49	7.069e+36	1.43e-05
18462	triHPacyl.tppmptmmpu	6.369e+44	10.92	10.92	7.060e+36	1.42e-05
18463	triHPacyl.tmttppppu	6.395e+44	10.92	10.92	7.050e+36	1.42e-05
18464	triHPacyl.pppmtpppu	1.488e+44	10.06	10.06	7.014e+36	1.42e-05
18465	triHPacyl.tmpmtmmpu	2.798e+44	10.43	10.43	7.007e+36	1.41e-05
18466	triHPacyl.pptpmtppu	1.127e+44	9.90	9.90	6.976e+36	1.41e-05
18467	triHPacyl.mptmmmtmmpu	1.444e+44	10.04	10.04	6.955e+36	1.4e-05
18468	triHPacyl.mmtmmtmpu	7.682e+44	11.04	11.04	6.921e+36	1.4e-05
18469	triHPacyl.mtmmtmmpu	1.462e+44	10.06	10.06	6.910e+36	1.39e-05
18470	triHPacyl.mtmmtmmpu	7.795e+43	9.68	9.68	6.907e+36	1.39e-05
18471	triHPacyl.pmtppptmpu	6.651e+43	9.59	9.59	6.882e+36	1.39e-05
18472	triHPacyl.ttpmptppu	7.037e+43	9.63	9.63	6.782e+36	1.37e-05
18473	triHPacyl.ttmmtmmpu	3.184e+44	10.53	10.53	6.774e+36	1.37e-05
18474	triHPacyl.tttmtmmpu	4.937e+44	10.80	10.80	6.741e+36	1.36e-05
18475	triHPacyl.tpppmpppu	1.819e+44	10.20	10.20	6.739e+36	1.36e-05
18476	triHPacyl.pmpptppmu	7.116e+43	9.64	9.64	6.701e+36	1.35e-05
18477	triHPacyl.tmpmmmmmu	5.788e+43	9.53	9.53	6.654e+36	1.34e-05
18478	triHPacyl.mtptmmpmu	2.158e+44	10.32	10.32	6.601e+36	1.33e-05
18479	triHPacyl.tmtpppppu	6.150e+43	9.57	9.57	6.520e+36	1.32e-05

18480	triHPacyl.tmpppppppu	8.610e+44	11.15	11.15	6.482e+36	1.31e-05
18481	triHPacyl.pttmmmtmpu	1.360e+44	10.05	10.05	6.480e+36	1.31e-05
18482	triHPacyl.mptppmtmpu	7.033e+43	9.66	9.66	6.459e+36	1.3e-05
18483	triHPacyl.tmpppmtmpu	4.797e+44	10.81	10.81	6.431e+36	1.3e-05
18484	triHPacyl.ttmmmtmmmu	2.399e+44	10.39	10.39	6.422e+36	1.3e-05
18485	triHPacyl.mmmmmmtmpu	5.133e+44	10.85	10.85	6.390e+36	1.29e-05
18486	triHPacyl.ttmpmttppu	1.624e+44	10.17	10.17	6.315e+36	1.27e-05
18487	triHPacyl.ttmppptppu	3.521e+43	9.26	9.26	6.314e+36	1.27e-05
18488	triHPacyl.ptppmttppu	3.504e+44	10.63	10.63	6.296e+36	1.27e-05
18489	triHPacyl.tmttptmpu	2.268e+44	10.37	10.37	6.286e+36	1.27e-05
18490	triHPacyl.mmpmmmtppu	3.090e+43	9.19	9.19	6.267e+36	1.26e-05
18491	triHPacyl.mtptptppu	8.365e+43	9.78	9.78	6.246e+36	1.26e-05
18492	triHPacyl.ppptmmmmu	1.104e+44	9.95	9.95	6.216e+36	1.25e-05
18493	triHPacyl.pmpmtmmpu	1.177e+44	9.99	9.99	6.186e+36	1.25e-05
18494	triHPacyl.tttmpptppu	9.401e+43	9.87	9.87	6.078e+36	1.23e-05
18495	triHPacyl.ttmpmttppu	3.340e+44	10.63	10.63	6.071e+36	1.23e-05
18496	triHPacyl.mtptptmpu	6.216e+43	9.63	9.63	6.047e+36	1.22e-05
18497	triHPacyl.mpppmmtppu	4.170e+44	10.76	10.76	6.035e+36	1.22e-05
18498	triHPacyl.tpttptppu	6.939e+44	11.08	11.08	5.905e+36	1.19e-05
18499	triHPacyl.ttptmmpmpu	1.178e+44	10.02	10.02	5.887e+36	1.19e-05
18500	triHPacyl.ttptmtmmu	1.800e+44	10.28	10.28	5.883e+36	1.19e-05
18501	triHPacyl.pmtmmmtppu	2.506e+44	10.48	10.48	5.783e+36	1.17e-05
18502	triHPacyl.mptmpmtmpu	7.501e+43	9.77	9.77	5.765e+36	1.16e-05
18503	triHPacyl.tptmmpmpu	1.003e+44	9.94	9.94	5.764e+36	1.16e-05
18504	triHPacyl.ttttmtmpu	3.035e+44	10.61	10.61	5.709e+36	1.15e-05
18505	triHPacyl.mptmmmmppu	3.586e+43	9.33	9.33	5.706e+36	1.15e-05
18506	triHPacyl.mtmppmmmpu	2.108e+44	10.39	10.39	5.684e+36	1.15e-05
18507	triHPacyl.mptpmtmpu	1.360e+44	10.13	10.13	5.654e+36	1.14e-05
18508	triHPacyl.ttptppmpu	1.930e+44	10.34	10.34	5.650e+36	1.14e-05
18509	triHPacyl.mtmmpmtppu	6.919e+43	9.73	9.73	5.605e+36	1.13e-05
18510	triHPacyl.tmpmpmtmpu	3.350e+43	9.31	9.31	5.575e+36	1.13e-05
18511	triHPacyl.mmttmtmpu	1.450e+44	10.18	10.18	5.531e+36	1.12e-05
18512	triHPacyl.mtttmtmpu	1.558e+44	10.23	10.23	5.524e+36	1.11e-05
18513	triHPacyl.ttmtpmmpu	3.206e+44	10.66	10.66	5.520e+36	1.11e-05
18514	triHPacyl.mttmpttppu	4.414e+43	9.48	9.48	5.481e+36	1.11e-05
18515	triHPacyl.mppmtppmpu	2.488e+44	10.51	10.51	5.478e+36	1.11e-05
18516	triHPacyl.mtmmpmmmpu	2.134e+44	10.42	10.42	5.477e+36	1.11e-05
18517	triHPacyl.mptppmmmpu	3.364e+43	9.32	9.32	5.465e+36	1.1e-05
18518	triHPacyl.mmmmtmmpu	5.529e+44	10.99	10.99	5.414e+36	1.09e-05
18519	triHPacyl.mmttppmmmpu	1.104e+45	11.41	11.41	5.410e+36	1.09e-05
18520	triHPacyl.mptmmmpmpu	1.079e+44	10.02	10.02	5.394e+36	1.09e-05
18521	triHPacyl.ttmtpttppu	1.096e+44	10.03	10.03	5.387e+36	1.09e-05
18522	triHPacyl.ptmpmmpmpu	1.056e+44	10.01	10.01	5.379e+36	1.09e-05
18523	triHPacyl.mtptppmpmpu	7.070e+43	9.77	9.77	5.368e+36	1.08e-05
18524	triHPacyl.pmpmtppmpu	4.828e+43	9.55	9.55	5.356e+36	1.08e-05
18525	triHPacyl.mmttmmmmmpu	7.013e+44	11.14	11.14	5.342e+36	1.08e-05
18526	triHPacyl.ttpttppmpu	1.161e+44	10.07	10.07	5.324e+36	1.07e-05
18527	triHPacyl.ttptmtppmpu	2.783e+44	10.60	10.60	5.269e+36	1.06e-05
18528	triHPacyl.pppmmmmmpu	1.651e+43	8.92	8.92	5.267e+36	1.06e-05
18529	triHPacyl.mtmtptmmpu	2.501e+44	10.54	10.54	5.247e+36	1.06e-05
18530	triHPacyl.tppmpptmpu	5.477e+43	9.64	9.64	5.243e+36	1.06e-05
18531	triHPacyl.ttmtptppmpu	1.323e+44	10.16	10.16	5.236e+36	1.06e-05
18532	triHPacyl.ttttptmmpu	2.870e+44	10.62	10.62	5.225e+36	1.05e-05
18533	triHPacyl.ttptptmpmpu	3.501e+44	10.74	10.74	5.221e+36	1.05e-05
18534	triHPacyl.mptmmmtmpu	2.330e+44	10.50	10.50	5.218e+36	1.05e-05
18535	triHPacyl.tmtppptppu	2.222e+44	10.47	10.47	5.218e+36	1.05e-05
18536	triHPacyl.ttmttppppu	9.030e+43	9.94	9.94	5.192e+36	1.05e-05
18537	triHPacyl.pmtmpmtmpu	3.828e+44	10.80	10.80	5.187e+36	1.05e-05
18538	triHPacyl.mpttpttppu	8.381e+43	9.90	9.90	5.178e+36	1.05e-05
18539	triHPacyl.mmpmpmpmpu	1.368e+44	10.19	10.19	5.137e+36	1.04e-05
18540	triHPacyl.tppppppmpu	3.450e+43	9.37	9.37	5.124e+36	1.03e-05
18541	triHPacyl.mtmmpptmpu	3.076e+44	10.68	10.68	5.075e+36	1.02e-05
18542	triHPacyl.mtmtptmmpu	1.859e+44	10.38	10.38	5.071e+36	1.02e-05
18543	triHPacyl.ttmmpmpmpu	3.215e+43	9.34	9.34	5.057e+36	1.02e-05
18544	triHPacyl.pptmpmmmpu	3.606e+43	9.41	9.41	5.025e+36	1.01e-05
18545	triHPacyl.mptmmmpppu	9.396e+43	9.98	9.98	5.008e+36	1.01e-05
18546	triHPacyl.ptppmttppu	1.551e+44	10.28	10.28	5.002e+36	1.01e-05
18547	triHPacyl.mmttmmmmmpu	6.523e+44	11.14	11.14	5.000e+36	1.01e-05
18548	triHPacyl.tptppmpppu	1.397e+44	10.23	10.23	4.939e+36	9.97e-06
18549	triHPacyl.mppmpptmpu	1.100e+44	10.09	10.09	4.923e+36	9.94e-06
18550	triHPacyl.ttmtmmpppu	9.724e+43	10.02	10.02	4.908e+36	9.91e-06
18551	triHPacyl.ttppmmmtmpu	1.104e+44	10.09	10.09	4.888e+36	9.86e-06

18552	triHPacyl.mmttmmpmpu	7.985e+44	11.28	11.28	4.880e+36	9.85e-06
18553	triHPacyl.ttttppmpu	1.221e+44	10.16	10.16	4.865e+36	9.82e-06
18554	triHPacyl.ppttmppmpu	2.436e+44	10.57	10.57	4.864e+36	9.82e-06
18555	triHPacyl.tpmtppmpu	5.744e+43	9.71	9.71	4.864e+36	9.82e-06
18556	triHPacyl.pmpptppmpu	4.036e+43	9.50	9.50	4.858e+36	9.81e-06
18557	triHPacyl.ttmtpmmpu	4.745e+44	10.97	10.97	4.856e+36	9.8e-06
18558	triHPacyl.mpppttpmpu	1.832e+44	10.40	10.40	4.843e+36	9.77e-06
18559	triHPacyl.ttmtpmtpmpu	1.721e+44	10.37	10.37	4.813e+36	9.71e-06
18560	triHPacyl.ttpppmmpu	8.488e+43	9.95	9.95	4.798e+36	9.68e-06
18561	triHPacyl.mmtppmtpmpu	1.507e+44	10.29	10.29	4.781e+36	9.65e-06
18562	triHPacyl.ttmtpmmpu	5.635e+44	11.08	11.08	4.779e+36	9.64e-06
18563	triHPacyl.ttmmpmtpmpu	2.659e+44	10.63	10.63	4.760e+36	9.61e-06
18564	triHPacyl.mptmtpmpu	2.933e+44	10.70	10.70	4.710e+36	9.51e-06
18565	triHPacyl.mtmtpmmpu	8.398e+43	9.96	9.96	4.697e+36	9.48e-06
18566	triHPacyl.tpptmtpmpu	1.050e+45	11.46	11.46	4.681e+36	9.45e-06
18567	triHPacyl.mtpmtpmpu	6.391e+43	9.80	9.80	4.677e+36	9.44e-06
18568	triHPacyl.ttmppmmpu	6.102e+43	9.77	9.77	4.665e+36	9.42e-06
18569	triHPacyl.mtpmmpu	1.617e+44	10.35	10.35	4.664e+36	9.41e-06
18570	triHPacyl.pmtppmtpmpu	3.107e+44	10.74	10.74	4.658e+36	9.4e-06
18571	triHPacyl.mmpmtpmpu	1.082e+43	8.74	8.74	4.648e+36	9.38e-06
18572	triHPacyl.ttttmmpu	3.776e+44	10.87	10.87	4.580e+36	9.24e-06
18573	triHPacyl.ttpmtpmpu	9.502e+43	10.05	10.05	4.569e+36	9.22e-06
18574	triHPacyl.ppmtpmpu	2.048e+44	10.50	10.50	4.566e+36	9.22e-06
18575	triHPacyl.pppmmpu	8.076e+43	9.95	9.95	4.555e+36	9.19e-06
18576	triHPacyl.tmpmtpmpu	3.868e+43	9.51	9.51	4.554e+36	9.19e-06
18577	triHPacyl.tmpmmpu	4.763e+43	9.64	9.64	4.550e+36	9.18e-06
18578	triHPacyl.ptmtpmpu	5.177e+44	11.06	11.06	4.543e+36	9.17e-06
18579	triHPacyl.pmpmtpmpu	3.674e+44	10.87	10.87	4.466e+36	9.01e-06
18580	triHPacyl.mppmmpu	4.309e+43	9.59	9.59	4.431e+36	8.94e-06
18581	triHPacyl.pptmmpu	4.436e+43	9.61	9.61	4.429e+36	8.94e-06
18582	triHPacyl.mtpmtpmpu	1.228e+44	10.22	10.22	4.415e+36	8.91e-06
18583	triHPacyl.ttmppmmpu	2.403e+43	9.25	9.25	4.400e+36	8.88e-06
18584	triHPacyl.tmtptmpu	8.548e+44	11.38	11.38	4.397e+36	8.87e-06
18585	triHPacyl.mmtmmpu	6.938e+43	9.88	9.88	4.390e+36	8.86e-06
18586	triHPacyl.pppmmpu	9.585e+43	10.08	10.08	4.381e+36	8.84e-06
18587	triHPacyl.ptmtpmpu	3.442e+44	10.85	10.85	4.323e+36	8.73e-06
18588	triHPacyl.ttmtpmtpmpu	2.363e+43	9.27	9.27	4.154e+36	8.38e-06
18589	triHPacyl.mppmtpmpu	4.827e+44	11.08	11.08	4.097e+36	8.27e-06
18590	triHPacyl.ttttppmpu	1.778e+44	10.49	10.49	4.088e+36	8.25e-06
18591	triHPacyl.mtpmtpmpu	4.969e+43	9.74	9.74	4.018e+36	8.11e-06
18592	triHPacyl.pppmtpmpu	6.588e+43	9.91	9.91	4.007e+36	8.09e-06
18593	triHPacyl.ppmtpmmpu	8.997e+43	10.09	10.09	4.007e+36	8.09e-06
18594	triHPacyl.ttmtpmmpu	5.631e+44	11.19	11.19	4.001e+36	8.07e-06
18595	triHPacyl.tmpmtpmpu	4.218e+44	11.01	11.01	3.998e+36	8.07e-06
18596	triHPacyl.mptmmpu	1.396e+44	10.36	10.36	3.941e+36	7.95e-06
18597	triHPacyl.pmpmtpmpu	2.288e+44	10.66	10.66	3.929e+36	7.93e-06
18598	triHPacyl.mtmtpmtpmpu	6.380e+44	11.27	11.27	3.906e+36	7.88e-06
18599	triHPacyl.mtppmtpmpu	1.875e+44	10.55	10.55	3.899e+36	7.87e-06
18600	triHPacyl.mptmmpu	2.353e+44	10.68	10.68	3.886e+36	7.84e-06
18601	triHPacyl.tttmtpmpu	4.250e+44	11.04	11.04	3.868e+36	7.81e-06
18602	triHPacyl.mmpmmpu	2.616e+44	10.75	10.75	3.844e+36	7.76e-06
18603	triHPacyl.mtmmpmtpmpu	3.443e+44	10.92	10.92	3.821e+36	7.71e-06
18604	triHPacyl.mppmmpu	2.204e+43	9.28	9.28	3.814e+36	7.7e-06
18605	triHPacyl.mtmmpmmpu	3.069e+44	10.86	10.86	3.780e+36	7.63e-06
18606	triHPacyl.ttmtpmtpmpu	6.572e+44	11.31	11.31	3.770e+36	7.61e-06
18607	triHPacyl.mtmppmtpmpu	4.234e+43	9.68	9.68	3.754e+36	7.58e-06
18608	triHPacyl.mppmmpu	1.473e+44	10.43	10.43	3.708e+36	7.48e-06
18609	triHPacyl.mmpmtpmpu	3.155e+43	9.51	9.51	3.700e+36	7.47e-06
18610	triHPacyl.tmtppmtpmpu	1.159e+44	10.29	10.29	3.678e+36	7.42e-06
18611	triHPacyl.ttmtpmmpu	4.705e+44	11.13	11.13	3.672e+36	7.41e-06
18612	triHPacyl.tmpmtpmpu	8.843e+44	11.51	11.51	3.661e+36	7.39e-06
18613	triHPacyl.tmmpmmpu	6.732e+43	9.97	9.97	3.645e+36	7.36e-06
18614	triHPacyl.mtpmmpu	1.536e+44	10.47	10.47	3.617e+36	7.3e-06
18615	triHPacyl.ttmppmmpu	1.067e+44	10.26	10.26	3.591e+36	7.25e-06
18616	triHPacyl.tmmpmtpmpu	1.373e+43	9.04	9.04	3.578e+36	7.22e-06
18617	triHPacyl.ttmtpmtpmpu	5.663e+44	11.26	11.26	3.567e+36	7.2e-06
18618	triHPacyl.pmpmtpmpu	2.429e+45	12.13	12.13	3.561e+36	7.19e-06
18619	triHPacyl.pmpmtpmpu	1.261e+45	11.74	11.74	3.557e+36	7.18e-06
18620	triHPacyl.tmmpmmpu	3.943e+43	9.67	9.67	3.552e+36	7.17e-06
18621	triHPacyl.mtmmpmmpu	1.176e+44	10.33	10.33	3.497e+36	7.06e-06
18622	triHPacyl.mmpmtpmpu	7.607e+44	11.45	11.45	3.478e+36	7.02e-06
18623	triHPacyl.pmpmtpmpu	4.211e+44	11.10	11.10	3.451e+36	6.97e-06

18624	triHPacyl.tpptmtmmu	1.229e+45	11.74	11.74	3.422e+36	6.91e-06
18625	triHPacyl.mttmmtmpu	6.138e+43	9.96	9.96	3.408e+36	6.88e-06
18626	triHPacyl.mpmmmmmmpu	2.398e+43	9.40	9.40	3.393e+36	6.85e-06
18627	triHPacyl.mtmppttmmu	7.369e+43	10.07	10.07	3.382e+36	6.83e-06
18628	triHPacyl.tmtmptpmu	7.583e+44	11.47	11.47	3.366e+36	6.79e-06
18629	triHPacyl.ppptmmmpu	8.774e+43	10.19	10.19	3.315e+36	6.69e-06
18630	triHPacyl.mtppppppu	3.537e+43	9.65	9.65	3.313e+36	6.69e-06
18631	triHPacyl.mtppmpmpu	1.821e+44	10.63	10.63	3.303e+36	6.67e-06
18632	triHPacyl.mptpmpppu	1.633e+44	10.57	10.57	3.284e+36	6.63e-06
18633	triHPacyl.pmtppptpu	9.330e+43	10.23	10.23	3.278e+36	6.62e-06
18634	triHPacyl.mptpmmtpmu	2.263e+44	10.77	10.77	3.251e+36	6.56e-06
18635	triHPacyl.mtppppmmu	3.207e+43	9.61	9.61	3.225e+36	6.51e-06
18636	triHPacyl.mttmmmpmmu	1.571e+44	10.55	10.55	3.220e+36	6.5e-06
18637	triHPacyl.mttmmtmpu	8.149e+43	10.17	10.17	3.196e+36	6.45e-06
18638	triHPacyl.mptpmmtmmu	6.570e+43	10.04	10.04	3.168e+36	6.39e-06
18639	triHPacyl.mtptmpmpmu	9.500e+43	10.26	10.26	3.166e+36	6.39e-06
18640	triHPacyl.mpmpttpmu	4.938e+44	11.25	11.25	3.165e+36	6.39e-06
18641	triHPacyl.ttpttptmu	8.586e+44	11.59	11.59	3.118e+36	6.29e-06
18642	triHPacyl.ttmpppppu	1.077e+44	10.35	10.35	3.105e+36	6.27e-06
18643	triHPacyl.mptmttmu	2.196e+44	10.78	10.78	3.097e+36	6.25e-06
18644	triHPacyl.ptmmmpmmu	5.019e+43	9.90	9.90	3.082e+36	6.22e-06
18645	triHPacyl.ptmptmpu	2.905e+43	9.58	9.58	3.073e+36	6.2e-06
18646	triHPacyl.mtttppmpmu	1.411e+44	10.52	10.52	3.051e+36	6.16e-06
18647	triHPacyl.ttttmmmmu	1.422e+44	10.53	10.53	3.041e+36	6.14e-06
18648	triHPacyl.mtppppptpu	2.006e+44	10.74	10.74	3.009e+36	6.07e-06
18649	triHPacyl.mtmtptmpu	8.460e+43	10.23	10.23	3.005e+36	6.07e-06
18650	triHPacyl.ttttppmpmu	2.426e+44	10.86	10.86	2.961e+36	5.98e-06
18651	triHPacyl.ttppptmpu	4.894e+44	11.28	11.28	2.953e+36	5.96e-06
18652	triHPacyl.pmpptpmu	1.025e+44	10.35	10.35	2.935e+36	5.92e-06
18653	triHPacyl.ttttmmmmu	4.468e+44	11.23	11.23	2.931e+36	5.92e-06
18654	triHPacyl.ptptmtmpu	4.746e+44	11.27	11.27	2.913e+36	5.88e-06
18655	triHPacyl.tppppmpmpu	2.640e+43	9.56	9.56	2.879e+36	5.81e-06
18656	triHPacyl.mmtmtmpu	1.449e+45	11.95	11.95	2.864e+36	5.78e-06
18657	triHPacyl.mtpttptmpu	8.631e+43	10.27	10.27	2.844e+36	5.74e-06
18658	triHPacyl.ttmtptmpu	3.638e+44	11.13	11.13	2.839e+36	5.73e-06
18659	triHPacyl.ppttmtmpu	8.644e+44	11.65	11.65	2.829e+36	5.71e-06
18660	triHPacyl.ppmptppmu	1.537e+43	9.25	9.25	2.792e+36	5.63e-06
18661	triHPacyl.mtmpttpmu	1.331e+44	10.54	10.54	2.788e+36	5.63e-06
18662	triHPacyl.mtmpppmmpu	1.745e+44	10.70	10.70	2.782e+36	5.62e-06
18663	triHPacyl.tmtptmmu	1.807e+45	12.11	12.11	2.738e+36	5.53e-06
18664	triHPacyl.pmttmmmmu	1.057e+45	11.79	11.79	2.708e+36	5.47e-06
18665	triHPacyl.ttmtptmmu	4.009e+44	11.22	11.22	2.703e+36	5.46e-06
18666	triHPacyl.ttptmtpu	1.662e+45	12.07	12.07	2.688e+36	5.43e-06
18667	triHPacyl.mmtmmptmpu	9.139e+44	11.71	11.71	2.676e+36	5.4e-06
18668	triHPacyl.mppptmpu	1.764e+44	10.74	10.74	2.663e+36	5.37e-06
18669	triHPacyl.mpppttppu	1.715e+44	10.72	10.72	2.655e+36	5.36e-06
18670	triHPacyl.mtmppptmpu	4.343e+43	9.90	9.90	2.650e+36	5.35e-06
18671	triHPacyl.tttppmpmu	5.755e+43	10.07	10.07	2.638e+36	5.33e-06
18672	triHPacyl.mtttmtmpu	1.845e+44	10.77	10.77	2.630e+36	5.31e-06
18673	triHPacyl.ttmppmtppu	8.826e+43	10.33	10.33	2.613e+36	5.27e-06
18674	triHPacyl.mtppmtmpu	9.783e+43	10.40	10.40	2.601e+36	5.25e-06
18675	triHPacyl.ptmpttmmpu	8.505e+43	10.33	10.33	2.556e+36	5.16e-06
18676	triHPacyl.mtmmmtppu	1.528e+44	10.68	10.68	2.550e+36	5.15e-06
18677	triHPacyl.ttppmpmpu	4.908e+43	10.00	10.00	2.543e+36	5.13e-06
18678	triHPacyl.mtttmtmpu	1.429e+44	10.64	10.64	2.541e+36	5.13e-06
18679	triHPacyl.mptmptmmu	1.232e+44	10.55	10.55	2.527e+36	5.1e-06
18680	triHPacyl.pmttmtmpu	1.397e+44	10.63	10.63	2.511e+36	5.07e-06
18681	triHPacyl.tmmtpttppu	8.127e+44	11.69	11.69	2.476e+36	5e-06
18682	triHPacyl.tppmptmpu	1.215e+44	10.56	10.56	2.465e+36	4.98e-06
18683	triHPacyl.pmpmpmpmpu	1.013e+43	9.08	9.08	2.459e+36	4.96e-06
18684	triHPacyl.tpttptmpu	2.677e+44	11.04	11.04	2.422e+36	4.89e-06
18685	triHPacyl.tptmptmpu	3.218e+44	11.16	11.16	2.400e+36	4.84e-06
18686	triHPacyl.tppmptppu	7.939e+43	10.32	10.32	2.396e+36	4.84e-06
18687	triHPacyl.pptmmmmmpu	3.514e+43	9.84	9.84	2.382e+36	4.81e-06
18688	triHPacyl.tpmtmmmmmpu	8.163e+43	10.34	10.34	2.379e+36	4.8e-06
18689	triHPacyl.mpmpttmmpu	1.223e+44	10.59	10.59	2.377e+36	4.8e-06
18690	triHPacyl.mmtmptmpu	1.171e+44	10.56	10.56	2.364e+36	4.77e-06
18691	triHPacyl.mttmmpmpu	5.885e+43	10.15	10.15	2.361e+36	4.77e-06
18692	triHPacyl.ttppmptppu	1.066e+44	10.51	10.51	2.358e+36	4.76e-06
18693	triHPacyl.ttttmtmpu	4.203e+44	11.33	11.33	2.351e+36	4.74e-06
18694	triHPacyl.mttmmmpmpu	5.109e+43	10.07	10.07	2.349e+36	4.74e-06
18695	triHPacyl.pmtmtmpmu	3.104e+44	11.15	11.15	2.336e+36	4.71e-06

18696	triHPacyl.pmptmmmpu	2.388e+44	11.00	11.00	2.323e+36	4.69e-06
18697	triHPacyl.tttmptmmpu	1.135e+44	10.56	10.56	2.320e+36	4.68e-06
18698	triHPacyl.ppttptmmpu	3.220e+44	11.18	11.18	2.313e+36	4.67e-06
18699	triHPacyl.tttmptmmpu	9.142e+43	10.43	10.43	2.301e+36	4.64e-06
18700	triHPacyl.mttmmtppmu	8.326e+43	10.38	10.38	2.284e+36	4.61e-06
18701	triHPacyl.pppmpmmpu	7.136e+42	8.93	8.93	2.236e+36	4.51e-06
18702	triHPacyl.mtmtmmpu	9.572e+43	10.48	10.48	2.231e+36	4.5e-06
18703	triHPacyl.tttmmtmmpu	2.086e+44	10.95	10.95	2.210e+36	4.46e-06
18704	triHPacyl.ttmptmmpu	3.961e+44	11.33	11.33	2.193e+36	4.43e-06
18705	triHPacyl.mtppmmpu	2.329e+43	9.65	9.65	2.189e+36	4.42e-06
18706	triHPacyl.mtppmtpu	3.351e+43	9.87	9.87	2.163e+36	4.37e-06
18707	triHPacyl.tppmtpu	1.504e+44	10.77	10.77	2.158e+36	4.36e-06
18708	triHPacyl.ttpmtpu	3.693e+44	11.31	11.31	2.122e+36	4.28e-06
18709	triHPacyl.ttpmmpu	2.498e+44	11.08	11.08	2.120e+36	4.28e-06
18710	triHPacyl.mmpmtmmpu	2.389e+44	11.06	11.06	2.112e+36	4.26e-06
18711	triHPacyl.mptmtpu	1.910e+44	10.92	10.92	2.105e+36	4.25e-06
18712	triHPacyl.ttpmtpu	6.455e+43	10.29	10.29	2.060e+36	4.16e-06
18713	triHPacyl.mmpmtmmpu	1.072e+44	10.60	10.60	2.044e+36	4.13e-06
18714	triHPacyl.mttmtpu	1.437e+44	10.77	10.77	2.035e+36	4.11e-06
18715	triHPacyl.tttmmpu	3.025e+44	11.22	11.22	2.019e+36	4.07e-06
18716	triHPacyl.mmpmtmmpu	6.995e+44	11.73	11.73	2.002e+36	4.04e-06
18717	triHPacyl.mtmtmmpu	4.592e+44	11.48	11.48	1.991e+36	4.02e-06
18718	triHPacyl.tppmtpu	7.191e+43	10.38	10.38	1.983e+36	4e-06
18719	triHPacyl.tppmtpu	8.296e+43	10.46	10.46	1.981e+36	4e-06
18720	triHPacyl.mmpmtmmpu	2.479e+44	11.12	11.12	1.980e+36	4e-06
18721	triHPacyl.pptmmtmmpu	3.206e+44	11.27	11.27	1.975e+36	3.99e-06
18722	triHPacyl.pptmmtmmpu	1.227e+44	10.70	10.70	1.972e+36	3.98e-06
18723	triHPacyl.tmmmpmmpu	5.091e+43	10.18	10.18	1.963e+36	3.96e-06
18724	triHPacyl.ptttmtpu	2.910e+44	11.22	11.22	1.954e+36	3.94e-06
18725	triHPacyl.ttmtpmmpu	3.237e+44	11.28	11.28	1.948e+36	3.93e-06
18726	triHPacyl.tppmtpu	2.946e+44	11.23	11.23	1.946e+36	3.93e-06
18727	triHPacyl.ttmppmmpu	1.825e+44	10.95	10.95	1.937e+36	3.91e-06
18728	triHPacyl.pmpmtpmmpu	1.356e+44	10.78	10.78	1.911e+36	3.86e-06
18729	triHPacyl.pmpmtpmmpu	2.294e+43	9.72	9.72	1.890e+36	3.82e-06
18730	triHPacyl.pmttptmmpu	1.285e+45	12.12	12.12	1.889e+36	3.81e-06
18731	triHPacyl.pmttptmmpu	2.117e+44	11.05	11.05	1.883e+36	3.8e-06
18732	triHPacyl.tppmmpu	5.367e+43	10.23	10.23	1.881e+36	3.8e-06
18733	triHPacyl.tppmmpu	1.145e+44	10.69	10.69	1.877e+36	3.79e-06
18734	triHPacyl.mttmtpmmpu	7.861e+43	10.46	10.46	1.874e+36	3.78e-06
18735	triHPacyl.tttmtpmmpu	1.588e+44	10.88	10.88	1.872e+36	3.78e-06
18736	triHPacyl.tppmtpmmpu	2.099e+44	11.06	11.06	1.828e+36	3.69e-06
18737	triHPacyl.ttpmtpmmpu	1.679e+44	10.93	10.93	1.820e+36	3.67e-06
18738	triHPacyl.mtppmtpmmpu	1.281e+44	10.77	10.77	1.815e+36	3.66e-06
18739	triHPacyl.mtppmtpmmpu	5.167e+43	10.24	10.24	1.798e+36	3.63e-06
18740	triHPacyl.pptmmpmmpu	9.780e+43	10.62	10.62	1.793e+36	3.62e-06
18741	triHPacyl.tppmmtmmpu	2.030e+44	11.07	11.07	1.763e+36	3.56e-06
18742	triHPacyl.tppmmpmmpu	2.011e+43	9.69	9.69	1.763e+36	3.56e-06
18743	triHPacyl.tmpmtpmmpu	1.517e+44	10.89	10.89	1.760e+36	3.55e-06
18744	triHPacyl.ttmmtmmpu	4.734e+43	10.20	10.20	1.754e+36	3.54e-06
18745	triHPacyl.mtmtmmpu	1.155e+44	10.73	10.73	1.754e+36	3.54e-06
18746	triHPacyl.mtppmtpmmpu	4.757e+43	10.21	10.21	1.742e+36	3.52e-06
18747	triHPacyl.mtppmtpmmpu	1.868e+44	11.03	11.03	1.722e+36	3.48e-06
18748	triHPacyl.mmtppmtpmmpu	1.301e+44	10.81	10.81	1.721e+36	3.47e-06
18749	triHPacyl.pppmmpmmpu	1.122e+43	9.35	9.35	1.721e+36	3.47e-06
18750	triHPacyl.mppmtpmmpu	3.588e+43	10.05	10.05	1.710e+36	3.45e-06
18751	triHPacyl.mttmtpmtpu	7.370e+43	10.49	10.49	1.692e+36	3.41e-06
18752	triHPacyl.mttmtpmmpu	1.728e+44	10.99	10.99	1.691e+36	3.41e-06
18753	triHPacyl.mmtmtpmmpu	8.973e+44	11.98	11.98	1.669e+36	3.37e-06
18754	triHPacyl.ttmppmmpu	2.192e+44	11.15	11.15	1.657e+36	3.34e-06
18755	triHPacyl.tmttptmtpu	7.538e+44	11.89	11.89	1.651e+36	3.33e-06
18756	triHPacyl.pmpmmpmmpu	9.457e+42	9.28	9.28	1.650e+36	3.33e-06
18757	triHPacyl.tmpmtpmtpu	7.652e+44	11.90	11.90	1.634e+36	3.3e-06
18758	triHPacyl.mmtmtpmtpu	3.313e+44	11.40	11.40	1.631e+36	3.29e-06
18759	triHPacyl.mtppmmpmmpu	2.521e+44	11.24	11.24	1.628e+36	3.29e-06
18760	triHPacyl.ttmppmmpu	1.578e+44	10.97	10.97	1.620e+36	3.27e-06
18761	triHPacyl.tppmmpmmpu	3.271e+43	10.03	10.03	1.609e+36	3.25e-06
18762	triHPacyl.mptmmtmmpu	2.013e+44	11.12	11.12	1.606e+36	3.24e-06
18763	triHPacyl.tttmtpmmpu	2.698e+44	11.29	11.29	1.603e+36	3.24e-06
18764	triHPacyl.mtmtmtpmmpu	6.421e+43	10.44	10.44	1.600e+36	3.23e-06
18765	triHPacyl.mptmmpmmpu	1.624e+44	10.99	10.99	1.599e+36	3.23e-06
18766	triHPacyl.mtmmmpmmpu	1.596e+44	10.99	10.99	1.578e+36	3.19e-06
18767	triHPacyl.tttmtpmmpu	2.194e+44	11.18	11.18	1.570e+36	3.17e-06

18768	triHPacyl.mtptppmmmu	1.165e+44	10.80	10.80	1.570e+36	3.17e-06
18769	triHPacyl.mtppmttppu	6.838e+44	11.86	11.86	1.561e+36	3.15e-06
18770	triHPacyl.ptttmmtppu	2.231e+44	11.19	11.19	1.560e+36	3.15e-06
18771	triHPacyl.mmpmpmtppu	5.408e+44	11.73	11.73	1.542e+36	3.11e-06
18772	triHPacyl.mpptpmpmpu	1.438e+44	10.94	10.94	1.541e+36	3.11e-06
18773	triHPacyl.mtmmtmmmmu	2.354e+44	11.24	11.24	1.527e+36	3.08e-06
18774	triHPacyl.mtptpppppu	1.738e+44	11.06	11.06	1.522e+36	3.07e-06
18775	triHPacyl.tpptptmmpu	3.482e+44	11.48	11.48	1.498e+36	3.02e-06
18776	triHPacyl.mtmtppmmmpu	3.069e+44	11.41	11.41	1.494e+36	3.02e-06
18777	triHPacyl.mtmmtttmmu	1.208e+44	10.86	10.86	1.486e+36	3e-06
18778	triHPacyl.tptmppmmmu	7.989e+44	12.01	12.01	1.435e+36	2.9e-06
18779	triHPacyl.mttmmmpmpu	1.075e+44	10.81	10.81	1.432e+36	2.89e-06
18780	triHPacyl.mtmmpmmmpu	1.230e+44	10.89	10.89	1.431e+36	2.89e-06
18781	triHPacyl.mpmtptmmmu	6.003e+43	10.47	10.47	1.427e+36	2.88e-06
18782	triHPacyl.mpptmttppu	6.823e+44	11.92	11.92	1.425e+36	2.88e-06
18783	triHPacyl.mtptttmmu	7.587e+43	10.61	10.61	1.410e+36	2.85e-06
18784	triHPacyl.mmpmpppppu	3.890e+44	11.59	11.59	1.395e+36	2.82e-06
18785	triHPacyl.pmttptmpu	6.565e+44	11.91	11.91	1.391e+36	2.81e-06
18786	triHPacyl.tmtptpppu	1.175e+44	10.89	10.89	1.374e+36	2.77e-06
18787	triHPacyl.tpmmtmmmu	5.764e+43	10.47	10.47	1.369e+36	2.76e-06
18788	triHPacyl.ttmtptppu	5.831e+44	11.85	11.85	1.355e+36	2.73e-06
18789	triHPacyl.ttttptmmpu	7.181e+44	11.98	11.98	1.348e+36	2.72e-06
18790	triHPacyl.tmpppppmpu	1.413e+44	11.01	11.01	1.343e+36	2.71e-06
18791	triHPacyl.mtppmtppu	1.263e+44	10.95	10.95	1.326e+36	2.68e-06
18792	triHPacyl.ttmppmmmpu	1.009e+44	10.82	10.82	1.323e+36	2.67e-06
18793	triHPacyl.mpmmpppmmu	6.489e+43	10.56	10.56	1.318e+36	2.66e-06
18794	triHPacyl.tpptptppu	9.220e+44	12.15	12.15	1.302e+36	2.63e-06
18795	triHPacyl.ttmmpmpmpu	6.050e+43	10.53	10.53	1.296e+36	2.62e-06
18796	triHPacyl.tppppmmmpu	2.548e+44	11.39	11.39	1.277e+36	2.58e-06
18797	triHPacyl.tpmmpmtmmu	3.826e+44	11.64	11.64	1.271e+36	2.57e-06
18798	triHPacyl.mtmtptmpu	2.768e+44	11.46	11.46	1.240e+36	2.5e-06
18799	triHPacyl.tpmppmtppu	8.949e+43	10.79	10.79	1.238e+36	2.5e-06
18800	triHPacyl.ttmppptmmu	2.022e+44	11.27	11.27	1.238e+36	2.5e-06
18801	triHPacyl.mpttpttppu	2.539e+44	11.41	11.41	1.235e+36	2.49e-06
18802	triHPacyl.pttpmttppu	1.161e+44	10.95	10.95	1.230e+36	2.48e-06
18803	triHPacyl.pmttpttppu	4.122e+44	11.70	11.70	1.228e+36	2.48e-06
18804	triHPacyl.ttttptmmmu	7.593e+44	12.07	12.07	1.216e+36	2.45e-06
18805	triHPacyl.ttmmtmmmpu	4.538e+43	10.40	10.40	1.213e+36	2.45e-06
18806	triHPacyl.ptpmpmmmpu	1.140e+44	10.95	10.95	1.206e+36	2.43e-06
18807	triHPacyl.tpptptmmpu	1.268e+45	12.38	12.38	1.206e+36	2.43e-06
18808	triHPacyl.mppptpmmmpu	1.085e+44	10.92	10.92	1.205e+36	2.43e-06
18809	triHPacyl.tptpttppu	2.132e+44	11.32	11.32	1.203e+36	2.43e-06
18810	triHPacyl.mtppmtppu	6.823e+43	10.64	10.64	1.202e+36	2.43e-06
18811	triHPacyl.tppmpmpmpu	6.910e+43	10.65	10.65	1.202e+36	2.43e-06
18812	triHPacyl.mtmppmmmpu	6.530e+43	10.62	10.62	1.196e+36	2.41e-06
18813	triHPacyl.mmpmmppppu	1.813e+44	11.23	11.23	1.187e+36	2.4e-06
18814	triHPacyl.pmttpttppu	1.870e+45	12.63	12.63	1.182e+36	2.39e-06
18815	triHPacyl.mtptmtmpu	1.970e+44	11.30	11.30	1.164e+36	2.35e-06
18816	triHPacyl.mtttmmmpu	2.384e+44	11.41	11.41	1.153e+36	2.33e-06
18817	triHPacyl.ttpmpmmmpu	8.346e+43	10.79	10.79	1.153e+36	2.33e-06
18818	triHPacyl.tpttppmpu	3.140e+44	11.58	11.58	1.148e+36	2.32e-06
18819	triHPacyl.ttmtppmmmpu	5.421e+44	11.91	11.91	1.140e+36	2.3e-06
18820	triHPacyl.mpttmtmpu	2.548e+44	11.47	11.47	1.125e+36	2.27e-06
18821	triHPacyl.mppmmtppu	5.133e+44	11.89	11.89	1.111e+36	2.24e-06
18822	triHPacyl.ppttmmmpu	1.674e+44	11.23	11.23	1.107e+36	2.23e-06
18823	triHPacyl.mtmmpmtppu	3.435e+44	11.66	11.66	1.103e+36	2.23e-06
18824	triHPacyl.tmpmptppu	6.952e+43	10.71	10.71	1.099e+36	2.22e-06
18825	triHPacyl.mpttmmmpu	4.173e+44	11.78	11.78	1.097e+36	2.21e-06
18826	triHPacyl.mtppmmtpu	2.380e+44	11.44	11.44	1.097e+36	2.21e-06
18827	triHPacyl.tmpppptmpu	4.950e+44	11.89	11.89	1.085e+36	2.19e-06
18828	triHPacyl.pmppttmmu	6.236e+44	12.02	12.02	1.085e+36	2.19e-06
18829	triHPacyl.mmtmmmpmpu	2.154e+44	11.40	11.40	1.075e+36	2.17e-06
18830	triHPacyl.ttmtptmpu	4.726e+44	11.87	11.87	1.065e+36	2.15e-06
18831	triHPacyl.pmptmtmmu	4.446e+44	11.84	11.84	1.062e+36	2.14e-06
18832	triHPacyl.tppppmmmpu	9.031e+44	12.26	12.26	1.053e+36	2.13e-06
18833	triHPacyl.mtptpttmmu	3.342e+44	11.67	11.67	1.046e+36	2.11e-06
18834	triHPacyl.tttpttppu	1.980e+44	11.37	11.37	1.034e+36	2.09e-06
18835	triHPacyl.mppmttppu	9.733e+43	10.95	10.95	1.033e+36	2.09e-06
18836	triHPacyl.mptmmmpmpu	2.993e+44	11.62	11.62	1.031e+36	2.08e-06
18837	triHPacyl.mtmtppmmppu	7.111e+44	12.14	12.14	1.016e+36	2.05e-06
18838	triHPacyl.tpttptppu	5.099e+44	11.95	11.95	1.009e+36	2.04e-06
18839	triHPacyl.tpttpttmmu	2.711e+44	11.57	11.57	1.006e+36	2.03e-06

18840	triHPacyl.tmpppptppu	4.492e+44	11.87	11.87	1.005e+36	2.03e-06
18841	triHPacyl.pmttmppmmu	2.508e+44	11.53	11.53	9.978e+35	2.01e-06
18842	triHPacyl.mppmtttmmu	8.677e+44	12.27	12.27	9.974e+35	2.01e-06
18843	triHPacyl.tttmpptppu	7.744e+43	10.83	10.83	9.949e+35	2.01e-06
18844	triHPacyl.mppmmtpppu	3.512e+43	10.37	10.37	9.758e+35	1.97e-06
18845	triHPacyl.mpttmmpmmu	1.260e+44	11.13	11.13	9.753e+35	1.97e-06
18846	triHPacyl.mttmtttmmu	1.570e+44	11.27	11.27	9.740e+35	1.97e-06
18847	triHPacyl.tttppmmmmu	1.217e+44	11.12	11.12	9.671e+35	1.95e-06
18848	triHPacyl.mtmppmmmmu	1.433e+44	11.22	11.22	9.598e+35	1.94e-06
18849	triHPacyl.mtmppmtmpu	1.312e+44	11.17	11.17	9.545e+35	1.93e-06
18850	triHPacyl.tppmmmtppu	1.184e+44	11.11	11.11	9.486e+35	1.91e-06
18851	triHPacyl.mpppmtmpu	9.795e+43	11.00	11.00	9.477e+35	1.91e-06
18852	triHPacyl.mppppmmmpu	2.682e+44	11.60	11.60	9.475e+35	1.91e-06
18853	triHPacyl.ttttppmpu	1.614e+44	11.30	11.30	9.426e+35	1.9e-06
18854	triHPacyl.pppmpmpppu	3.837e+43	10.45	10.45	9.400e+35	1.9e-06
18855	triHPacyl.mtmppppmmu	4.585e+43	10.56	10.56	9.314e+35	1.88e-06
18856	triHPacyl.tptmptmpu	9.872e+43	11.02	11.02	9.288e+35	1.87e-06
18857	triHPacyl.mttptpppu	5.243e+43	10.64	10.64	9.232e+35	1.86e-06
18858	triHPacyl.mpttpmmmpu	1.948e+44	11.43	11.43	9.200e+35	1.86e-06
18859	triHPacyl.mmtptmpu	4.520e+44	11.93	11.93	9.162e+35	1.85e-06
18860	triHPacyl.mpmmtmpu	6.081e+43	10.74	10.74	9.139e+35	1.84e-06
18861	triHPacyl.mtptmtppu	1.143e+44	11.12	11.12	9.131e+35	1.84e-06
18862	triHPacyl.pmpptmpu	6.708e+43	10.80	10.80	9.108e+35	1.84e-06
18863	triHPacyl.tppmptppu	7.397e+43	10.87	10.87	8.966e+35	1.81e-06
18864	triHPacyl.ttpmptmmu	8.285e+43	10.95	10.95	8.800e+35	1.78e-06
18865	triHPacyl.tppmpmpu	2.822e+43	10.31	10.31	8.754e+35	1.77e-06
18866	triHPacyl.ttptmtmmu	2.230e+45	12.91	12.91	8.731e+35	1.76e-06
18867	triHPacyl.ppmmtmmmmu	1.229e+44	11.19	11.19	8.730e+35	1.76e-06
18868	triHPacyl.mttmmmtmmu	2.151e+44	11.53	11.53	8.511e+35	1.72e-06
18869	triHPacyl.tmppttmmu	9.191e+44	12.40	12.40	8.472e+35	1.71e-06
18870	triHPacyl.mtppmmpu	2.143e+44	11.54	11.54	8.358e+35	1.69e-06
18871	triHPacyl.mppmmmmmmu	3.151e+43	10.41	10.41	8.281e+35	1.67e-06
18872	triHPacyl.mtmpttppu	3.857e+44	11.91	11.91	8.187e+35	1.65e-06
18873	triHPacyl.mttppmpu	9.584e+43	11.08	11.08	8.178e+35	1.65e-06
18874	triHPacyl.ttmtpmpu	6.932e+43	10.89	10.89	8.142e+35	1.64e-06
18875	triHPacyl.mmpmptmmu	8.956e+43	11.04	11.04	8.140e+35	1.64e-06
18876	triHPacyl.ttmppptppu	7.393e+43	10.93	10.93	8.125e+35	1.64e-06
18877	triHPacyl.pmpptmpu	1.566e+43	10.01	10.01	8.058e+35	1.63e-06
18878	triHPacyl.ttptppmmu	3.057e+44	11.79	11.79	7.933e+35	1.6e-06
18879	triHPacyl.mmpmtmpmmu	2.819e+44	11.74	11.74	7.907e+35	1.6e-06
18880	triHPacyl.mpttpmtmpu	1.165e+44	11.22	11.22	7.808e+35	1.58e-06
18881	triHPacyl.mttppptmmu	8.866e+43	11.06	11.06	7.725e+35	1.56e-06
18882	triHPacyl.mpmtpptppu	6.120e+43	10.85	10.85	7.658e+35	1.55e-06
18883	triHPacyl.mtptpmtppu	5.580e+44	12.17	12.17	7.648e+35	1.54e-06
18884	triHPacyl.tmpptpppu	1.523e+44	11.40	11.40	7.557e+35	1.53e-06
18885	triHPacyl.mppmtmpmpu	1.012e+44	11.16	11.16	7.556e+35	1.53e-06
18886	triHPacyl.mpptpmmmpu	8.100e+43	11.04	11.04	7.405e+35	1.49e-06
18887	triHPacyl.tmppttppu	1.110e+45	12.60	12.60	7.358e+35	1.49e-06
18888	triHPacyl.mppmpmtmpu	8.672e+44	12.45	12.45	7.343e+35	1.48e-06
18889	triHPacyl.mtmtpmpmmu	9.603e+43	11.14	11.14	7.315e+35	1.48e-06
18890	triHPacyl.tpptppmmu	3.206e+44	11.86	11.86	7.293e+35	1.47e-06
18891	triHPacyl.tttmpmmmpu	1.528e+44	11.42	11.42	7.284e+35	1.47e-06
18892	triHPacyl.pptpmmmmu	9.307e+43	11.13	11.13	7.247e+35	1.46e-06
18893	triHPacyl.mptmmmmmmu	3.585e+44	11.94	11.94	7.222e+35	1.46e-06
18894	triHPacyl.pmppttppu	9.105e+44	12.49	12.49	7.220e+35	1.46e-06
18895	triHPacyl.mmpmtmpmpu	1.808e+45	12.92	12.92	6.999e+35	1.41e-06
18896	triHPacyl.mpmmtppmu	1.372e+43	10.01	10.01	6.992e+35	1.41e-06
18897	triHPacyl.mtmmtmpmpu	8.068e+43	11.07	11.07	6.987e+35	1.41e-06
18898	triHPacyl.tppmptmpu	7.118e+43	11.00	11.00	6.871e+35	1.39e-06
18899	triHPacyl.ttptpmtmpu	3.556e+44	11.96	11.96	6.865e+35	1.39e-06
18900	triHPacyl.tptpmtmmu	4.765e+44	12.14	12.14	6.857e+35	1.38e-06
18901	triHPacyl.ttmppptppu	1.713e+44	11.54	11.54	6.733e+35	1.36e-06
18902	triHPacyl.ttptpmtmmu	3.442e+44	11.96	11.96	6.698e+35	1.35e-06
18903	triHPacyl.tttppmmppu	1.480e+44	11.46	11.46	6.619e+35	1.34e-06
18904	triHPacyl.mmttmmtmpu	1.248e+45	12.75	12.75	6.458e+35	1.3e-06
18905	triHPacyl.mmpmtppmmu	2.960e+44	11.89	11.89	6.446e+35	1.3e-06
18906	triHPacyl.mptmtpppu	4.709e+44	12.17	12.17	6.431e+35	1.3e-06
18907	triHPacyl.mtmppmpppu	4.498e+43	10.77	10.77	6.430e+35	1.3e-06
18908	triHPacyl.mmpmpmpmpu	2.962e+43	10.52	10.52	6.412e+35	1.29e-06
18909	triHPacyl.mttpttppu	2.808e+44	11.87	11.87	6.324e+35	1.28e-06
18910	triHPacyl.mtmptmpmpu	6.702e+43	11.02	11.02	6.318e+35	1.28e-06
18911	triHPacyl.tppmpmtmpu	1.014e+44	11.27	11.27	6.233e+35	1.26e-06

18912	triHPacyl.tmptpppppu	8.886e+43	11.19	11.19	6.232e+35	1.26e-06
18913	triHPacyl.ttmptpppu	1.556e+43	10.16	10.16	6.218e+35	1.26e-06
18914	triHPacyl.tppmpmtmmu	1.763e+44	11.61	11.61	6.195e+35	1.25e-06
18915	triHPacyl.tmpptpppu	9.556e+44	12.61	12.61	6.188e+35	1.25e-06
18916	triHPacyl.tpmtptppu	4.073e+44	12.11	12.11	6.153e+35	1.24e-06
18917	triHPacyl.mtttmppmmu	1.550e+44	11.54	11.54	6.123e+35	1.24e-06
18918	triHPacyl.mpptpmtppu	2.419e+44	11.81	11.81	6.056e+35	1.22e-06
18919	triHPacyl.pmtptpppu	7.048e+44	12.45	12.45	6.033e+35	1.22e-06
18920	triHPacyl.pmpptpppu	1.673e+44	11.60	11.60	5.938e+35	1.2e-06
18921	triHPacyl.mpttmtmmu	2.339e+44	11.80	11.80	5.937e+35	1.2e-06
18922	triHPacyl.mmptmtmpu	7.319e+44	12.48	12.48	5.884e+35	1.19e-06
18923	triHPacyl.ttmptmpu	3.824e+44	12.11	12.11	5.800e+35	1.17e-06
18924	triHPacyl.mtttmtpu	1.330e+44	11.48	11.48	5.797e+35	1.17e-06
18925	triHPacyl.tmmmpmtmpu	5.838e+44	12.36	12.36	5.772e+35	1.16e-06
18926	triHPacyl.mppmtmtmpu	9.696e+43	11.30	11.30	5.732e+35	1.16e-06
18927	triHPacyl.mppmtmpmpu	6.567e+43	11.08	11.08	5.571e+35	1.12e-06
18928	triHPacyl.tmtppptppu	2.015e+44	11.76	11.76	5.484e+35	1.11e-06
18929	triHPacyl.mppmpmtmpu	1.323e+44	11.51	11.51	5.479e+35	1.11e-06
18930	triHPacyl.mppmpmtppu	6.380e+44	12.45	12.45	5.435e+35	1.1e-06
18931	triHPacyl.mppmpmmpu	1.329e+44	11.52	11.52	5.345e+35	1.08e-06
18932	triHPacyl.mttppmmppu	1.601e+44	11.64	11.64	5.328e+35	1.08e-06
18933	triHPacyl.tmtppmpu	2.232e+44	11.84	11.84	5.321e+35	1.07e-06
18934	triHPacyl.tmpptppmpu	5.919e+43	11.07	11.07	5.146e+35	1.04e-06
18935	triHPacyl.tppmmmmmmu	4.518e+43	10.91	10.91	5.122e+35	1.03e-06
18936	triHPacyl.mptmmmmmpu	3.195e+44	12.08	12.08	5.105e+35	1.03e-06
18937	triHPacyl.ppmmmmmmpu	1.491e+44	11.62	11.62	5.105e+35	1.03e-06
18938	triHPacyl.mtmtptppu	4.523e+44	12.29	12.29	5.038e+35	1.02e-06
18939	triHPacyl.mptmtmpu	1.142e+44	11.47	11.47	5.011e+35	1.01e-06
18940	triHPacyl.tttpttpu	6.740e+44	12.54	12.54	4.942e+35	9.97e-07
18941	triHPacyl.ttmppmmpu	1.104e+44	11.47	11.47	4.885e+35	9.86e-07
18942	triHPacyl.mpptpmtppu	2.568e+44	11.98	11.98	4.830e+35	9.75e-07
18943	triHPacyl.pmtpttpu	2.484e+44	11.96	11.96	4.821e+35	9.73e-07
18944	triHPacyl.ttmptmpu	1.262e+44	11.56	11.56	4.749e+35	9.58e-07
18945	triHPacyl.mttpttpu	3.078e+44	12.11	12.11	4.667e+35	9.42e-07
18946	triHPacyl.tppmpmpmpu	4.402e+43	10.95	10.95	4.663e+35	9.41e-07
18947	triHPacyl.mptmppppu	6.984e+43	11.23	11.23	4.637e+35	9.36e-07
18948	triHPacyl.mtptpmpu	1.772e+44	11.78	11.78	4.629e+35	9.34e-07
18949	triHPacyl.mppmtmmmu	1.912e+44	11.83	11.83	4.609e+35	9.3e-07
18950	triHPacyl.tptptmpu	9.278e+44	12.77	12.77	4.608e+35	9.3e-07
18951	triHPacyl.pppmpptppu	1.970e+44	11.85	11.85	4.592e+35	9.27e-07
18952	triHPacyl.tptpmpmpu	1.517e+44	11.71	11.71	4.500e+35	9.08e-07
18953	triHPacyl.mttppmppu	1.652e+44	11.76	11.76	4.440e+35	8.96e-07
18954	triHPacyl.tmtmpmpmpu	1.041e+44	11.50	11.50	4.400e+35	8.88e-07
18955	triHPacyl.tttmpmpmpu	1.473e+44	11.72	11.72	4.302e+35	8.68e-07
18956	triHPacyl.mppmpmtmpu	1.407e+44	11.71	11.71	4.172e+35	8.42e-07
18957	triHPacyl.mtmtptmpu	2.650e+44	12.09	12.09	4.158e+35	8.39e-07
18958	triHPacyl.mtptpmpu	3.146e+44	12.20	12.20	4.087e+35	8.25e-07
18959	triHPacyl.tmtppmpu	5.525e+44	12.53	12.53	4.082e+35	8.24e-07
18960	triHPacyl.ttpmpmmpu	1.732e+45	13.22	13.22	4.069e+35	8.21e-07
18961	triHPacyl.mpttmtmmu	1.871e+44	11.89	11.89	4.062e+35	8.2e-07
18962	triHPacyl.mmmmtmmmpu	1.371e+44	11.71	11.71	4.053e+35	8.18e-07
18963	triHPacyl.pmtptmpu	1.187e+44	11.62	11.62	4.040e+35	8.15e-07
18964	triHPacyl.tttptmmmu	4.875e+44	12.47	12.47	4.029e+35	8.13e-07
18965	triHPacyl.mppmttmmu	5.100e+44	12.50	12.50	3.965e+35	8e-07
18966	triHPacyl.mptpmtmpu	5.476e+44	12.55	12.55	3.963e+35	8e-07
18967	triHPacyl.tmptppmpu	2.207e+45	13.39	13.39	3.875e+35	7.82e-07
18968	triHPacyl.tpmtptmpu	3.962e+44	12.38	12.38	3.794e+35	7.66e-07
18969	triHPacyl.ttpmpmmmu	1.393e+44	11.76	11.76	3.771e+35	7.61e-07
18970	triHPacyl.pppmpptmpu	1.237e+44	11.70	11.70	3.736e+35	7.54e-07
18971	triHPacyl.mptpmmmmu	1.048e+44	11.60	11.60	3.730e+35	7.53e-07
18972	triHPacyl.tttmpmpmmu	1.596e+44	11.86	11.86	3.656e+35	7.38e-07
18973	triHPacyl.mmttmptppu	1.299e+45	13.12	13.12	3.603e+35	7.27e-07
18974	triHPacyl.pmpptppmpu	9.775e+43	11.59	11.59	3.547e+35	7.16e-07
18975	triHPacyl.pppppptppu	1.385e+44	11.80	11.80	3.491e+35	7.05e-07
18976	triHPacyl.ttmpppmpu	7.292e+43	11.42	11.42	3.474e+35	7.01e-07
18977	triHPacyl.mppmpmmmmu	9.411e+43	11.59	11.59	3.398e+35	6.86e-07
18978	triHPacyl.tpmtptppu	1.451e+44	11.86	11.86	3.352e+35	6.77e-07
18979	triHPacyl.mpttmtmpu	3.747e+44	12.43	12.43	3.310e+35	6.68e-07
18980	triHPacyl.pppppptmpu	7.292e+43	11.45	11.45	3.307e+35	6.67e-07
18981	triHPacyl.tpmtptmmu	2.558e+44	12.20	12.20	3.304e+35	6.67e-07
18982	triHPacyl.pmpptpppu	9.125e+44	12.97	12.97	3.276e+35	6.61e-07
18983	triHPacyl.mttptmpu	2.331e+44	12.17	12.17	3.174e+35	6.41e-07

18984	triHPacyl.tmmtpmtppu	8.957e+44	12.97	12.97	3.171e+35	6.4e-07
18985	triHPacyl.mtmtpmtpmu	6.914e+44	12.82	12.82	3.160e+35	6.38e-07
18986	triHPacyl.ttmpmtmmpu	8.533e+43	11.59	11.59	3.068e+35	6.19e-07
18987	triHPacyl.ttmppmtmpu	5.097e+43	11.28	11.28	3.068e+35	6.19e-07
18988	triHPacyl.mtttmmpppu	1.334e+44	11.86	11.86	3.055e+35	6.17e-07
18989	triHPacyl.mmptmttppu	7.312e+44	12.88	12.88	3.038e+35	6.13e-07
18990	triHPacyl.ttptmmpmpu	3.361e+44	12.42	12.42	3.010e+35	6.08e-07
18991	triHPacyl.pppmpmpmpu	1.552e+43	10.59	10.59	3.000e+35	6.05e-07
18992	triHPacyl.mtmtpmmpmu	1.426e+44	11.92	11.92	2.972e+35	6e-07
18993	triHPacyl.mpptmtmmpu	2.461e+44	12.25	12.25	2.946e+35	5.95e-07
18994	triHPacyl.mtttmmpmpu	2.036e+44	12.14	12.14	2.933e+35	5.92e-07
18995	triHPacyl.mmptmtpppu	5.572e+43	11.37	11.37	2.927e+35	5.91e-07
18996	triHPacyl.mmptmtmmu	1.259e+45	13.23	13.23	2.890e+35	5.83e-07
18997	triHPacyl.mpttpmtmmu	1.219e+44	11.84	11.84	2.876e+35	5.8e-07
18998	triHPacyl.tpttpmpppu	3.662e+44	12.51	12.51	2.809e+35	5.67e-07
18999	triHPacyl.pmpmtmmppu	7.436e+43	11.57	11.57	2.793e+35	5.64e-07
19000	triHPacyl.mmptmppppu	1.109e+44	11.81	11.81	2.752e+35	5.55e-07
19001	triHPacyl.ttttmmmpu	5.557e+44	12.77	12.77	2.751e+35	5.55e-07
19002	triHPacyl.1.642e+44	12.05	12.05	2.714e+35	5.48e-07	
19003	triHPacyl.tpttpmpppu	8.013e+44	13.01	13.01	2.683e+35	5.41e-07
19004	triHPacyl.mpptmmtmpu	7.956e+44	13.01	13.01	2.670e+35	5.39e-07
19005	triHPacyl.ttmpmpmpu	6.942e+43	11.55	11.55	2.668e+35	5.38e-07
19006	triHPacyl.mpmtpmmpu	1.879e+44	12.16	12.16	2.608e+35	5.26e-07
19007	triHPacyl.tmttpttpu	5.465e+44	12.80	12.80	2.584e+35	5.22e-07
19008	triHPacyl.mpttmtppu	5.064e+44	12.78	12.78	2.498e+35	5.04e-07
19009	triHPacyl.mmpmtppmu	8.731e+43	11.73	11.73	2.491e+35	5.03e-07
19010	triHPacyl.mppmmpmpu	2.559e+43	11.00	11.00	2.478e+35	5e-07
19011	triHPacyl.tmttpttpu	9.049e+44	13.13	13.13	2.467e+35	4.98e-07
19012	triHPacyl.mtptmtpppu	4.208e+43	11.30	11.30	2.464e+35	4.97e-07
19013	triHPacyl.ttptptpmu	6.299e+44	12.91	12.91	2.462e+35	4.97e-07
19014	triHPacyl.mtptmttppu	9.288e+44	13.16	13.16	2.418e+35	4.88e-07
19015	triHPacyl.ttptmmmmu	2.759e+44	12.44	12.44	2.405e+35	4.85e-07
19016	triHPacyl.mmptmptppu	1.428e+45	13.43	13.43	2.369e+35	4.78e-07
19017	triHPacyl.mpmtmtmmu	2.423e+43	11.00	11.00	2.365e+35	4.77e-07
19018	triHPacyl.mtttptmpu	3.791e+44	12.64	12.64	2.330e+35	4.7e-07
19019	triHPacyl.mtmppmpmpu	1.285e+44	12.00	12.00	2.316e+35	4.67e-07
19020	triHPacyl.mpttpmtmpu	3.270e+44	12.57	12.57	2.270e+35	4.58e-07
19021	triHPacyl.mpptmtpppu	9.966e+43	11.87	11.87	2.254e+35	4.55e-07
19022	triHPacyl.ttmtmppppu	2.191e+44	12.35	12.35	2.223e+35	4.49e-07
19023	triHPacyl.tmmtpmmppu	1.654e+44	12.18	12.18	2.212e+35	4.46e-07
19024	triHPacyl.mpptmmtmmu	7.919e+44	13.12	13.12	2.188e+35	4.42e-07
19025	triHPacyl.mtmmmmtmpu	2.023e+44	12.31	12.31	2.174e+35	4.39e-07
19026	triHPacyl.tpmmpptppu	6.095e+43	11.60	11.60	2.163e+35	4.37e-07
19027	triHPacyl.mppmtmmpu	1.000e+44	11.91	11.91	2.124e+35	4.29e-07
19028	triHPacyl.ttttpttpu	5.617e+44	12.93	12.93	2.124e+35	4.29e-07
19029	triHPacyl.tpmmpptmpu	2.866e+44	12.54	12.54	2.103e+35	4.24e-07
19030	triHPacyl.tttppmmmpu	4.041e+44	12.76	12.76	2.060e+35	4.16e-07
19031	triHPacyl.tpmppmtmpu	7.713e+43	11.78	11.78	2.033e+35	4.1e-07
19032	triHPacyl.mmttmpmpmu	2.084e+44	12.37	12.37	2.032e+35	4.1e-07
19033	triHPacyl.tpmppmtppu	8.984e+43	11.87	11.87	2.010e+35	4.06e-07
19034	triHPacyl.tmtpttmmu	1.368e+45	13.51	13.51	1.980e+35	4e-07
19035	triHPacyl.mtmppmtppu	2.304e+44	12.45	12.45	1.977e+35	3.99e-07
19036	triHPacyl.mpmtmmpmpu	1.476e+43	10.81	10.81	1.955e+35	3.95e-07
19037	triHPacyl.mtmppptmpu	3.649e+43	11.36	11.36	1.934e+35	3.9e-07
19038	triHPacyl.tmpptptppu	7.509e+44	13.17	13.17	1.910e+35	3.85e-07
19039	triHPacyl.mmpmtmmpmu	3.701e+43	11.38	11.38	1.895e+35	3.82e-07
19040	triHPacyl.ttpmmmmmmu	1.177e+44	12.08	12.08	1.854e+35	3.74e-07
19041	triHPacyl.mppmmptmpu	7.811e+44	13.21	13.21	1.847e+35	3.73e-07
19042	triHPacyl.mtmppptmmu	1.259e+44	12.13	12.13	1.847e+35	3.73e-07
19043	triHPacyl.mmmmpmmmpu	1.488e+43	10.86	10.86	1.832e+35	3.7e-07
19044	triHPacyl.pptpmmtppu	9.419e+44	13.34	13.34	1.805e+35	3.64e-07
19045	triHPacyl.tpttpmtmpu	1.083e+45	13.42	13.42	1.804e+35	3.64e-07
19046	triHPacyl.tpmptmmpu	1.153e+44	12.09	12.09	1.803e+35	3.64e-07
19047	triHPacyl.mpmmmmtmpu	2.299e+43	11.13	11.13	1.802e+35	3.64e-07
19048	triHPacyl.mptpmmpmpu	3.597e+45	14.14	14.14	1.800e+35	3.63e-07
19049	triHPacyl.mtmtpmmpmu	2.097e+44	12.45	12.45	1.797e+35	3.63e-07
19050	triHPacyl.mtmppmmppu	9.952e+43	12.00	12.00	1.792e+35	3.62e-07
19051	triHPacyl.tmpmptppmu	9.556e+43	11.98	11.98	1.788e+35	3.61e-07
19052	triHPacyl.mttppmtmmu	1.164e+44	12.10	12.10	1.786e+35	3.6e-07
19053	triHPacyl.mtmtmtpmmu	1.097e+44	12.07	12.07	1.764e+35	3.56e-07
19054	triHPacyl.pmtppmtppu	4.448e+44	12.93	12.93	1.702e+35	3.43e-07
19055	triHPacyl.mpttmttppu	2.280e+44	12.53	12.53	1.700e+35	3.43e-07

19056	triHPacyl.pppmpttpmu	1.165e+44	12.15	12.15	1.645e+35	3.32e-07
19057	triHPacyl.mtmtmttmmu	7.323e+43	11.87	11.87	1.639e+35	3.31e-07
19058	triHPacyl.mpmtpmmmmu	1.145e+44	12.14	12.14	1.637e+35	3.3e-07
19059	triHPacyl.mtprnmpptpu	1.386e+44	12.26	12.26	1.623e+35	3.27e-07
19060	triHPacyl.mmpmtmtmmu	1.873e+45	13.81	13.81	1.621e+35	3.27e-07
19061	triHPacyl.mtppptppu	5.237e+43	11.68	11.68	1.618e+35	3.27e-07
19062	triHPacyl.tmpmpttmmu	1.626e+44	12.38	12.38	1.549e+35	3.13e-07
19063	triHPacyl.tmpmpmppmu	2.184e+44	12.56	12.56	1.546e+35	3.12e-07
19064	triHPacyl.pppmnmmpu	3.301e+43	11.44	11.44	1.520e+35	3.07e-07
19065	triHPacyl.mtppmtppmu	5.579e+43	11.76	11.76	1.518e+35	3.06e-07
19066	triHPacyl.pppmnmmpu	7.370e+43	11.93	11.93	1.492e+35	3.01e-07
19067	triHPacyl.tpttpmmmu	7.369e+44	13.31	13.31	1.489e+35	3.01e-07
19068	triHPacyl.ttpmnmmtmu	7.214e+44	13.30	13.30	1.480e+35	2.99e-07
19069	triHPacyl.mtmmmttppu	3.854e+44	12.93	12.93	1.459e+35	2.95e-07
19070	triHPacyl.mtmtmmpmpu	1.063e+44	12.17	12.17	1.458e+35	2.94e-07
19071	triHPacyl.tmpmpmmmmu	3.679e+43	11.54	11.54	1.448e+35	2.92e-07
19072	triHPacyl.ttmtppmmpu	7.573e+43	11.97	11.97	1.441e+35	2.91e-07
19073	triHPacyl.mtptmtmmpu	5.961e+43	11.83	11.83	1.430e+35	2.89e-07
19074	triHPacyl.mtpppttppu	7.733e+43	11.99	11.99	1.427e+35	2.88e-07
19075	triHPacyl.mppmmmtppu	1.217e+44	12.26	12.26	1.421e+35	2.87e-07
19076	triHPacyl.tppmtppppu	1.363e+44	12.33	12.33	1.411e+35	2.85e-07
19077	triHPacyl.mtppmpmpu	7.698e+43	12.00	12.00	1.394e+35	2.81e-07
19078	triHPacyl.mtmmptppmu	6.843e+43	11.93	11.93	1.392e+35	2.81e-07
19079	triHPacyl.ttmtptppmu	1.556e+44	12.42	12.42	1.390e+35	2.8e-07
19080	triHPacyl.tppmnmmtmu	2.795e+44	12.78	12.78	1.370e+35	2.77e-07
19081	triHPacyl.tmpptppmpu	2.659e+44	12.76	12.76	1.351e+35	2.73e-07
19082	triHPacyl.mpttmppppu	4.669e+44	13.11	13.11	1.316e+35	2.66e-07
19083	triHPacyl.mppmmmtmmu	8.378e+44	13.46	13.46	1.306e+35	2.64e-07
19084	triHPacyl.mppmtmtpmpu	1.488e+44	12.43	12.43	1.301e+35	2.63e-07
19085	triHPacyl.tmpmpttppu	1.859e+44	12.57	12.57	1.290e+35	2.6e-07
19086	triHPacyl.tmpmpmpmpu	2.495e+43	11.37	11.37	1.290e+35	2.6e-07
19087	triHPacyl.pppmmpmtpu	1.392e+44	12.43	12.43	1.232e+35	2.49e-07
19088	triHPacyl.mptmmmtppu	1.111e+45	13.67	13.67	1.224e+35	2.47e-07
19089	triHPacyl.mppmtppppu	8.468e+43	12.16	12.16	1.167e+35	2.36e-07
19090	triHPacyl.mttmtmtpu	2.571e+44	12.83	12.83	1.157e+35	2.34e-07
19091	triHPacyl.mppmtmmtmmu	3.189e+43	11.59	11.59	1.155e+35	2.33e-07
19092	triHPacyl.mttptmtpu	3.265e+44	12.98	12.98	1.142e+35	2.3e-07
19093	triHPacyl.mmpmtmtpu	8.786e+44	13.58	13.58	1.122e+35	2.26e-07
19094	triHPacyl.mtptmtmtpu	1.334e+44	12.46	12.46	1.119e+35	2.26e-07
19095	triHPacyl.mtppppmpu	1.425e+44	12.51	12.51	1.097e+35	2.21e-07
19096	triHPacyl.mmpmtmtpu	1.665e+44	12.61	12.61	1.080e+35	2.18e-07
19097	triHPacyl.tpttpmmpu	1.145e+45	13.77	13.77	1.061e+35	2.14e-07
19098	triHPacyl.tmpmpmmpu	1.611e+43	11.24	11.24	1.041e+35	2.1e-07
19099	triHPacyl.mttppmmpmpu	1.153e+44	12.42	12.42	1.039e+35	2.1e-07
19100	triHPacyl.mppmmmtmmu	5.127e+43	11.93	11.93	1.039e+35	2.1e-07
19101	triHPacyl.mttmtmtpu	4.322e+44	13.22	13.22	1.011e+35	2.04e-07
19102	triHPacyl.tptppmmpu	1.927e+44	12.75	12.75	9.987e+34	2.02e-07
19103	triHPacyl.tppmnmmtmu	4.229e+44	13.23	13.23	9.784e+34	1.97e-07
19104	triHPacyl.mmtmmpmpu	2.516e+44	12.92	12.92	9.676e+34	1.95e-07
19105	triHPacyl.ttptpmtmu	1.128e+45	13.84	13.84	9.383e+34	1.89e-07
19106	triHPacyl.mtppmpmpu	5.751e+43	12.07	12.07	9.325e+34	1.88e-07
19107	triHPacyl.mppmtmtpu	4.119e+44	13.24	13.24	9.318e+34	1.88e-07
19108	triHPacyl.mtmtppmpu	1.314e+44	12.57	12.57	9.202e+34	1.86e-07
19109	triHPacyl.mmtppmpmpu	1.643e+44	12.71	12.71	9.018e+34	1.82e-07
19110	triHPacyl.tttptmtpu	7.295e+44	13.61	13.61	8.914e+34	1.8e-07
19111	triHPacyl.mtmmmpmtpu	3.869e+44	13.25	13.25	8.656e+34	1.75e-07
19112	triHPacyl.ttptppppu	4.966e+44	13.40	13.40	8.642e+34	1.74e-07
19113	triHPacyl.mtmtmmtppu	2.761e+44	13.05	13.05	8.526e+34	1.72e-07
19114	triHPacyl.tmpmpmmpu	1.315e+44	12.61	12.61	8.521e+34	1.72e-07
19115	triHPacyl.mtppmnmmtmu	9.657e+43	12.43	12.43	8.462e+34	1.71e-07
19116	triHPacyl.mtmtmtpmmu	4.036e+44	13.30	13.30	8.240e+34	1.66e-07
19117	triHPacyl.mttptmtpu	4.135e+44	13.32	13.32	8.123e+34	1.64e-07
19118	triHPacyl.mptmmtppu	6.907e+44	13.64	13.64	7.997e+34	1.61e-07
19119	triHPacyl.mppmnmmpu	1.946e+44	12.89	12.89	7.869e+34	1.59e-07
19120	triHPacyl.mtmmmtppu	5.274e+43	12.12	12.12	7.834e+34	1.58e-07
19121	triHPacyl.mmpmtmtpu	1.689e+45	14.19	14.19	7.711e+34	1.56e-07
19122	triHPacyl.mtppmmtmmu	3.414e+44	13.25	13.25	7.595e+34	1.53e-07
19123	triHPacyl.pppmptmmmu	3.270e+43	11.85	11.85	7.588e+34	1.53e-07
19124	triHPacyl.mptmnmmtmu	3.224e+44	13.23	13.23	7.410e+34	1.5e-07
19125	triHPacyl.mptmtpmpu	2.613e+44	13.11	13.11	7.357e+34	1.48e-07
19126	triHPacyl.tptmnmmpu	1.713e+44	12.87	12.87	7.210e+34	1.46e-07
19127	triHPacyl.ttppmpmpu	3.691e+43	11.96	11.96	7.149e+34	1.44e-07

19128	triHPacyl.mpttmmtpmu	1.846e+45	14.30	14.30	7.055e+34	1.42e-07
19129	triHPacyl.ttttptmtpu	1.000e+45	13.94	13.94	7.022e+34	1.42e-07
19130	triHPacyl.ttttppmmpu	1.948e+44	12.97	12.97	6.975e+34	1.41e-07
19131	triHPacyl.tttppppmpu	6.754e+43	12.34	12.34	6.967e+34	1.41e-07
19132	triHPacyl.mtppmmmmu	1.832e+44	12.94	12.94	6.824e+34	1.38e-07
19133	triHPacyl.mpmmtmmppu	6.052e+43	12.29	12.29	6.745e+34	1.36e-07
19134	triHPacyl.mmpmmppmu	6.865e+43	12.39	12.39	6.465e+34	1.3e-07
19135	triHPacyl.mmpmmtmmu	9.770e+43	12.60	12.60	6.461e+34	1.3e-07
19136	triHPacyl.tmpptpmpu	9.457e+44	13.96	13.96	6.443e+34	1.3e-07
19137	triHPacyl.mmpmpmpmu	1.751e+44	12.96	12.96	6.357e+34	1.28e-07
19138	triHPacyl.tpmptmmu	7.385e+43	12.46	12.46	6.225e+34	1.26e-07
19139	triHPacyl.ttttppmpu	3.150e+44	13.33	13.33	6.151e+34	1.24e-07
19140	triHPacyl.mtttmmppmu	1.976e+44	13.05	13.05	6.119e+34	1.24e-07
19141	triHPacyl.tpmtptmpu	4.589e+44	13.56	13.56	6.082e+34	1.23e-07
19142	triHPacyl.tpmptmtpu	3.822e+44	13.45	13.45	6.077e+34	1.23e-07
19143	triHPacyl.mtmtmtmmu	2.387e+43	11.82	11.82	5.843e+34	1.18e-07
19144	triHPacyl.mtmtmtmmu	5.912e+44	13.73	13.73	5.839e+34	1.18e-07
19145	triHPacyl.mtmmtpmmu	4.756e+43	12.25	12.25	5.665e+34	1.14e-07
19146	triHPacyl.mppmmpmmu	2.120e+44	13.18	13.18	5.273e+34	1.06e-07
19147	triHPacyl.mpttmmppmu	4.944e+44	13.69	13.69	5.271e+34	1.06e-07
19148	triHPacyl.mtttmtmmu	2.193e+44	13.20	13.20	5.270e+34	1.06e-07
19149	triHPacyl.mppmmpmmu	2.821e+44	13.36	13.36	5.226e+34	1.05e-07
19150	triHPacyl.mtmmmtppu	1.429e+44	12.98	12.98	5.031e+34	1.02e-07
19151	triHPacyl.ttpmpmmmu	9.489e+43	12.74	12.74	4.989e+34	1.01e-07
19152	triHPacyl.mtttppmpmu	5.102e+44	13.74	13.74	4.972e+34	1e-07
19153	triHPacyl.mtmmmpmmu	1.194e+44	12.88	12.88	4.948e+34	9.99e-08
19154	triHPacyl.mmpmmppmu	9.677e+43	12.79	12.79	4.673e+34	9.43e-08
19155	triHPacyl.tmpmpppmu	1.338e+44	12.99	12.99	4.609e+34	9.3e-08
19156	triHPacyl.mtmmppmmu	7.804e+43	12.67	12.67	4.581e+34	9.25e-08
19157	triHPacyl.tpmtptmmu	2.751e+44	13.42	13.42	4.569e+34	9.22e-08
19158	triHPacyl.mmpmmtppmu	7.884e+43	12.70	12.70	4.430e+34	8.94e-08
19159	triHPacyl.mtttmtmmu	2.707e+44	13.46	13.46	4.251e+34	8.58e-08
19160	triHPacyl.mtmmptmmu	7.349e+43	12.68	12.68	4.239e+34	8.56e-08
19161	triHPacyl.tpmptmmpu	2.373e+43	12.01	12.01	4.237e+34	8.55e-08
19162	triHPacyl.mpttmmmpu	5.297e+44	13.88	13.88	4.081e+34	8.24e-08
19163	triHPacyl.mtmtmtpmu	1.081e+44	12.96	12.96	3.914e+34	7.9e-08
19164	triHPacyl.mtmmmpmmu	1.033e+44	12.95	12.95	3.833e+34	7.74e-08
19165	triHPacyl.tpmtmppmu	1.602e+44	13.25	13.25	3.553e+34	7.17e-08
19166	triHPacyl.ttptppmmu	5.091e+44	13.96	13.96	3.467e+34	7e-08
19167	triHPacyl.pppmmpmmu	2.523e+43	12.18	12.18	3.389e+34	6.84e-08
19168	triHPacyl.tmpmptmmu	8.369e+43	12.96	12.96	3.049e+34	6.15e-08
19169	triHPacyl.mppmtpmmu	2.706e+44	13.66	13.66	3.006e+34	6.07e-08
19170	triHPacyl.mtmtmmpmu	1.675e+44	13.39	13.39	2.932e+34	5.92e-08
19171	triHPacyl.ttmmpmmpu	5.850e+43	12.79	12.79	2.827e+34	5.71e-08
19172	triHPacyl.tttppmpmu	2.177e+44	13.57	13.57	2.818e+34	5.69e-08
19173	triHPacyl.mppmmtpmu	1.052e+44	13.16	13.16	2.716e+34	5.48e-08
19174	triHPacyl.mtmtmmmpu	3.890e+44	13.95	13.95	2.661e+34	5.37e-08
19175	triHPacyl.tpmptppmu	3.827e+43	12.57	12.57	2.648e+34	5.35e-08
19176	triHPacyl.mtmmppmmu	9.950e+43	13.16	13.16	2.592e+34	5.23e-08
19177	triHPacyl.ppmtpppmu	6.553e+44	14.30	14.30	2.510e+34	5.07e-08
19178	triHPacyl.mppmmpmmu	2.789e+44	13.80	13.80	2.487e+34	5.02e-08
19179	triHPacyl.tpmmpmtpmu	3.013e+44	13.87	13.87	2.380e+34	4.8e-08
19180	triHPacyl.mmpmmtmmu	5.621e+43	12.87	12.87	2.369e+34	4.78e-08
19181	triHPacyl.mtmtmmmpu	2.460e+44	13.76	13.76	2.341e+34	4.72e-08
19182	triHPacyl.mppmmmpmu	3.286e+43	12.57	12.57	2.308e+34	4.66e-08
19183	triHPacyl.mmpmmtpmu	1.111e+44	13.29	13.29	2.297e+34	4.64e-08
19184	triHPacyl.mtptptppu	3.460e+44	13.98	13.98	2.257e+34	4.55e-08
19185	triHPacyl.mppmmmtmmu	4.861e+43	12.83	12.83	2.194e+34	4.43e-08
19186	triHPacyl.tpmmpmpmu	8.881e+43	13.22	13.22	2.076e+34	4.19e-08
19187	triHPacyl.tpmtpmpmu	1.727e+44	13.65	13.65	1.952e+34	3.94e-08
19188	triHPacyl.mmpmmtmpmu	6.790e+43	13.12	13.12	1.896e+34	3.83e-08
19189	triHPacyl.mtmmmtmpu	1.384e+44	13.58	13.58	1.765e+34	3.56e-08
19190	triHPacyl.mmpmmtmmu	1.088e+44	13.47	13.47	1.686e+34	3.4e-08
19191	triHPacyl.mpmmtppmu	6.217e+43	13.14	13.14	1.651e+34	3.33e-08
19192	triHPacyl.mtmmtpmmu	5.826e+43	13.12	13.12	1.615e+34	3.26e-08
19193	triHPacyl.ppmtpppmu	4.377e+44	14.32	14.32	1.607e+34	3.24e-08
19194	triHPacyl.mtmmmmmpu	8.942e+44	14.77	14.77	1.559e+34	3.15e-08
19195	triHPacyl.tmpmptmpu	1.508e+44	13.73	13.73	1.506e+34	3.04e-08
19196	triHPacyl.tmpmptmmu	1.399e+44	13.72	13.72	1.423e+34	2.87e-08
19197	triHPacyl.ttmtmmpmu	1.288e+44	13.68	13.68	1.389e+34	2.8e-08
19198	triHPacyl.mtmtmtpmu	4.571e+44	14.45	14.45	1.362e+34	2.75e-08
19199	triHPacyl.mtmtmmmpu	1.402e+44	13.75	13.75	1.354e+34	2.73e-08

19200	triHPacyl.mtptmtpmu	4.953e+44	14.52	14.52	1.313e+34	2.65e-08
19201	triHPacyl.mpmmmmtppu	9.269e+43	13.52	13.52	1.307e+34	2.64e-08
19202	triHPacyl.mtptmtpmu	6.682e+44	14.72	14.72	1.262e+34	2.55e-08
19203	triHPacyl.mtmppptpmu	9.573e+43	13.58	13.58	1.226e+34	2.48e-08
19204	triHPacyl.mtmmmmpmmu	7.669e+43	13.46	13.46	1.195e+34	2.41e-08
19205	triHPacyl.mttmtmtmpu	5.158e+44	14.62	14.62	1.148e+34	2.32e-08
19206	triHPacyl.mtmmmmmmpu	2.313e+44	14.19	14.19	1.066e+34	2.15e-08
19207	triHPacyl.mtmmttpppu	1.060e+44	13.77	13.77	9.937e+33	2.01e-08
19208	triHPacyl.tpmtmmpmu	1.320e+44	13.90	13.90	9.830e+33	1.98e-08
19209	triHPacyl.mtmmtmtmpu	2.084e+44	14.20	14.20	9.417e+33	1.9e-08
19210	triHPacyl.mtmmpmpppu	4.631e+43	13.31	13.31	9.397e+33	1.9e-08
19211	triHPacyl.mtmmpmmpmu	9.435e+43	13.73	13.73	9.390e+33	1.9e-08
19212	triHPacyl.mtmmtmmpmu	1.591e+44	14.06	14.06	9.162e+33	1.85e-08
19213	triHPacyl.mmpmmmmmmu	8.320e+43	13.76	13.76	7.918e+33	1.6e-08
19214	triHPacyl.mmpmmmmmpu	1.272e+44	14.04	14.04	7.540e+33	1.52e-08
19215	triHPacyl.mtmmpmmpmu	1.312e+44	14.08	14.08	7.217e+33	1.46e-08
19216	triHPacyl.mtmptmmpmu	1.467e+44	14.21	14.21	6.557e+33	1.32e-08
19217	triHPacyl.mtmmpmtmpu	1.503e+44	14.22	14.22	6.525e+33	1.32e-08
19218	triHPacyl.mtmmpmpppu	6.361e+44	15.11	15.11	6.270e+33	1.27e-08
19219	triHPacyl.mtmmmmmmpu	8.108e+44	15.27	15.27	6.138e+33	1.24e-08
19220	triHPacyl.mtmmpmmpmu	3.838e+44	14.82	14.82	6.126e+33	1.24e-08
19221	triHPacyl.tpmppmpppu	4.291e+43	13.54	13.54	5.847e+33	1.18e-08
19222	triHPacyl.tpmppmmpu	3.632e+43	13.45	13.45	5.831e+33	1.18e-08
19223	triHPacyl.mtmptmmpmu	2.726e+44	14.76	14.76	4.846e+33	9.78e-09
19224	triHPacyl.tmpmpmmpmu	1.122e+44	14.25	14.25	4.663e+33	9.41e-09
19225	triHPacyl.ppmptmpppu	4.583e+44	15.10	15.10	4.592e+33	9.27e-09
19226	triHPacyl.mtmptmtpu	4.815e+44	15.14	15.14	4.477e+33	9.04e-09
19227	triHPacyl.mtmmtmpppu	1.796e+44	14.57	14.57	4.357e+33	8.79e-09
19228	triHPacyl.mpmmttppu	8.611e+43	14.21	14.21	3.829e+33	7.73e-09
19229	triHPacyl.mtmmpmmpu	9.715e+43	14.28	14.28	3.818e+33	7.71e-09
19230	triHPacyl.tpmmpmmpmu	9.093e+43	14.27	14.27	3.688e+33	7.44e-09
19231	triHPacyl.mtmmtmmpu	5.511e+44	15.40	15.40	3.306e+33	6.67e-09
19232	triHPacyl.mpmmtmpppu	6.147e+43	14.10	14.10	3.303e+33	6.67e-09
19233	triHPacyl.mpmmttmpu	1.738e+44	14.72	14.72	3.280e+33	6.62e-09
19234	triHPacyl.mtmmtmmpu	3.748e+44	15.21	15.21	3.142e+33	6.34e-09
19235	triHPacyl.mtmmpmmpu	6.265e+43	14.14	14.14	3.132e+33	6.32e-09
19236	triHPacyl.mtmmmmmmmu	8.068e+44	15.72	15.72	2.838e+33	5.73e-09
19237	triHPacyl.mtmptmpppu	6.068e+43	14.19	14.19	2.799e+33	5.65e-09
19238	triHPacyl.mpmmtmmpu	8.643e+43	14.44	14.44	2.608e+33	5.26e-09
19239	triHPacyl.mtmmtmtpu	1.888e+45	16.31	16.31	2.489e+33	5.02e-09
19240	triHPacyl.mtmmtmmpu	9.362e+44	15.91	15.91	2.394e+33	4.83e-09
19241	triHPacyl.mtmmtmmpu	4.469e+44	15.48	15.48	2.366e+33	4.78e-09
19242	triHPacyl.ttmmpmmpu	1.235e+44	14.81	14.81	2.004e+33	4.05e-09
19243	triHPacyl.mtmmtmmpu	5.902e+43	14.38	14.38	1.975e+33	3.99e-09
19244	triHPacyl.mpmmtmmpu	1.383e+44	15.02	15.02	1.590e+33	3.21e-09
19245	triHPacyl.mpmmtmmpu	3.566e+43	14.22	14.22	1.565e+33	3.16e-09
19246	triHPacyl.mtmmtmmpu	1.084e+45	16.34	16.34	1.362e+33	2.75e-09
19247	triHPacyl.mtmmtmmpu	7.706e+44	16.15	16.15	1.315e+33	2.65e-09
19248	triHPacyl.mtmmtmmpu	6.873e+44	16.16	16.16	1.154e+33	2.33e-09
19249	triHPacyl.mtmmtmmpu	2.189e+44	15.51	15.51	1.103e+33	2.23e-09
19250	triHPacyl.mpmmtmmpu	1.435e+44	15.35	15.35	9.496e+32	1.92e-09
19251	triHPacyl.mpmmtmmpu	1.872e+44	15.57	15.57	8.490e+32	1.71e-09
19252	triHPacyl.mpmmttppu	7.406e+44	16.57	16.57	6.239e+32	1.26e-09
19253	triHPacyl.mtmptmmpu	4.185e+44	16.25	16.25	6.100e+32	1.23e-09
19254	triHPacyl.mtmmpmmpu	7.903e+43	15.40	15.40	4.765e+32	9.62e-10
19255	triHPacyl.mpmmmmpmmpu	1.383e+44	15.78	15.78	4.440e+32	8.96e-10
19256	triHPacyl.mtmptmmpu	4.972e+44	16.67	16.67	3.598e+32	7.26e-10
19257	triHPacyl.ppmppptppu	3.591e+43	15.41	15.41	2.128e+32	4.3e-10
19258	triHPacyl.mpmmmmtmmpu	4.973e+43	15.87	15.87	1.355e+32	2.74e-10
19259	triHPacyl.mpmmmmtmpu	1.680e+44	17.24	17.24	4.656e+31	9.4e-11
19260	triHPacyl.ppmppmpppu	3.536e+43	16.52	16.52	3.254e+31	6.57e-11
19261	triHPacyl.mpmmmmtmpu	2.172e+44	18.25	18.25	1.108e+31	2.24e-11
19262	triHPacyl.mpmmmmpmmpu	3.877e+43	17.46	17.46	7.451e+30	1.5e-11
19263	Total				4.955e+43	100

CO elimination from (2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)

Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

19272	n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.					
19273	%: contribution to the population (with current data set assumed 100%)					
19274	Compound	Qtot	Erel	Erel2	n*Q*MB	%
19275	-----					
19276	TS.triHPacyl.COelim.pppmmmpmpu	3.520e+43	0.01	0.01	3.464e+43	13.8
19277	TS.triHPacyl.COelim.tmmmmmtmpu	2.706e+43	0.13	0.13	2.176e+43	8.65
19278	TS.triHPacyl.COelim.pppmptmpu	2.055e+43	0.00	0.00	2.055e+43	8.17
19279	TS.triHPacyl.COelim.tmmmmmtmpu	3.101e+43	0.34	0.34	1.743e+43	6.93
19280	TS.triHPacyl.COelim.pttpmmpmpu	1.223e+44	1.72	1.72	6.824e+42	2.71
19281	TS.triHPacyl.COelim.pppmptmpu	2.171e+43	0.71	0.71	6.558e+42	2.61
19282	TS.triHPacyl.COelim.ptppmmpmpu	4.244e+43	1.21	1.21	5.588e+42	2.22
19283	TS.triHPacyl.COelim.tmtptppmu	1.221e+44	1.95	1.95	4.620e+42	1.84
19284	TS.triHPacyl.COelim.ptppmmmpmu	5.385e+43	1.48	1.48	4.511e+42	1.79
19285	TS.triHPacyl.COelim.ptmmmmmtmpu	1.446e+44	2.09	2.09	4.322e+42	1.72
19286	TS.triHPacyl.COelim.pttpmtppmu	9.205e+43	1.95	1.95	3.515e+42	1.4
19287	TS.triHPacyl.COelim.tmmmmmtmpu	6.227e+43	1.86	1.86	2.758e+42	1.1
19288	TS.triHPacyl.COelim.pppmmppmpu	1.975e+43	1.19	1.19	2.698e+42	1.07
19289	TS.triHPacyl.COelim.ptppmmpmpu	6.426e+43	1.97	1.97	2.374e+42	0.944
19290	TS.triHPacyl.COelim.pppmptmpu	1.697e+43	1.23	1.23	2.156e+42	0.857
19291	TS.triHPacyl.COelim.tmmmmmtmpu	7.094e+43	2.10	2.10	2.093e+42	0.832
19292	TS.triHPacyl.COelim.ptppmtppmu	4.730e+43	1.86	1.86	2.085e+42	0.829
19293	TS.triHPacyl.COelim.pmtppppmu	8.987e+43	2.25	2.25	2.048e+42	0.814
19294	TS.triHPacyl.COelim.ppppmpmpu	1.840e+44	2.70	2.70	1.971e+42	0.784
19295	TS.triHPacyl.COelim.pppmptmpu	2.213e+43	1.48	1.48	1.848e+42	0.735
19296	TS.triHPacyl.COelim.pptmptmpu	5.339e+43	2.01	2.01	1.826e+42	0.726
19297	TS.triHPacyl.COelim.ptppmmmmmu	7.164e+43	2.19	2.19	1.821e+42	0.724
19298	TS.triHPacyl.COelim.ptmmmmppmu	1.471e+44	2.69	2.69	1.622e+42	0.645
19299	TS.triHPacyl.COelim.pppmmmtmpu	2.519e+43	1.66	1.66	1.559e+42	0.62
19300	TS.triHPacyl.COelim.ptmmmtmpu	9.762e+43	2.48	2.48	1.532e+42	0.609
19301	TS.triHPacyl.COelim.ptmmpmpmpu	6.941e+43	2.31	2.31	1.435e+42	0.571
19302	TS.triHPacyl.COelim.pppmptmpu	3.301e+43	1.92	1.92	1.318e+42	0.524
19303	TS.triHPacyl.COelim.tppmptmpu	2.656e+44	3.19	3.19	1.265e+42	0.503
19304	TS.triHPacyl.COelim.ptppmpmpmu	4.680e+43	2.16	2.16	1.247e+42	0.496
19305	TS.triHPacyl.COelim.tppmmmtppu	4.120e+43	2.09	2.09	1.234e+42	0.491
19306	TS.triHPacyl.COelim.ptmmmmppmu	9.077e+43	2.60	2.60	1.163e+42	0.462
19307	TS.triHPacyl.COelim.ptmmmmmtmpu	2.154e+44	3.11	3.11	1.162e+42	0.462
19308	TS.triHPacyl.COelim.pttpmmpmpu	1.787e+44	3.03	3.03	1.108e+42	0.441
19309	TS.triHPacyl.COelim.pppmmmpmpu	2.532e+43	1.89	1.89	1.068e+42	0.425
19310	TS.triHPacyl.COelim.ptmmmtmpu	7.037e+43	2.51	2.51	1.048e+42	0.417
19311	TS.triHPacyl.COelim.ptmmmtppmu	1.246e+44	2.85	2.85	1.046e+42	0.416
19312	TS.triHPacyl.COelim.pppmmmtppu	1.936e+43	1.75	1.75	1.032e+42	0.41
19313	TS.triHPacyl.COelim.pptmptmpu	6.103e+43	2.44	2.44	1.025e+42	0.407
19314	TS.triHPacyl.COelim.tmtppmmpmpu	1.323e+44	2.92	2.92	9.943e+41	0.395
19315	TS.triHPacyl.COelim.tmtppmmpmpu	1.133e+44	2.85	2.85	9.481e+41	0.377
19316	TS.triHPacyl.COelim.pmtppmmpmpu	2.034e+44	3.22	3.22	9.192e+41	0.366
19317	TS.triHPacyl.COelim.tppmmpmpmu	5.788e+43	2.49	2.49	8.921e+41	0.355
19318	TS.triHPacyl.COelim.ptpppmpmpu	8.475e+43	2.72	2.72	8.903e+41	0.354
19319	TS.triHPacyl.COelim.pmtmptpppu	6.673e+43	2.58	2.58	8.763e+41	0.348
19320	TS.triHPacyl.COelim.tppmmpmpmu	3.265e+44	3.54	3.54	8.573e+41	0.341
19321	TS.triHPacyl.COelim.pttmmmpmpu	3.004e+44	3.51	3.51	8.279e+41	0.329
19322	TS.triHPacyl.COelim.tmtmmtpppu	1.232e+44	2.99	2.99	8.150e+41	0.324
19323	TS.triHPacyl.COelim.mppmmpmpmpu	7.099e+43	2.67	2.67	8.047e+41	0.32
19324	TS.triHPacyl.COelim.tmtmmmtmpu	2.970e+44	3.53	3.53	7.903e+41	0.314
19325	TS.triHPacyl.COelim.pttppppmpu	9.895e+43	2.88	2.88	7.838e+41	0.312
19326	TS.triHPacyl.COelim.pppmmpmpmpu	1.307e+43	1.68	1.68	7.798e+41	0.31
19327	TS.triHPacyl.COelim.pptpmtmpu	1.652e+44	3.24	3.24	7.214e+41	0.287
19328	TS.triHPacyl.COelim.mppmptmpmpu	7.448e+43	2.77	2.77	7.163e+41	0.285
19329	TS.triHPacyl.COelim.tmtmmmtmpu	1.475e+44	3.18	3.18	7.074e+41	0.281
19330	TS.triHPacyl.COelim.pppmptmpu	3.837e+43	2.39	2.39	7.015e+41	0.279
19331	TS.triHPacyl.COelim.ptmmmtmpu	2.169e+44	3.42	3.42	6.975e+41	0.277
19332	TS.triHPacyl.COelim.pmtppppmpu	6.888e+43	2.77	2.77	6.659e+41	0.265
19333	TS.triHPacyl.COelim.pppmmmpmpu	1.979e+43	2.03	2.03	6.598e+41	0.262
19334	TS.triHPacyl.COelim.pttpmmtmpu	3.802e+44	3.79	3.79	6.592e+41	0.262
19335	TS.triHPacyl.COelim.tppmmpmpmu	7.383e+43	2.82	2.82	6.490e+41	0.258
19336	TS.triHPacyl.COelim.ptppmmpmpu	1.025e+44	3.02	3.02	6.477e+41	0.258
19337	TS.triHPacyl.COelim.ttpmmpmpmu	1.484e+44	3.27	3.27	6.142e+41	0.244
19338	TS.triHPacyl.COelim.tmtmmtmpu	5.358e+44	4.05	4.05	5.963e+41	0.237
19339	TS.triHPacyl.COelim.pptpmtppmu	3.554e+43	2.44	2.44	5.952e+41	0.237
19340	TS.triHPacyl.COelim.pttpptppmu	8.701e+43	2.98	2.98	5.910e+41	0.235
19341	TS.triHPacyl.COelim.ptmmpmpmpu	5.891e+43	2.75	2.75	5.848e+41	0.233
19342	TS.triHPacyl.COelim.ptmmmmmpu	1.326e+44	3.24	3.24	5.773e+41	0.23
19343	TS.triHPacyl.COelim.tmtmtpppu	1.570e+44	3.35	3.35	5.731e+41	0.228

19344	TS.triHPacyl.COelim.ppppptppu	4.949e+44	4.03	4.03	5.708e+41	0.227
19345	TS.triHPacyl.COelim.pttpmtpppu	1.305e+44	3.25	3.25	5.600e+41	0.223
19346	TS.triHPacyl.COelim.tpppmppmpu	1.708e+44	3.43	3.43	5.401e+41	0.215
19347	TS.triHPacyl.COelim.pptmpttmmu	1.196e+44	3.22	3.22	5.379e+41	0.214
19348	TS.triHPacyl.COelim.tptmmtmpu	1.490e+44	3.37	3.37	5.248e+41	0.209
19349	TS.triHPacyl.COelim.ttpmmmpmu	7.649e+43	2.98	2.98	5.185e+41	0.206
19350	TS.triHPacyl.COelim.tptmmtmpu	1.340e+44	3.34	3.34	4.944e+41	0.197
19351	TS.triHPacyl.COelim.pttmmmtmmu	6.064e+44	4.25	4.25	4.871e+41	0.194
19352	TS.triHPacyl.COelim.mpppmtppmu	2.395e+44	3.71	3.71	4.757e+41	0.189
19353	TS.triHPacyl.COelim.tpmmmmmppu	3.378e+43	2.55	2.55	4.719e+41	0.188
19354	TS.triHPacyl.COelim.pppmptppmu	3.007e+43	2.48	2.48	4.686e+41	0.186
19355	TS.triHPacyl.COelim.tttppmppmu	1.197e+44	3.33	3.33	4.504e+41	0.179
19356	TS.triHPacyl.COelim.pppppppmpu	3.607e+44	3.99	3.99	4.482e+41	0.178
19357	TS.triHPacyl.COelim.mmmmmmtmpu	2.851e+44	3.88	3.88	4.286e+41	0.17
19358	TS.triHPacyl.COelim.pttpptppmu	1.249e+44	3.39	3.39	4.235e+41	0.168
19359	TS.triHPacyl.COelim.pppmptppmu	1.276e+44	3.41	3.41	4.205e+41	0.167
19360	TS.triHPacyl.COelim.pttmtmpu	8.162e+44	4.53	4.53	4.066e+41	0.162
19361	TS.triHPacyl.COelim.ptmmpptmpu	1.382e+44	3.48	3.48	4.050e+41	0.161
19362	TS.triHPacyl.COelim.tpppptppmu	3.226e+44	4.00	4.00	3.903e+41	0.155
19363	TS.triHPacyl.COelim.pttpmmpmpu	3.438e+44	4.06	4.06	3.822e+41	0.152
19364	TS.triHPacyl.COelim.tmmpttppmu	7.715e+43	3.17	3.17	3.778e+41	0.15
19365	TS.triHPacyl.COelim.mppmptmpu	3.622e+43	2.72	2.72	3.768e+41	0.15
19366	TS.triHPacyl.COelim.ttmmtppmu	8.127e+43	3.21	3.21	3.739e+41	0.149
19367	TS.triHPacyl.COelim.pmtppptppu	1.681e+44	3.66	3.66	3.622e+41	0.144
19368	TS.triHPacyl.COelim.tmtmmmtmmu	8.519e+44	4.63	4.63	3.591e+41	0.143
19369	TS.triHPacyl.COelim.ttmmtmpu	1.429e+44	3.58	3.58	3.501e+41	0.139
19370	TS.triHPacyl.COelim.ptmmpmmpu	1.681e+44	3.68	3.68	3.490e+41	0.139
19371	TS.triHPacyl.COelim.ptmtmmpmpu	3.395e+44	4.10	4.10	3.486e+41	0.139
19372	TS.triHPacyl.COelim.pttmmmmmmu	8.769e+44	4.67	4.67	3.464e+41	0.138
19373	TS.triHPacyl.COelim.tmtmmtmmu	3.702e+44	4.16	4.16	3.422e+41	0.136
19374	TS.triHPacyl.COelim.pppmmpmmpu	4.757e+43	2.94	2.94	3.408e+41	0.136
19375	TS.triHPacyl.COelim.pppmptppmu	4.451e+43	2.91	2.91	3.406e+41	0.135
19376	TS.triHPacyl.COelim.pttppmpppu	9.551e+43	3.36	3.36	3.400e+41	0.135
19377	TS.triHPacyl.COelim.pptppptmpu	1.871e+44	3.76	3.76	3.397e+41	0.135
19378	TS.triHPacyl.COelim.pmpppptppmu	8.630e+43	3.31	3.31	3.361e+41	0.134
19379	TS.triHPacyl.COelim.tppmptmpu	4.941e+43	2.99	2.99	3.284e+41	0.131
19380	TS.triHPacyl.COelim.pttmmppppu	1.570e+44	3.69	3.69	3.214e+41	0.128
19381	TS.triHPacyl.COelim.ptmmpptmpu	1.394e+44	3.62	3.62	3.200e+41	0.127
19382	TS.triHPacyl.COelim.ttpmmtmpu	5.866e+44	4.51	4.51	3.031e+41	0.121
19383	TS.triHPacyl.COelim.ttmmmmmppu	1.887e+44	3.84	3.84	3.025e+41	0.12
19384	TS.triHPacyl.COelim.pttmmptmpu	1.528e+44	3.72	3.72	2.970e+41	0.118
19385	TS.triHPacyl.COelim.pttmmmtmmu	2.158e+45	5.30	5.30	2.959e+41	0.118
19386	TS.triHPacyl.COelim.mppmppppmu	2.689e+43	2.69	2.69	2.959e+41	0.118
19387	TS.triHPacyl.COelim.pttmtpppu	2.034e+44	3.90	3.90	2.936e+41	0.117
19388	TS.triHPacyl.COelim.pttpptppmu	1.588e+44	3.75	3.75	2.934e+41	0.117
19389	TS.triHPacyl.COelim.tppmpttmmu	1.740e+44	3.81	3.81	2.934e+41	0.117
19390	TS.triHPacyl.COelim.mmtppmppmu	2.357e+44	3.99	3.99	2.922e+41	0.116
19391	TS.triHPacyl.COelim.tmmmpmpppu	1.063e+44	3.52	3.52	2.883e+41	0.115
19392	TS.triHPacyl.COelim.mptppptmmu	1.635e+44	3.78	3.78	2.862e+41	0.114
19393	TS.triHPacyl.COelim.tttmmppppu	9.278e+43	3.45	3.45	2.858e+41	0.114
19394	TS.triHPacyl.COelim.tptmptppmu	1.361e+44	3.68	3.68	2.840e+41	0.113
19395	TS.triHPacyl.COelim.ptppmmpmmu	1.272e+44	3.66	3.66	2.764e+41	0.11
19396	TS.triHPacyl.COelim.pttmtpppu	8.299e+43	3.41	3.41	2.718e+41	0.108
19397	TS.triHPacyl.COelim.pmtpppppu	9.547e+43	3.50	3.50	2.708e+41	0.108
19398	TS.triHPacyl.COelim.tmtmptmpu	2.217e+44	4.00	4.00	2.686e+41	0.107
19399	TS.triHPacyl.COelim.tmmmmmpmpu	4.772e+43	3.09	3.09	2.655e+41	0.106
19400	TS.triHPacyl.COelim.pppmmtmpu	1.337e+44	3.71	3.71	2.654e+41	0.106
19401	TS.triHPacyl.COelim.mptppmtmpu	1.631e+44	3.83	3.83	2.646e+41	0.105
19402	TS.triHPacyl.COelim.tttppmmmpmu	1.815e+44	3.89	3.89	2.644e+41	0.105
19403	TS.triHPacyl.COelim.mppmppmmpu	5.793e+43	3.23	3.23	2.563e+41	0.102
19404	TS.triHPacyl.COelim.ptmmptmmu	1.171e+44	3.65	3.65	2.560e+41	0.102
19405	TS.triHPacyl.COelim.tptmptppmu	2.130e+44	4.01	4.01	2.553e+41	0.102
19406	TS.triHPacyl.COelim.pttpmtppmu	1.270e+44	3.70	3.70	2.543e+41	0.101
19407	TS.triHPacyl.COelim.ptppmmpmmu	1.443e+44	3.79	3.79	2.519e+41	0.1
19408	TS.triHPacyl.COelim.pttpmtmpu	3.344e+44	4.30	4.30	2.479e+41	0.0986
19409	TS.triHPacyl.COelim.ptppmmtmmu	1.304e+44	3.74	3.74	2.473e+41	0.0983
19410	TS.triHPacyl.COelim.ptppmmpmu	7.457e+43	3.41	3.41	2.450e+41	0.0974
19411	TS.triHPacyl.COelim.ppppmtmmu	5.011e+43	3.18	3.18	2.425e+41	0.0964
19412	TS.triHPacyl.COelim.pttmttppmu	1.492e+44	3.83	3.83	2.417e+41	0.0961
19413	TS.triHPacyl.COelim.tmmmmppppu	3.792e+43	3.01	3.01	2.415e+41	0.096
19414	TS.triHPacyl.COelim.ttpmptppmu	6.254e+43	3.31	3.31	2.407e+41	0.0957
19415	TS.triHPacyl.COelim.tppmmtmmu	2.350e+44	4.11	4.11	2.387e+41	0.0949

19416	TS.triHPacyl.COelim.pppppptppu	4.734e+44	4.53	4.53	2.355e+41	0.0936
19417	TS.triHPacyl.COelim.pttmmptmmu	3.703e+44	4.39	4.39	2.346e+41	0.0933
19418	TS.triHPacyl.COelim.ptmmmtmmu	1.430e+44	3.85	3.85	2.226e+41	0.0885
19419	TS.triHPacyl.COelim.tttppmppmu	6.363e+44	4.75	4.75	2.207e+41	0.0878
19420	TS.triHPacyl.COelim.ttmmmpmpu	7.491e+43	3.48	3.48	2.202e+41	0.0876
19421	TS.triHPacyl.COelim.tmtmpmpppu	1.565e+44	3.92	3.92	2.199e+41	0.0874
19422	TS.triHPacyl.COelim.ptpppmtpmmu	9.202e+43	3.61	3.61	2.169e+41	0.0863
19423	TS.triHPacyl.COelim.ptmmmmmpmu	3.628e+44	4.43	4.43	2.162e+41	0.086
19424	TS.triHPacyl.COelim.ptmmpptmpu	1.257e+44	3.80	3.80	2.132e+41	0.0848
19425	TS.triHPacyl.COelim.pppmpmmpmu	2.595e+43	2.87	2.87	2.114e+41	0.0841
19426	TS.triHPacyl.COelim.pptmpptmmu	1.205e+44	3.79	3.79	2.107e+41	0.0838
19427	TS.triHPacyl.COelim.pttppppmmu	1.218e+44	3.81	3.81	2.056e+41	0.0818
19428	TS.triHPacyl.COelim.mppmmptppu	1.216e+44	3.81	3.81	2.048e+41	0.0814
19429	TS.triHPacyl.COelim.pttppptmpu	2.655e+44	4.27	4.27	2.046e+41	0.0814
19430	TS.triHPacyl.COelim.mppmpmmpu	4.278e+43	3.21	3.21	1.979e+41	0.0787
19431	TS.triHPacyl.COelim.tptmpmmpmu	1.219e+44	3.83	3.83	1.978e+41	0.0786
19432	TS.triHPacyl.COelim.pttppmmpmu	1.604e+44	4.00	4.00	1.955e+41	0.0777
19433	TS.triHPacyl.COelim.tttptmtpmu	2.419e+44	4.25	4.25	1.934e+41	0.0769
19434	TS.triHPacyl.COelim.mppmptmpu	1.275e+43	2.96	2.96	1.930e+41	0.0767
19435	TS.triHPacyl.COelim.tptmmpmmpu	1.217e+44	3.86	3.86	1.890e+41	0.0751
19436	TS.triHPacyl.COelim.pptmptppu	8.624e+43	3.66	3.66	1.863e+41	0.0741
19437	TS.triHPacyl.COelim.tmtppmpppu	1.883e+44	4.12	4.12	1.863e+41	0.0741
19438	TS.triHPacyl.COelim.tpmmmtppu	2.542e+44	4.31	4.31	1.835e+41	0.073
19439	TS.triHPacyl.COelim.pttmmmpmmpu	4.935e+44	4.72	4.72	1.810e+41	0.072
19440	TS.triHPacyl.COelim.pppppptmpu	3.003e+44	4.43	4.43	1.779e+41	0.0707
19441	TS.triHPacyl.COelim.ptmmpptppu	2.688e+44	4.36	4.36	1.777e+41	0.0707
19442	TS.triHPacyl.COelim.tpmmmtmmpu	6.289e+43	3.50	3.50	1.775e+41	0.0706
19443	TS.triHPacyl.COelim.tmtppmpppu	2.113e+44	4.22	4.22	1.772e+41	0.0704
19444	TS.triHPacyl.COelim.pmmmpptppu	2.478e+43	2.95	2.95	1.771e+41	0.0704
19445	TS.triHPacyl.COelim.pttmtptmpu	2.197e+44	4.26	4.26	1.741e+41	0.0692
19446	TS.triHPacyl.COelim.tmmmtmmu	8.397e+43	3.69	3.69	1.725e+41	0.0686
19447	TS.triHPacyl.COelim.tmmmtpppu	2.138e+43	2.87	2.87	1.723e+41	0.0685
19448	TS.triHPacyl.COelim.pppppmmpu	2.247e+44	4.28	4.28	1.710e+41	0.068
19449	TS.triHPacyl.COelim.pttmmmpmpu	7.512e+44	5.01	5.01	1.673e+41	0.0665
19450	TS.triHPacyl.COelim.ptmmpmmpu	9.980e+43	3.81	3.81	1.660e+41	0.066
19451	TS.triHPacyl.COelim.tppppppmu	2.229e+44	4.30	4.30	1.656e+41	0.0658
19452	TS.triHPacyl.COelim.tmmmttppu	7.483e+43	3.65	3.65	1.653e+41	0.0657
19453	TS.triHPacyl.COelim.ptmmmmmpu	2.451e+44	4.36	4.36	1.641e+41	0.0653
19454	TS.triHPacyl.COelim.tmtmppppu	7.878e+43	3.69	3.69	1.617e+41	0.0643
19455	TS.triHPacyl.COelim.tmmmttmpu	2.781e+44	4.46	4.46	1.559e+41	0.062
19456	TS.triHPacyl.COelim.pttmmppmpu	6.270e+44	4.96	4.96	1.523e+41	0.0606
19457	TS.triHPacyl.COelim.tppmptmpu	4.044e+43	3.34	3.34	1.500e+41	0.0596
19458	TS.triHPacyl.COelim.tmmmtmmpu	1.895e+44	4.26	4.26	1.482e+41	0.0589
19459	TS.triHPacyl.COelim.tmmppppmpu	1.062e+44	3.92	3.92	1.474e+41	0.0586
19460	TS.triHPacyl.COelim.tptmmmpmpu	4.261e+44	4.76	4.76	1.462e+41	0.0581
19461	TS.triHPacyl.COelim.tttptmmpmu	1.567e+44	4.16	4.16	1.457e+41	0.0579
19462	TS.triHPacyl.COelim.pttmtmmu	2.949e+44	4.54	4.54	1.449e+41	0.0576
19463	TS.triHPacyl.COelim.tmtpppppmu	1.554e+44	4.17	4.17	1.418e+41	0.0564
19464	TS.triHPacyl.COelim.pmmmpmpppu	2.261e+43	3.03	3.03	1.404e+41	0.0558
19465	TS.triHPacyl.COelim.pppppptmpu	4.672e+44	4.84	4.84	1.393e+41	0.0554
19466	TS.triHPacyl.COelim.pmmmpptmmu	1.375e+44	4.11	4.11	1.384e+41	0.055
19467	TS.triHPacyl.COelim.pppmptppu	1.300e+44	4.08	4.08	1.384e+41	0.055
19468	TS.triHPacyl.COelim.tpmmmtpppu	1.480e+44	4.16	4.16	1.382e+41	0.055
19469	TS.triHPacyl.COelim.tmpmptppmu	4.463e+43	3.45	3.45	1.365e+41	0.0543
19470	TS.triHPacyl.COelim.pttmmmpmmpu	4.845e+44	4.88	4.88	1.354e+41	0.0538
19471	TS.triHPacyl.COelim.pptptmpmu	4.283e+44	4.83	4.83	1.301e+41	0.0517
19472	TS.triHPacyl.COelim.pmmmmpppu	2.321e+43	3.10	3.10	1.288e+41	0.0512
19473	TS.triHPacyl.COelim.tmtmptmmu	5.687e+44	5.01	5.01	1.269e+41	0.0505
19474	TS.triHPacyl.COelim.tppmptmmpu	8.882e+43	3.93	3.93	1.225e+41	0.0487
19475	TS.triHPacyl.COelim.tppmmpmmpu	4.900e+43	3.58	3.58	1.206e+41	0.048
19476	TS.triHPacyl.COelim.tmmptppmu	6.236e+43	3.73	3.73	1.202e+41	0.0478
19477	TS.triHPacyl.COelim.tptmmpmmpu	8.896e+43	3.94	3.94	1.200e+41	0.0477
19478	TS.triHPacyl.COelim.tpppmtppu	6.964e+44	5.18	5.18	1.182e+41	0.047
19479	TS.triHPacyl.COelim.tmmmmmpmu	1.030e+44	4.04	4.04	1.180e+41	0.0469
19480	TS.triHPacyl.COelim.ptmmpptppu	2.399e+44	4.54	4.54	1.179e+41	0.0469
19481	TS.triHPacyl.COelim.pttppppppu	2.499e+44	4.57	4.57	1.170e+41	0.0465
19482	TS.triHPacyl.COelim.tppmmpmmpu	2.900e+44	4.67	4.67	1.142e+41	0.0454
19483	TS.triHPacyl.COelim.tppmptmpu	1.666e+44	4.34	4.34	1.141e+41	0.0454
19484	TS.triHPacyl.COelim.tpmmmmmpu	7.101e+43	3.84	3.84	1.139e+41	0.0453
19485	TS.triHPacyl.COelim.pttmmmpmmpu	5.329e+44	5.04	5.04	1.130e+41	0.0449
19486	TS.triHPacyl.COelim.tmmmmmtppu	1.001e+44	4.05	4.05	1.117e+41	0.0444
19487	TS.triHPacyl.COelim.ptpppmtmpu	9.467e+43	4.02	4.02	1.107e+41	0.044

19488	TS.triHPacyl.COelim.pmtppppppu	1.076e+44	4.11	4.11	1.092e+41	0.0434
19489	TS.triHPacyl.COelim.tttmmmtmmu	4.011e+44	4.89	4.89	1.091e+41	0.0434
19490	TS.triHPacyl.COelim.tmtppmmpmmu	2.361e+44	4.58	4.58	1.089e+41	0.0433
19491	TS.triHPacyl.COelim.ptttmmtmpu	6.401e+44	5.18	5.18	1.086e+41	0.0432
19492	TS.triHPacyl.COelim.tmtpptmpu	5.141e+44	5.05	5.05	1.083e+41	0.0431
19493	TS.triHPacyl.COelim.tptmmtppu	1.739e+44	4.41	4.41	1.065e+41	0.0423
19494	TS.triHPacyl.COelim.tmtmmtppmu	2.451e+44	4.62	4.62	1.056e+41	0.042
19495	TS.triHPacyl.COelim.ttpptpppu	4.789e+43	3.65	3.65	1.050e+41	0.0418
19496	TS.triHPacyl.COelim.tptmmtppmu	1.979e+44	4.50	4.50	1.047e+41	0.0416
19497	TS.triHPacyl.COelim.tppmmtppu	1.058e+45	5.50	5.50	1.044e+41	0.0415
19498	TS.triHPacyl.COelim.tttmmpmpu	8.527e+44	5.37	5.37	1.040e+41	0.0413
19499	TS.triHPacyl.COelim.tttmmmtmpu	1.489e+44	4.34	4.34	1.024e+41	0.0407
19500	TS.triHPacyl.COelim.pmpppppmmu	2.675e+43	3.32	3.32	1.020e+41	0.0405
19501	TS.triHPacyl.COelim.pptmptpppu	2.929e+43	3.37	3.37	1.019e+41	0.0405
19502	TS.triHPacyl.COelim.tttmptppmu	9.902e+43	4.10	4.10	1.013e+41	0.0403
19503	TS.triHPacyl.COelim.mmmmmmtmpu	7.917e+43	3.98	3.98	9.939e+40	0.0395
19504	TS.triHPacyl.COelim.ptmmtmpppu	2.691e+44	4.74	4.74	9.542e+40	0.0379
19505	TS.triHPacyl.COelim.ptmmtppmu	2.471e+44	4.70	4.70	9.363e+40	0.0372
19506	TS.triHPacyl.COelim.ptppmtppmu	1.263e+44	4.30	4.30	9.302e+40	0.037
19507	TS.triHPacyl.COelim.ptmmtmpmu	8.802e+44	5.46	5.46	9.197e+40	0.0366
19508	TS.triHPacyl.COelim.mtppmppmu	1.501e+44	4.41	4.41	9.184e+40	0.0365
19509	TS.triHPacyl.COelim.pmpmmpmmmu	4.193e+43	3.65	3.65	9.155e+40	0.0364
19510	TS.triHPacyl.COelim.tppmtpmpu	1.774e+44	4.51	4.51	9.140e+40	0.0363
19511	TS.triHPacyl.COelim.mptmptmpu	1.869e+45	5.92	5.92	9.062e+40	0.036
19512	TS.triHPacyl.COelim.pptpppppmu	3.089e+43	3.48	3.48	8.993e+40	0.0358
19513	TS.triHPacyl.COelim.pmtmptmpu	4.341e+44	5.06	5.06	8.961e+40	0.0356
19514	TS.triHPacyl.COelim.ptmmpmpmu	3.189e+44	4.88	4.88	8.928e+40	0.0355
19515	TS.triHPacyl.COelim.ttpmtpmpu	2.331e+44	4.69	4.69	8.922e+40	0.0355
19516	TS.triHPacyl.COelim.pptpptmpu	1.625e+44	4.48	4.48	8.900e+40	0.0354
19517	TS.triHPacyl.COelim.ptmtpppmu	1.588e+44	4.47	4.47	8.860e+40	0.0352
19518	TS.triHPacyl.COelim.tptmmtmmu	3.636e+44	4.97	4.97	8.731e+40	0.0347
19519	TS.triHPacyl.COelim.tppmmpmpu	4.859e+43	3.78	3.78	8.558e+40	0.034
19520	TS.triHPacyl.COelim.mppppmtpu	4.192e+44	5.07	5.07	8.516e+40	0.0339
19521	TS.triHPacyl.COelim.tmmmtmpmu	7.396e+43	4.04	4.04	8.416e+40	0.0335
19522	TS.triHPacyl.COelim.ppppmtppu	1.984e+44	4.64	4.64	8.246e+40	0.0328
19523	TS.triHPacyl.COelim.tpmmtmpmu	9.259e+43	4.19	4.19	8.205e+40	0.0326
19524	TS.triHPacyl.COelim.pttpptmpu	2.761e+44	4.85	4.85	8.153e+40	0.0324
19525	TS.triHPacyl.COelim.tppmmtmpu	1.524e+45	5.87	5.87	8.025e+40	0.0319
19526	TS.triHPacyl.COelim.pptmtpmpu	7.824e+43	4.11	4.11	7.982e+40	0.0317
19527	TS.triHPacyl.COelim.tptmmtmpu	4.073e+44	5.10	5.10	7.887e+40	0.0314
19528	TS.triHPacyl.COelim.pmmptppmu	7.424e+43	4.09	4.09	7.843e+40	0.0312
19529	TS.triHPacyl.COelim.tptmmtppu	1.585e+44	4.55	4.55	7.741e+40	0.0308
19530	TS.triHPacyl.COelim.pmtmptmpu	1.077e+44	4.32	4.32	7.624e+40	0.0303
19531	TS.triHPacyl.COelim.tppmmpmpu	8.666e+43	4.20	4.20	7.604e+40	0.0302
19532	TS.triHPacyl.COelim.pttmmmpmu	3.140e+44	4.96	4.96	7.597e+40	0.0302
19533	TS.triHPacyl.COelim.tppmmtmmu	8.932e+43	4.22	4.22	7.586e+40	0.0302
19534	TS.triHPacyl.COelim.mppppmtpu	5.468e+44	5.30	5.30	7.580e+40	0.0301
19535	TS.triHPacyl.COelim.mmtmmpmpmu	2.845e+44	4.91	4.91	7.535e+40	0.03
19536	TS.triHPacyl.COelim.tpmmpmmpmu	5.362e+43	3.92	3.92	7.518e+40	0.0299
19537	TS.triHPacyl.COelim.mppmmpmpmu	1.501e+43	3.16	3.16	7.463e+40	0.0297
19538	TS.triHPacyl.COelim.pttpptmpu	1.907e+44	4.68	4.68	7.422e+40	0.0295
19539	TS.triHPacyl.COelim.pmmptmmpu	1.130e+44	4.38	4.38	7.319e+40	0.0291
19540	TS.triHPacyl.COelim.tmmmtmmpu	6.555e+43	4.07	4.07	7.140e+40	0.0284
19541	TS.triHPacyl.COelim.tppmmpmpmu	7.484e+43	4.15	4.15	7.139e+40	0.0284
19542	TS.triHPacyl.COelim.ptmmpmmpmu	4.072e+44	5.16	5.16	7.082e+40	0.0282
19543	TS.triHPacyl.COelim.tppmmpmpmu	5.449e+43	3.96	3.96	7.064e+40	0.0281
19544	TS.triHPacyl.COelim.pptmptppu	1.042e+44	4.35	4.35	7.058e+40	0.0281
19545	TS.triHPacyl.COelim.pttmtppmu	2.583e+44	4.90	4.90	7.011e+40	0.0279
19546	TS.triHPacyl.COelim.tttmmpmpmu	1.238e+44	4.46	4.46	6.968e+40	0.0277
19547	TS.triHPacyl.COelim.tppppmpmu	3.524e+44	5.09	5.09	6.936e+40	0.0276
19548	TS.triHPacyl.COelim.tmmmmmtmmu	1.237e+44	4.46	4.46	6.932e+40	0.0276
19549	TS.triHPacyl.COelim.pttmtppu	1.707e+44	4.66	4.66	6.931e+40	0.0276
19550	TS.triHPacyl.COelim.tttmtpppu	1.119e+44	4.41	4.41	6.906e+40	0.0275
19551	TS.triHPacyl.COelim.tptmmtppu	2.986e+44	5.00	5.00	6.828e+40	0.0272
19552	TS.triHPacyl.COelim.pttmtppmu	4.207e+44	5.20	5.20	6.826e+40	0.0271
19553	TS.triHPacyl.COelim.tpmmmpppu	1.045e+44	4.38	4.38	6.764e+40	0.0269
19554	TS.triHPacyl.COelim.pptmtpmpu	7.611e+43	4.19	4.19	6.743e+40	0.0268
19555	TS.triHPacyl.COelim.pttmtppu	1.274e+44	4.50	4.50	6.693e+40	0.0266
19556	TS.triHPacyl.COelim.tptmmpmpu	1.523e+44	4.61	4.61	6.636e+40	0.0264
19557	TS.triHPacyl.COelim.tpmmpmtpu	2.362e+44	4.88	4.88	6.615e+40	0.0263
19558	TS.triHPacyl.COelim.pmpppmmpmu	5.726e+43	4.03	4.03	6.600e+40	0.0262
19559	TS.triHPacyl.COelim.tpppmtmpu	6.697e+43	4.13	4.13	6.587e+40	0.0262

19560	TS.triHPacyl.COelim.ppppmtmpu	1.400e+44	4.57	4.57	6.540e+40	0.026
19561	TS.triHPacyl.COelim.ttmppmtmpu	4.279e+44	5.24	5.24	6.506e+40	0.0259
19562	TS.triHPacyl.COelim.ptppmptmmu	1.466e+44	4.61	4.61	6.451e+40	0.0257
19563	TS.triHPacyl.COelim.ppmmpmpu	5.178e+43	3.99	3.99	6.434e+40	0.0256
19564	TS.triHPacyl.COelim.pttmppmpu	5.626e+44	5.41	5.41	6.407e+40	0.0255
19565	TS.triHPacyl.COelim.ptmpppmpu	6.927e+43	4.17	4.17	6.395e+40	0.0254
19566	TS.triHPacyl.COelim.tttmpmpu	4.506e+44	5.29	5.29	6.325e+40	0.0251
19567	TS.triHPacyl.COelim.ppmmttmu	1.229e+44	4.52	4.52	6.304e+40	0.0251
19568	TS.triHPacyl.COelim.pptppptmpu	2.132e+44	4.85	4.85	6.234e+40	0.0248
19569	TS.triHPacyl.COelim.tpmmpmtmpu	1.721e+44	4.73	4.73	6.182e+40	0.0246
19570	TS.triHPacyl.COelim.pptmmppu	9.616e+43	4.39	4.39	6.134e+40	0.0244
19571	TS.triHPacyl.COelim.tpmmmtpu	1.812e+44	4.77	4.77	6.093e+40	0.0242
19572	TS.triHPacyl.COelim.pppmmmpu	2.586e+44	4.98	4.98	6.054e+40	0.0241
19573	TS.triHPacyl.COelim.tmtppmpu	7.235e+43	4.23	4.23	6.034e+40	0.024
19574	TS.triHPacyl.COelim.mmtpmppu	5.178e+44	5.35	5.35	6.023e+40	0.0239
19575	TS.triHPacyl.COelim.tmpmtmpu	1.239e+44	4.55	4.55	6.012e+40	0.0239
19576	TS.triHPacyl.COelim.ppmppptmpu	1.168e+44	4.52	4.52	5.973e+40	0.0238
19577	TS.triHPacyl.COelim.tpmmpmpu	4.155e+44	5.28	5.28	5.938e+40	0.0236
19578	TS.triHPacyl.COelim.pppmptmpu	2.917e+44	5.07	5.07	5.932e+40	0.0236
19579	TS.triHPacyl.COelim.pmtmptmpu	1.441e+44	4.65	4.65	5.919e+40	0.0235
19580	TS.triHPacyl.COelim.ttmmtmpu	3.358e+44	5.16	5.16	5.886e+40	0.0234
19581	TS.triHPacyl.COelim.tmtmptmpu	1.515e+44	4.68	4.68	5.861e+40	0.0233
19582	TS.triHPacyl.COelim.pptptmpu	5.170e+44	5.42	5.42	5.824e+40	0.0232
19583	TS.triHPacyl.COelim.tpmmmmpu	1.711e+44	4.76	4.76	5.795e+40	0.023
19584	TS.triHPacyl.COelim.ppmmpmpu	3.427e+43	3.81	3.81	5.762e+40	0.0229
19585	TS.triHPacyl.COelim.ttpmtmpu	1.729e+44	4.77	4.77	5.745e+40	0.0228
19586	TS.triHPacyl.COelim.tptmptmpu	4.924e+44	5.40	5.40	5.697e+40	0.0227
19587	TS.triHPacyl.COelim.mpmmpmpu	5.020e+43	4.05	4.05	5.647e+40	0.0225
19588	TS.triHPacyl.COelim.ppttptmpu	2.208e+44	4.93	4.93	5.633e+40	0.0224
19589	TS.triHPacyl.COelim.ppmppmpu	3.743e+43	3.88	3.88	5.578e+40	0.0222
19590	TS.triHPacyl.COelim.tppmmtmpu	1.321e+45	6.01	6.01	5.539e+40	0.022
19591	TS.triHPacyl.COelim.mppmmpmpu	2.939e+45	6.49	6.49	5.512e+40	0.0219
19592	TS.triHPacyl.COelim.mmtmmppu	3.089e+44	5.15	5.15	5.476e+40	0.0218
19593	TS.triHPacyl.COelim.pttmmpmpu	2.738e+44	5.08	5.08	5.448e+40	0.0217
19594	TS.triHPacyl.COelim.mpmmpmpu	1.233e+44	4.62	4.62	5.347e+40	0.0213
19595	TS.triHPacyl.COelim.pptmmpmpu	7.106e+43	4.29	4.29	5.330e+40	0.0212
19596	TS.triHPacyl.COelim.tmtmmmpu	1.937e+44	4.89	4.89	5.324e+40	0.0212
19597	TS.triHPacyl.COelim.tptmmmpu	3.038e+44	5.16	5.16	5.317e+40	0.0211
19598	TS.triHPacyl.COelim.mptppptmpu	1.833e+44	4.86	4.86	5.301e+40	0.0211
19599	TS.triHPacyl.COelim.pttmmmpu	8.139e+44	5.75	5.75	5.291e+40	0.021
19600	TS.triHPacyl.COelim.tptmmtmpu	3.517e+44	5.25	5.25	5.274e+40	0.021
19601	TS.triHPacyl.COelim.pmmmpmpu	5.012e+43	4.09	4.09	5.270e+40	0.021
19602	TS.triHPacyl.COelim.pttmmpmpu	5.121e+44	5.48	5.48	5.250e+40	0.0209
19603	TS.triHPacyl.COelim.tmtmptmpu	9.304e+43	4.46	4.46	5.245e+40	0.0209
19604	TS.triHPacyl.COelim.pptmptmpu	1.070e+44	4.54	4.54	5.239e+40	0.0208
19605	TS.triHPacyl.COelim.pttmmmpmpu	4.514e+44	5.40	5.40	5.227e+40	0.0208
19606	TS.triHPacyl.COelim.pptmptmpu	3.909e+44	5.32	5.32	5.182e+40	0.0206
19607	TS.triHPacyl.COelim.tptmptmpu	3.021e+44	5.17	5.17	5.155e+40	0.0205
19608	TS.triHPacyl.COelim.mmtmmmpu	3.747e+44	5.31	5.31	5.112e+40	0.0203
19609	TS.triHPacyl.COelim.pttmtmpu	4.163e+44	5.37	5.37	5.075e+40	0.0202
19610	TS.triHPacyl.COelim.tpmmtmpu	9.334e+43	4.49	4.49	5.039e+40	0.02
19611	TS.triHPacyl.COelim.pptmtpmpu	8.416e+43	4.43	4.43	4.988e+40	0.0198
19612	TS.triHPacyl.COelim.mpmmpmpu	1.166e+44	4.62	4.62	4.983e+40	0.0198
19613	TS.triHPacyl.COelim.tptmptmpu	8.691e+43	4.45	4.45	4.967e+40	0.0198
19614	TS.triHPacyl.COelim.tmtmtmpu	6.459e+44	5.66	5.66	4.879e+40	0.0194
19615	TS.triHPacyl.COelim.tptmtpmpu	5.455e+44	5.56	5.56	4.818e+40	0.0192
19616	TS.triHPacyl.COelim.mpppmpmpu	1.995e+44	4.98	4.98	4.687e+40	0.0186
19617	TS.triHPacyl.COelim.ttpmmpmpu	1.585e+44	4.85	4.85	4.677e+40	0.0186
19618	TS.triHPacyl.COelim.tppmmpmpu	1.476e+44	4.81	4.81	4.650e+40	0.0185
19619	TS.triHPacyl.COelim.ppmmtmpu	1.045e+44	4.61	4.61	4.605e+40	0.0183
19620	TS.triHPacyl.COelim.ptmmpmpu	1.675e+44	4.89	4.89	4.557e+40	0.0181
19621	TS.triHPacyl.COelim.tmtmmmpu	5.343e+45	6.96	6.96	4.513e+40	0.0179
19622	TS.triHPacyl.COelim.tppmmpmpu	1.673e+44	4.91	4.91	4.462e+40	0.0177
19623	TS.triHPacyl.COelim.pppmptmpu	2.130e+44	5.05	5.05	4.443e+40	0.0177
19624	TS.triHPacyl.COelim.ptmmpmpu	2.106e+44	5.05	5.05	4.439e+40	0.0176
19625	TS.triHPacyl.COelim.pttmmmpu	9.607e+44	5.95	5.95	4.438e+40	0.0176
19626	TS.triHPacyl.COelim.tptpmpu	1.476e+44	4.84	4.84	4.428e+40	0.0176
19627	TS.triHPacyl.COelim.tptmmpmpu	1.101e+45	6.04	6.04	4.364e+40	0.0174
19628	TS.triHPacyl.COelim.ptmmtmpu	4.455e+44	5.51	5.51	4.319e+40	0.0172
19629	TS.triHPacyl.COelim.tptmmpmpu	1.019e+44	4.64	4.64	4.260e+40	0.0169
19630	TS.triHPacyl.COelim.tppmmpmpu	8.207e+43	4.51	4.51	4.231e+40	0.0168
19631	TS.triHPacyl.COelim.mptpmpmpu	9.922e+43	4.63	4.63	4.223e+40	0.0168

19632	TS.triHPacyl.COelim.tttpmmtpmu	8.899e+44	5.94	5.94	4.212e+40	0.0167
19633	TS.triHPacyl.COelim.ptmmpmpmpu	2.095e+44	5.08	5.08	4.198e+40	0.0167
19634	TS.triHPacyl.COelim.ptmpmpmpu	6.480e+43	4.38	4.38	4.188e+40	0.0167
19635	TS.triHPacyl.COelim.ptmtmtpppu	1.749e+44	4.98	4.98	4.108e+40	0.0163
19636	TS.triHPacyl.COelim.ppmmpptppu	2.783e+44	5.26	5.26	4.099e+40	0.0163
19637	TS.triHPacyl.COelim.tptmpmpmpu	1.812e+44	5.01	5.01	4.028e+40	0.016
19638	TS.triHPacyl.COelim.ptttmmpmpu	7.372e+44	5.85	5.85	4.018e+40	0.016
19639	TS.triHPacyl.COelim.ptmmpmpmpu	3.873e+44	5.47	5.47	4.012e+40	0.016
19640	TS.triHPacyl.COelim.tptpmmtpmu	4.861e+44	5.61	5.61	4.008e+40	0.0159
19641	TS.triHPacyl.COelim.tmmptmtmmu	1.808e+44	5.02	5.02	3.989e+40	0.0159
19642	TS.triHPacyl.COelim.pptpmpmpu	9.704e+43	4.65	4.65	3.980e+40	0.0158
19643	TS.triHPacyl.COelim.ptpmmpmpu	7.043e+43	4.47	4.47	3.901e+40	0.0155
19644	TS.triHPacyl.COelim.ptmmpmpmpu	3.141e+44	5.36	5.36	3.898e+40	0.0155
19645	TS.triHPacyl.COelim.pttmtptmpu	3.604e+44	5.44	5.44	3.896e+40	0.0155
19646	TS.triHPacyl.COelim.tppmmpmpu	4.707e+44	5.62	5.62	3.877e+40	0.0154
19647	TS.triHPacyl.COelim.pmmmpmpmpu	3.301e+43	4.02	4.02	3.868e+40	0.0154
19648	TS.triHPacyl.COelim.pttppppmpu	2.565e+44	5.25	5.25	3.852e+40	0.0153
19649	TS.triHPacyl.COelim.ptppppmpu	1.549e+44	4.95	4.95	3.820e+40	0.0152
19650	TS.triHPacyl.COelim.tpmmpmpmpu	7.249e+43	4.50	4.50	3.803e+40	0.0151
19651	TS.triHPacyl.COelim.tttmmtmpu	2.141e+44	5.15	5.15	3.800e+40	0.0151
19652	TS.triHPacyl.COelim.tmmmtmpu	1.293e+44	4.86	4.86	3.710e+40	0.0148
19653	TS.triHPacyl.COelim.tppmtpmpu	1.414e+45	6.29	6.29	3.707e+40	0.0147
19654	TS.triHPacyl.COelim.ptptmpmpu	2.491e+44	5.26	5.26	3.700e+40	0.0147
19655	TS.triHPacyl.COelim.mpmmpmpmpu	1.230e+44	4.83	4.83	3.696e+40	0.0147
19656	TS.triHPacyl.COelim.tpptmpmpu	6.505e+44	5.84	5.84	3.649e+40	0.0145
19657	TS.triHPacyl.COelim.pmpmpmpmpu	9.473e+43	4.69	4.69	3.649e+40	0.0145
19658	TS.triHPacyl.COelim.pppmptmpu	1.372e+44	4.91	4.91	3.640e+40	0.0145
19659	TS.triHPacyl.COelim.pmtmmmtmpu	2.012e+44	5.14	5.14	3.639e+40	0.0145
19660	TS.triHPacyl.COelim.ptttmtmpu	4.697e+44	5.64	5.64	3.628e+40	0.0144
19661	TS.triHPacyl.COelim.ttpmmpmpu	6.868e+43	4.50	4.50	3.619e+40	0.0144
19662	TS.triHPacyl.COelim.ptmpptmpu	7.442e+43	4.55	4.55	3.614e+40	0.0144
19663	TS.triHPacyl.COelim.pttmmpmpu	2.767e+44	5.34	5.34	3.582e+40	0.0142
19664	TS.triHPacyl.COelim.pttmtppmpu	2.404e+44	5.25	5.25	3.575e+40	0.0142
19665	TS.triHPacyl.COelim.ptmmpmpmpu	1.642e+44	5.03	5.03	3.543e+40	0.0141
19666	TS.triHPacyl.COelim.tpmmpmpmpu	5.058e+43	4.33	4.33	3.529e+40	0.014
19667	TS.triHPacyl.COelim.mmpmpmpmpu	1.762e+44	5.08	5.08	3.514e+40	0.014
19668	TS.triHPacyl.COelim.ptmmpmpmpu	1.212e+44	4.86	4.86	3.498e+40	0.0139
19669	TS.triHPacyl.COelim.pttmtppmpu	2.123e+44	5.20	5.20	3.483e+40	0.0138
19670	TS.triHPacyl.COelim.tmmmtmpmpu	1.420e+44	4.96	4.96	3.443e+40	0.0137
19671	TS.triHPacyl.COelim.tmtmtmpmpu	8.043e+44	6.01	6.01	3.393e+40	0.0135
19672	TS.triHPacyl.COelim.tppmpmpmpu	4.056e+44	5.60	5.60	3.379e+40	0.0134
19673	TS.triHPacyl.COelim.pttppppmpu	5.700e+44	5.81	5.81	3.361e+40	0.0134
19674	TS.triHPacyl.COelim.pttmtmpmpu	5.731e+44	5.81	5.81	3.355e+40	0.0133
19675	TS.triHPacyl.COelim.tmtppppmpu	2.428e+44	5.30	5.30	3.340e+40	0.0133
19676	TS.triHPacyl.COelim.tpmmpmpmpu	2.354e+44	5.29	5.29	3.323e+40	0.0132
19677	TS.triHPacyl.COelim.tmmmpmpmpu	9.684e+43	4.76	4.76	3.321e+40	0.0132
19678	TS.triHPacyl.COelim.tttmmpmpu	1.672e+44	5.08	5.08	3.319e+40	0.0132
19679	TS.triHPacyl.COelim.ppmmpmpmpu	2.872e+43	4.04	4.04	3.289e+40	0.0131
19680	TS.triHPacyl.COelim.ptmmpmpmpu	1.308e+44	4.94	4.94	3.280e+40	0.013
19681	TS.triHPacyl.COelim.ptpmmpmpu	4.907e+43	4.36	4.36	3.265e+40	0.013
19682	TS.triHPacyl.COelim.tpptmpmpu	5.127e+44	5.76	5.76	3.243e+40	0.0129
19683	TS.triHPacyl.COelim.pttmtppmpu	2.198e+44	5.26	5.26	3.223e+40	0.0128
19684	TS.triHPacyl.COelim.mmpmpmpmpu	8.828e+43	4.72	4.72	3.222e+40	0.0128
19685	TS.triHPacyl.COelim.tmmmpmpmpu	1.971e+44	5.20	5.20	3.197e+40	0.0127
19686	TS.triHPacyl.COelim.tppmptmpu	7.288e+43	4.62	4.62	3.156e+40	0.0125
19687	TS.triHPacyl.COelim.ptttmmpmpu	8.654e+44	6.09	6.09	3.154e+40	0.0125
19688	TS.triHPacyl.COelim.mttppppmpu	1.167e+44	4.90	4.90	3.128e+40	0.0124
19689	TS.triHPacyl.COelim.pmtppppmpu	2.413e+44	5.34	5.34	3.094e+40	0.0123
19690	TS.triHPacyl.COelim.tmtppppmpu	1.296e+44	4.98	4.98	3.060e+40	0.0122
19691	TS.triHPacyl.COelim.mptppppmpu	8.740e+43	4.74	4.74	3.057e+40	0.0122
19692	TS.triHPacyl.COelim.tttppppmpu	1.271e+45	6.34	6.34	3.034e+40	0.0121
19693	TS.triHPacyl.COelim.pmtmpmtmpu	7.376e+44	6.02	6.02	3.034e+40	0.0121
19694	TS.triHPacyl.COelim.tptmtpppu	2.227e+44	5.31	5.31	3.028e+40	0.0121
19695	TS.triHPacyl.COelim.pmtmtmpmpu	1.060e+44	4.87	4.87	3.007e+40	0.012
19696	TS.triHPacyl.COelim.pttppppmpu	3.125e+44	5.52	5.52	2.988e+40	0.0119
19697	TS.triHPacyl.COelim.ttmmpmtppu	2.477e+45	6.76	6.76	2.949e+40	0.0117
19698	TS.triHPacyl.COelim.pptpmpmpu	8.160e+43	4.74	4.74	2.893e+40	0.0115
19699	TS.triHPacyl.COelim.pttmmmpmpu	1.032e+45	6.25	6.25	2.887e+40	0.0115
19700	TS.triHPacyl.COelim.ptppppppmpu	3.635e+44	5.63	5.63	2.878e+40	0.0114
19701	TS.triHPacyl.COelim.tmmmtppu	4.945e+44	5.81	5.81	2.875e+40	0.0114
19702	TS.triHPacyl.COelim.pttmpptmpu	7.117e+44	6.04	6.04	2.832e+40	0.0113
19703	TS.triHPacyl.COelim.mtmmpmtmpu	1.590e+44	5.15	5.15	2.811e+40	0.0112

19704	TS.triHPacyl.COelim.pptmmtmpu	8.124e+43	4.75	4.75	2.808e+40	0.0112
19705	TS.triHPacyl.COelim.tttmmmmppu	3.277e+44	5.58	5.58	2.807e+40	0.0112
19706	TS.triHPacyl.COelim.ptppmmtmpu	1.349e+44	5.06	5.06	2.787e+40	0.0111
19707	TS.triHPacyl.COelim.ptmmpmmpu	3.187e+44	5.58	5.58	2.756e+40	0.011
19708	TS.triHPacyl.COelim.pppmmmtppu	1.302e+44	5.05	5.05	2.733e+40	0.0109
19709	TS.triHPacyl.COelim.pmtmpptmpu	9.766e+43	4.88	4.88	2.729e+40	0.0109
19710	TS.triHPacyl.COelim.mppppptmpu	5.158e+44	5.87	5.87	2.726e+40	0.0108
19711	TS.triHPacyl.COelim.tttmpttmmu	6.431e+45	7.38	7.38	2.724e+40	0.0108
19712	TS.triHPacyl.COelim.ptmmpmmppu	4.343e+44	5.77	5.77	2.712e+40	0.0108
19713	TS.triHPacyl.COelim.mtmmpmmpu	1.009e+44	4.91	4.91	2.692e+40	0.0107
19714	TS.triHPacyl.COelim.ptmptppmu	1.280e+44	5.05	5.05	2.688e+40	0.0107
19715	TS.triHPacyl.COelim.ptppppmpu	1.402e+44	5.11	5.11	2.660e+40	0.0106
19716	TS.triHPacyl.COelim.pptmppmmu	6.134e+44	6.00	6.00	2.621e+40	0.0104
19717	TS.triHPacyl.COelim.tttmmmtppu	3.087e+44	5.59	5.59	2.613e+40	0.0104
19718	TS.triHPacyl.COelim.ppttpptmpu	2.212e+44	5.39	5.39	2.610e+40	0.0104
19719	TS.triHPacyl.COelim.tpmmpmtmpu	1.445e+44	5.14	5.14	2.601e+40	0.0103
19720	TS.triHPacyl.COelim.tttppppmpu	3.694e+45	7.07	7.07	2.594e+40	0.0103
19721	TS.triHPacyl.COelim.mppppmpppu	9.544e+44	6.27	6.27	2.590e+40	0.0103
19722	TS.triHPacyl.COelim.tmtpttppu	3.840e+44	5.73	5.73	2.580e+40	0.0103
19723	TS.triHPacyl.COelim.ttmmpmtmmu	8.865e+43	4.86	4.86	2.566e+40	0.0102
19724	TS.triHPacyl.COelim.mtppppmpu	4.761e+43	4.49	4.49	2.561e+40	0.0102
19725	TS.triHPacyl.COelim.tttmptmpu	1.369e+45	6.49	6.49	2.548e+40	0.0101
19726	TS.triHPacyl.COelim.tmtmmmpmmu	1.054e+45	6.34	6.34	2.545e+40	0.0101
19727	TS.triHPacyl.COelim.pmtmppmmpu	2.984e+44	5.59	5.59	2.532e+40	0.0101
19728	TS.triHPacyl.COelim.pmmmtppu	5.216e+43	4.55	4.55	2.531e+40	0.0101
19729	TS.triHPacyl.COelim.tppmptmpu	6.482e+43	4.68	4.68	2.530e+40	0.0101
19730	TS.triHPacyl.COelim.pttmttmmu	6.819e+44	6.08	6.08	2.530e+40	0.0101
19731	TS.triHPacyl.COelim.tmtmmpmpu	1.461e+44	5.17	5.17	2.521e+40	0.01
19732	TS.triHPacyl.COelim.tpmptppmu	4.291e+43	4.44	4.44	2.496e+40	0.00992
19733	TS.triHPacyl.COelim.tmtmptppu	3.542e+44	5.70	5.70	2.482e+40	0.00987
19734	TS.triHPacyl.COelim.tttmmtppu	4.364e+44	5.83	5.83	2.477e+40	0.00985
19735	TS.triHPacyl.COelim.pmtppptmpu	1.871e+44	5.32	5.32	2.473e+40	0.00983
19736	TS.triHPacyl.COelim.tppmppmmu	4.385e+43	4.46	4.46	2.459e+40	0.00978
19737	TS.triHPacyl.COelim.ptmtmmtmmu	5.730e+44	6.00	6.00	2.452e+40	0.00975
19738	TS.triHPacyl.COelim.tptmmpmpu	7.863e+43	4.81	4.81	2.451e+40	0.00975
19739	TS.triHPacyl.COelim.pmpmmtppu	3.402e+43	4.33	4.33	2.383e+40	0.00947
19740	TS.triHPacyl.COelim.tttmmmpmu	6.681e+44	6.11	6.11	2.377e+40	0.00945
19741	TS.triHPacyl.COelim.mppmmtppu	1.930e+44	5.37	5.37	2.354e+40	0.00936
19742	TS.triHPacyl.COelim.mppppptppu	3.445e+44	5.72	5.72	2.347e+40	0.00933
19743	TS.triHPacyl.COelim.ptttmmmmmu	7.921e+44	6.22	6.22	2.341e+40	0.00931
19744	TS.triHPacyl.COelim.pptmptppu	8.148e+43	4.86	4.86	2.340e+40	0.0093
19745	TS.triHPacyl.COelim.mptmptppu	2.988e+44	5.64	5.64	2.324e+40	0.00924
19746	TS.triHPacyl.COelim.pttmtmpu	1.940e+44	5.38	5.38	2.320e+40	0.00922
19747	TS.triHPacyl.COelim.tmtmmpmpu	1.821e+44	5.35	5.35	2.301e+40	0.00915
19748	TS.triHPacyl.COelim.pptmppppu	3.384e+43	4.35	4.35	2.298e+40	0.00914
19749	TS.triHPacyl.COelim.ptmmpmmpu	7.935e+43	4.86	4.86	2.275e+40	0.00904
19750	TS.triHPacyl.COelim.pppppmpmpu	3.251e+44	5.71	5.71	2.267e+40	0.00901
19751	TS.triHPacyl.COelim.pmpppptmpu	7.067e+43	4.80	4.80	2.252e+40	0.00895
19752	TS.triHPacyl.COelim.mppmptppu	1.364e+44	5.19	5.19	2.247e+40	0.00893
19753	TS.triHPacyl.COelim.tmtmmmtppu	4.169e+44	5.86	5.86	2.228e+40	0.00886
19754	TS.triHPacyl.COelim.pppmptppu	2.801e+44	5.63	5.63	2.217e+40	0.00881
19755	TS.triHPacyl.COelim.pptmmtppu	1.068e+44	5.06	5.06	2.214e+40	0.0088
19756	TS.triHPacyl.COelim.tttmmmtmmu	4.265e+44	5.88	5.88	2.207e+40	0.00878
19757	TS.triHPacyl.COelim.pppmptppu	3.577e+43	4.41	4.41	2.202e+40	0.00876
19758	TS.triHPacyl.COelim.mmtmmpmpu	4.026e+44	5.85	5.85	2.197e+40	0.00873
19759	TS.triHPacyl.COelim.pppmpttmmu	1.931e+44	5.42	5.42	2.171e+40	0.00863
19760	TS.triHPacyl.COelim.tttmmtppu	6.647e+44	6.16	6.16	2.169e+40	0.00862
19761	TS.triHPacyl.COelim.pptmmpmpu	7.192e+43	4.85	4.85	2.113e+40	0.0084
19762	TS.triHPacyl.COelim.tmmmmmpu	5.121e+43	4.65	4.65	2.106e+40	0.00837
19763	TS.triHPacyl.COelim.tptmtpmpu	5.768e+44	6.09	6.09	2.094e+40	0.00833
19764	TS.triHPacyl.COelim.tttmmppmu	1.895e+44	5.44	5.44	2.071e+40	0.00823
19765	TS.triHPacyl.COelim.pmpppptmmu	8.514e+43	4.96	4.96	2.069e+40	0.00823
19766	TS.triHPacyl.COelim.tttmmpmtmmu	1.026e+45	6.45	6.45	2.068e+40	0.00822
19767	TS.triHPacyl.COelim.ptmptmpu	8.825e+43	4.98	4.98	2.064e+40	0.00821
19768	TS.triHPacyl.COelim.tmtmmtmmu	8.767e+44	6.36	6.36	2.048e+40	0.00814
19769	TS.triHPacyl.COelim.pppmptppu	2.100e+43	4.13	4.13	2.047e+40	0.00814
19770	TS.triHPacyl.COelim.tttmtpmpu	8.753e+44	6.37	6.37	2.010e+40	0.00799
19771	TS.triHPacyl.COelim.mppmptmpu	6.318e+43	4.80	4.80	2.004e+40	0.00797
19772	TS.triHPacyl.COelim.ttpmmpmpu	7.444e+43	4.90	4.90	1.991e+40	0.00792
19773	TS.triHPacyl.COelim.pttppptmpu	5.211e+44	6.07	6.07	1.987e+40	0.0079
19774	TS.triHPacyl.COelim.mppmmtpmpu	4.103e+43	4.55	4.55	1.985e+40	0.00789
19775	TS.triHPacyl.COelim.mtppmpmpu	1.658e+44	5.39	5.39	1.979e+40	0.00787

19776	TS.triHPacyl.COelim.tpmptmnmnu	6.705e+43	4.85	4.85	1.962e+40	0.0078
19777	TS.triHPacyl.COelim.mmtpmntmpu	6.516e+44	6.21	6.21	1.960e+40	0.00779
19778	TS.triHPacyl.COelim.pppppptmmu	1.379e+44	5.28	5.28	1.953e+40	0.00777
19779	TS.triHPacyl.COelim.ppppppmpmu	3.373e+43	4.45	4.45	1.948e+40	0.00775
19780	TS.triHPacyl.COelim.tptpmppppu	1.805e+44	5.45	5.45	1.948e+40	0.00775
19781	TS.triHPacyl.COelim.ttmnmpppmu	1.870e+44	5.47	5.47	1.925e+40	0.00765
19782	TS.triHPacyl.COelim.ptmtmnmmpu	5.579e+44	6.13	6.13	1.919e+40	0.00763
19783	TS.triHPacyl.COelim.pppmnmppu	3.639e+43	4.50	4.50	1.919e+40	0.00763
19784	TS.triHPacyl.COelim.tpppmmpmu	1.957e+44	5.51	5.51	1.908e+40	0.00759
19785	TS.triHPacyl.COelim.ptttmtpppu	4.362e+44	5.98	5.98	1.904e+40	0.00757
19786	TS.triHPacyl.COelim.ptppptppu	5.558e+44	6.13	6.13	1.888e+40	0.00751
19787	TS.triHPacyl.COelim.ptmtmmtmpu	1.076e+45	6.54	6.54	1.862e+40	0.0074
19788	TS.triHPacyl.COelim.ptttmmpmmu	6.445e+44	6.24	6.24	1.844e+40	0.00733
19789	TS.triHPacyl.COelim.mmpmptttmpu	3.802e+44	5.93	5.93	1.827e+40	0.00727
19790	TS.triHPacyl.COelim.ptmmmmmmmu	6.368e+44	6.24	6.24	1.816e+40	0.00722
19791	TS.triHPacyl.COelim.ptpmmtmpu	1.098e+44	5.20	5.20	1.803e+40	0.00717
19792	TS.triHPacyl.COelim.tpptpmpmmu	1.054e+45	6.54	6.54	1.803e+40	0.00717
19793	TS.triHPacyl.COelim.pppmmpmpu	2.995e+44	5.80	5.80	1.797e+40	0.00715
19794	TS.triHPacyl.COelim.pptmptmpu	6.034e+44	6.21	6.21	1.792e+40	0.00712
19795	TS.triHPacyl.COelim.ptmmmtppu	4.885e+44	6.09	6.09	1.788e+40	0.00711
19796	TS.triHPacyl.COelim.mppmptmpu	6.839e+43	4.92	4.92	1.783e+40	0.00709
19797	TS.triHPacyl.COelim.ptpppptmpu	2.707e+44	5.74	5.74	1.772e+40	0.00705
19798	TS.triHPacyl.COelim.tppmmpmmu	1.261e+44	5.30	5.30	1.727e+40	0.00687
19799	TS.triHPacyl.COelim.tmtmmtppu	2.002e+44	5.58	5.58	1.727e+40	0.00687
19800	TS.triHPacyl.COelim.tmtpmmtmpu	4.470e+44	6.06	6.06	1.719e+40	0.00684
19801	TS.triHPacyl.COelim.pttptpmpmu	2.303e+44	5.67	5.67	1.692e+40	0.00673
19802	TS.triHPacyl.COelim.tmtmmtmpmu	5.220e+44	6.16	6.16	1.690e+40	0.00672
19803	TS.triHPacyl.COelim.pmmptmmpu	4.871e+43	4.76	4.76	1.670e+40	0.00664
19804	TS.triHPacyl.COelim.pttmppmpmu	5.328e+44	6.18	6.18	1.667e+40	0.00663
19805	TS.triHPacyl.COelim.mppmmpmpmu	3.948e+44	6.01	6.01	1.660e+40	0.0066
19806	TS.triHPacyl.COelim.pmptmmpmmu	1.995e+44	5.60	5.60	1.656e+40	0.00659
19807	TS.triHPacyl.COelim.mmtmmtmnu	6.792e+44	6.33	6.33	1.654e+40	0.00658
19808	TS.triHPacyl.COelim.tmtmmmmmmu	1.022e+45	6.58	6.58	1.654e+40	0.00658
19809	TS.triHPacyl.COelim.mtmmmmpmpu	1.004e+44	5.19	5.19	1.652e+40	0.00657
19810	TS.triHPacyl.COelim.ppppppmpu	1.202e+44	5.30	5.30	1.644e+40	0.00654
19811	TS.triHPacyl.COelim.pttppmmpmu	2.587e+44	5.77	5.77	1.629e+40	0.00648
19812	TS.triHPacyl.COelim.tttmmtmpmu	4.845e+44	6.15	6.15	1.609e+40	0.0064
19813	TS.triHPacyl.COelim.pppmmpmmpu	5.300e+43	4.83	4.83	1.595e+40	0.00634
19814	TS.triHPacyl.COelim.tmtmmtmnu	8.233e+44	6.48	6.48	1.577e+40	0.00627
19815	TS.triHPacyl.COelim.ppppmtmpu	1.789e+44	5.57	5.57	1.557e+40	0.00619
19816	TS.triHPacyl.COelim.tppppppmu	2.693e+44	5.82	5.82	1.550e+40	0.00617
19817	TS.triHPacyl.COelim.tptmnmppmu	5.054e+44	6.21	6.21	1.517e+40	0.00603
19818	TS.triHPacyl.COelim.pptpmppppu	1.279e+44	5.39	5.39	1.513e+40	0.00602
19819	TS.triHPacyl.COelim.mmmmmmpppu	2.982e+44	5.90	5.90	1.511e+40	0.00601
19820	TS.triHPacyl.COelim.pttpptmpu	5.134e+44	6.22	6.22	1.510e+40	0.006
19821	TS.triHPacyl.COelim.tmtppptmpu	3.824e+44	6.05	6.05	1.503e+40	0.00598
19822	TS.triHPacyl.COelim.ttmnmmpmu	3.269e+44	5.96	5.96	1.494e+40	0.00594
19823	TS.triHPacyl.COelim.pptpmtmpu	2.101e+44	5.70	5.70	1.475e+40	0.00587
19824	TS.triHPacyl.COelim.pppmptmnmnu	1.145e+44	5.34	5.34	1.471e+40	0.00585
19825	TS.triHPacyl.COelim.pptppppppu	4.342e+43	4.77	4.77	1.457e+40	0.0058
19826	TS.triHPacyl.COelim.ppmtpmpppu	9.804e+43	5.26	5.26	1.448e+40	0.00576
19827	TS.triHPacyl.COelim.ppppmtpppu	1.955e+44	5.68	5.68	1.413e+40	0.00562
19828	TS.triHPacyl.COelim.tmtmtpppu	3.363e+44	6.01	6.01	1.411e+40	0.00561
19829	TS.triHPacyl.COelim.ptmtmmpppu	3.266e+44	5.99	5.99	1.410e+40	0.00561
19830	TS.triHPacyl.COelim.mmtpmppppu	4.123e+44	6.13	6.13	1.408e+40	0.0056
19831	TS.triHPacyl.COelim.ttmmtmnu	2.585e+44	5.86	5.86	1.403e+40	0.00558
19832	TS.triHPacyl.COelim.mmpmptmnu	9.278e+44	6.62	6.62	1.385e+40	0.00551
19833	TS.triHPacyl.COelim.mmtmmppppu	3.724e+44	6.09	6.09	1.372e+40	0.00546
19834	TS.triHPacyl.COelim.ttmmpmmpu	1.078e+45	6.72	6.72	1.369e+40	0.00544
19835	TS.triHPacyl.COelim.pmtppmtmpu	7.066e+44	6.47	6.47	1.363e+40	0.00542
19836	TS.triHPacyl.COelim.pppptppmmu	4.539e+44	6.21	6.21	1.363e+40	0.00542
19837	TS.triHPacyl.COelim.tppmtpmpu	1.494e+44	5.55	5.55	1.360e+40	0.00541
19838	TS.triHPacyl.COelim.tppmmtmnu	1.601e+44	5.59	5.59	1.355e+40	0.00539
19839	TS.triHPacyl.COelim.ptmmpmmpu	2.423e+45	7.23	7.23	1.307e+40	0.0052
19840	TS.triHPacyl.COelim.pppptpppu	5.519e+44	6.35	6.35	1.304e+40	0.00519
19841	TS.triHPacyl.COelim.mptpmtmpu	7.558e+43	5.17	5.17	1.295e+40	0.00515
19842	TS.triHPacyl.COelim.tppmmtmpu	8.693e+44	6.63	6.63	1.293e+40	0.00514
19843	TS.triHPacyl.COelim.mmpmptppu	3.179e+44	6.03	6.03	1.282e+40	0.0051
19844	TS.triHPacyl.COelim.tttmmtmpu	4.241e+44	6.21	6.21	1.280e+40	0.00509
19845	TS.triHPacyl.COelim.ppmtpmmpu	1.142e+44	5.42	5.42	1.278e+40	0.00508
19846	TS.triHPacyl.COelim.pptmmtmpu	1.850e+44	5.71	5.71	1.273e+40	0.00506
19847	TS.triHPacyl.COelim.tppmmtmpu	1.784e+44	5.69	5.69	1.271e+40	0.00506

19848	TS.triHPacyl.COelim.pmttptpppu	3.314e+44	6.06	6.06	1.267e+40	0.00504
19849	TS.triHPacyl.COelim.tmtmmpmpmu	1.885e+44	5.73	5.73	1.263e+40	0.00502
19850	TS.triHPacyl.COelim.pppmpptmmu	2.964e+44	6.01	6.01	1.238e+40	0.00492
19851	TS.triHPacyl.COelim.tttmmtppmu	3.257e+44	6.07	6.07	1.235e+40	0.00491
19852	TS.triHPacyl.COelim.ptttmpmmpu	6.915e+44	6.52	6.52	1.231e+40	0.00489
19853	TS.triHPacyl.COelim.tttptmtpmu	7.400e+44	6.56	6.56	1.225e+40	0.00487
19854	TS.triHPacyl.COelim.ptttmpmmpu	8.625e+44	6.66	6.66	1.222e+40	0.00486
19855	TS.triHPacyl.COelim.mptmpmmpu	1.177e+44	5.47	5.47	1.215e+40	0.00483
19856	TS.triHPacyl.COelim.mtppmmpmmpu	6.238e+43	5.09	5.09	1.215e+40	0.00483
19857	TS.triHPacyl.COelim.tpptmmpmpu	2.537e+44	5.93	5.93	1.210e+40	0.00481
19858	TS.triHPacyl.COelim.pttpmmpmmpu	1.838e+44	5.74	5.74	1.209e+40	0.00481
19859	TS.triHPacyl.COelim.tptptpmpmu	6.399e+44	6.49	6.49	1.204e+40	0.00479
19860	TS.triHPacyl.COelim.mmpmptpmpu	2.272e+44	5.87	5.87	1.198e+40	0.00476
19861	TS.triHPacyl.COelim.tttptpppu	1.883e+44	5.76	5.76	1.195e+40	0.00475
19862	TS.triHPacyl.COelim.mppmmpmmpu	7.422e+43	5.21	5.21	1.195e+40	0.00475
19863	TS.triHPacyl.COelim.mmpmptmmpu	2.285e+45	7.25	7.25	1.194e+40	0.00475
19864	TS.triHPacyl.COelim.pmtmptmmpu	2.625e+44	5.96	5.96	1.188e+40	0.00472
19865	TS.triHPacyl.COelim.pmmmpmtppu	9.319e+43	5.35	5.35	1.187e+40	0.00472
19866	TS.triHPacyl.COelim.pptpmtpppu	1.163e+44	5.48	5.48	1.177e+40	0.00468
19867	TS.triHPacyl.COelim.mttmmppppu	2.080e+44	5.83	5.83	1.177e+40	0.00468
19868	TS.triHPacyl.COelim.tmpmmpmpu	4.981e+44	6.35	6.35	1.174e+40	0.00467
19869	TS.triHPacyl.COelim.tttptmtpu	1.509e+45	7.01	7.01	1.173e+40	0.00466
19870	TS.triHPacyl.COelim.pmmppmmpu	1.635e+43	4.32	4.32	1.171e+40	0.00466
19871	TS.triHPacyl.COelim.mtmmpmmpu	3.384e+44	6.12	6.12	1.168e+40	0.00465
19872	TS.triHPacyl.COelim.ptmtmmpu	1.111e+45	6.84	6.84	1.162e+40	0.00462
19873	TS.triHPacyl.COelim.pmtmmpmmpu	4.544e+44	6.31	6.31	1.159e+40	0.00461
19874	TS.triHPacyl.COelim.mmtmmpmmpu	1.593e+45	7.06	7.06	1.152e+40	0.00458
19875	TS.triHPacyl.COelim.tttmmppppu	1.797e+44	5.76	5.76	1.148e+40	0.00457
19876	TS.triHPacyl.COelim.pmmmpmtpu	1.297e+44	5.56	5.56	1.146e+40	0.00456
19877	TS.triHPacyl.COelim.tptmtpmmpu	9.564e+43	5.39	5.39	1.138e+40	0.00453
19878	TS.triHPacyl.COelim.tttmptmmpu	2.191e+44	5.89	5.89	1.128e+40	0.00449
19879	TS.triHPacyl.COelim.pppmmpmmpu	1.179e+44	5.52	5.52	1.128e+40	0.00449
19880	TS.triHPacyl.COelim.pmpmmpmmpu	1.396e+44	5.62	5.62	1.125e+40	0.00447
19881	TS.triHPacyl.COelim.pmpmptmmpu	8.447e+43	5.32	5.32	1.124e+40	0.00447
19882	TS.triHPacyl.COelim.ptptmmpu	5.995e+44	6.49	6.49	1.121e+40	0.00446
19883	TS.triHPacyl.COelim.pptmmpmmpu	1.107e+44	5.49	5.49	1.118e+40	0.00445
19884	TS.triHPacyl.COelim.pmpmptmmpu	6.213e+43	5.15	5.15	1.109e+40	0.00441
19885	TS.triHPacyl.COelim.pptppmmpu	1.432e+44	5.65	5.65	1.096e+40	0.00436
19886	TS.triHPacyl.COelim.ptttmmpmmpu	5.664e+44	6.47	6.47	1.096e+40	0.00436
19887	TS.triHPacyl.COelim.mtmmpmmpu	1.043e+44	5.46	5.46	1.095e+40	0.00435
19888	TS.triHPacyl.COelim.pptppmmpu	6.702e+43	5.20	5.20	1.094e+40	0.00435
19889	TS.triHPacyl.COelim.pptptmmpu	4.508e+44	6.34	6.34	1.092e+40	0.00434
19890	TS.triHPacyl.COelim.ptmtpmmpu	3.952e+44	6.26	6.26	1.091e+40	0.00434
19891	TS.triHPacyl.COelim.pmtmmpmmpu	7.109e+43	5.24	5.24	1.074e+40	0.00427
19892	TS.triHPacyl.COelim.mmpmptmmpu	5.383e+44	6.45	6.45	1.072e+40	0.00426
19893	TS.triHPacyl.COelim.tttptmmpu	1.265e+45	6.96	6.96	1.071e+40	0.00426
19894	TS.triHPacyl.COelim.pmmmpmmpu	5.888e+43	5.14	5.14	1.066e+40	0.00424
19895	TS.triHPacyl.COelim.pmpmtpmmpu	5.806e+44	6.50	6.50	1.064e+40	0.00423
19896	TS.triHPacyl.COelim.tptmtpmmpu	5.583e+44	6.48	6.48	1.055e+40	0.0042
19897	TS.triHPacyl.COelim.mtmmpmtpu	1.534e+44	5.72	5.72	1.054e+40	0.00419
19898	TS.triHPacyl.COelim.mmtmtpmmpu	2.535e+44	6.01	6.01	1.053e+40	0.00419
19899	TS.triHPacyl.COelim.ttmmtmmpu	3.074e+44	6.13	6.13	1.048e+40	0.00417
19900	TS.triHPacyl.COelim.tpptmmpmmpu	2.890e+44	6.10	6.10	1.045e+40	0.00416
19901	TS.triHPacyl.COelim.tmtptmmpu	8.266e+44	6.72	6.72	1.045e+40	0.00415
19902	TS.triHPacyl.COelim.pttpmmpmmpu	1.821e+44	5.83	5.83	1.038e+40	0.00413
19903	TS.triHPacyl.COelim.tpmmpmmpu	8.519e+43	5.38	5.38	1.023e+40	0.00407
19904	TS.triHPacyl.COelim.mmtmmpmmpu	1.985e+44	5.89	5.89	1.022e+40	0.00406
19905	TS.triHPacyl.COelim.mppmmpmmpu	3.908e+43	4.92	4.92	1.011e+40	0.00402
19906	TS.triHPacyl.COelim.ptppmmpu	2.415e+44	6.01	6.01	1.011e+40	0.00402
19907	TS.triHPacyl.COelim.ptmptmmpu	6.390e+43	5.22	5.22	1.010e+40	0.00401
19908	TS.triHPacyl.COelim.tttmmpmmpu	2.033e+44	5.91	5.91	1.009e+40	0.00401
19909	TS.triHPacyl.COelim.pmtmptmmpu	2.368e+44	6.00	6.00	1.007e+40	0.00401
19910	TS.triHPacyl.COelim.pmtptmmpu	5.217e+43	5.10	5.10	1.007e+40	0.00401
19911	TS.triHPacyl.COelim.mttmptmmpu	2.279e+44	5.98	5.98	1.005e+40	0.004
19912	TS.triHPacyl.COelim.tmtmmpmmpu	4.276e+43	4.98	4.98	1.001e+40	0.00398
19913	TS.triHPacyl.COelim.tpptmtpu	2.407e+45	7.39	7.39	9.970e+39	0.00396
19914	TS.triHPacyl.COelim.pttpmmpu	6.675e+44	6.63	6.63	9.952e+39	0.00396
19915	TS.triHPacyl.COelim.tttmtpmmpu	2.191e+44	5.96	5.96	9.949e+39	0.00396
19916	TS.triHPacyl.COelim.pptmtpmmpu	2.354e+44	6.01	6.01	9.899e+39	0.00394
19917	TS.triHPacyl.COelim.pptmmtmmpu	1.453e+44	5.72	5.72	9.875e+39	0.00393
19918	TS.triHPacyl.COelim.tmtmtpmmpu	1.167e+44	5.59	5.59	9.872e+39	0.00393
19919	TS.triHPacyl.COelim.pmpmtpmmpu	5.710e+43	5.17	5.17	9.811e+39	0.0039

19920	TS.triHPacyl.COelim.tmtmppmpu	7.939e+43	5.37	5.37	9.796e+39	0.00389
19921	TS.triHPacyl.COelim.tmtmmmpu	8.197e+44	6.76	6.76	9.720e+39	0.00387
19922	TS.triHPacyl.COelim.mptppmpu	1.711e+44	5.83	5.83	9.672e+39	0.00385
19923	TS.triHPacyl.COelim.tmpmmmpu	3.857e+44	6.32	6.32	9.619e+39	0.00382
19924	TS.triHPacyl.COelim.pttmppmpu	1.468e+45	7.12	7.12	9.551e+39	0.0038
19925	TS.triHPacyl.COelim.tpmtmpmpu	2.488e+44	6.06	6.06	9.544e+39	0.00379
19926	TS.triHPacyl.COelim.ptmtmpmpu	4.455e+44	6.41	6.41	9.459e+39	0.00376
19927	TS.triHPacyl.COelim.tmtmmmpu	4.894e+44	6.47	6.47	9.413e+39	0.00374
19928	TS.triHPacyl.COelim.tmmptmpu	3.896e+44	6.34	6.34	9.389e+39	0.00373
19929	TS.triHPacyl.COelim.mtppppmpu	4.684e+43	5.08	5.08	9.342e+39	0.00371
19930	TS.triHPacyl.COelim.tttmmmpu	2.779e+44	6.14	6.14	9.332e+39	0.00371
19931	TS.triHPacyl.COelim.ptppmpmpu	2.116e+44	5.98	5.98	9.316e+39	0.0037
19932	TS.triHPacyl.COelim.tmmptppmu	1.451e+44	5.76	5.76	9.313e+39	0.0037
19933	TS.triHPacyl.COelim.tmtmpmpu	4.417e+43	5.05	5.05	9.279e+39	0.00369
19934	TS.triHPacyl.COelim.tmtpmmpu	6.102e+44	6.62	6.62	9.253e+39	0.00368
19935	TS.triHPacyl.COelim.mtppmmmpu	1.538e+44	5.80	5.80	9.195e+39	0.00366
19936	TS.triHPacyl.COelim.pptmmppmu	1.964e+44	5.95	5.95	9.080e+39	0.00361
19937	TS.triHPacyl.COelim.mppmmmpu	6.973e+43	5.33	5.33	9.064e+39	0.0036
19938	TS.triHPacyl.COelim.tmpmtmpu	1.311e+44	5.71	5.71	9.032e+39	0.00359
19939	TS.triHPacyl.COelim.mtppmpmpu	1.167e+44	5.64	5.64	9.014e+39	0.00358
19940	TS.triHPacyl.COelim.tmmmtmpu	5.027e+44	6.52	6.52	9.006e+39	0.00358
19941	TS.triHPacyl.COelim.pmmmmtpmu	2.910e+44	6.19	6.19	8.966e+39	0.00357
19942	TS.triHPacyl.COelim.pmpmpmpu	8.603e+43	5.47	5.47	8.935e+39	0.00355
19943	TS.triHPacyl.COelim.mtppmmmpu	1.420e+44	5.77	5.77	8.907e+39	0.00354
19944	TS.triHPacyl.COelim.mppmtmpu	4.683e+44	6.48	6.48	8.868e+39	0.00353
19945	TS.triHPacyl.COelim.ppmmtmpu	3.614e+44	6.33	6.33	8.842e+39	0.00352
19946	TS.triHPacyl.COelim.pptmtmpu	5.606e+44	6.59	6.59	8.821e+39	0.00351
19947	TS.triHPacyl.COelim.pptptmpu	6.012e+44	6.64	6.64	8.805e+39	0.0035
19948	TS.triHPacyl.COelim.pmmmmmpu	8.419e+43	5.47	5.47	8.782e+39	0.00349
19949	TS.triHPacyl.COelim.pttmtppmu	3.876e+44	6.38	6.38	8.778e+39	0.00349
19950	TS.triHPacyl.COelim.mtmmptmpu	2.096e+44	6.01	6.01	8.722e+39	0.00347
19951	TS.triHPacyl.COelim.ptppmpmpu	2.756e+44	6.18	6.18	8.705e+39	0.00346
19952	TS.triHPacyl.COelim.tptpmpmu	2.846e+44	6.20	6.20	8.674e+39	0.00345
19953	TS.triHPacyl.COelim.ptpppmpu	4.655e+44	6.49	6.49	8.669e+39	0.00345
19954	TS.triHPacyl.COelim.pmpmpmpu	5.920e+44	6.64	6.64	8.623e+39	0.00343
19955	TS.triHPacyl.COelim.pttmtmpu	5.982e+44	6.65	6.65	8.604e+39	0.00342
19956	TS.triHPacyl.COelim.tmmmtmpu	1.792e+44	5.93	5.93	8.545e+39	0.0034
19957	TS.triHPacyl.COelim.tpppmpu	4.876e+44	6.53	6.53	8.533e+39	0.00339
19958	TS.triHPacyl.COelim.ptmtmpu	5.596e+44	6.62	6.62	8.438e+39	0.00335
19959	TS.triHPacyl.COelim.mtppptmpu	1.702e+44	5.91	5.91	8.426e+39	0.00335
19960	TS.triHPacyl.COelim.tmtptmpu	1.338e+45	7.14	7.14	8.400e+39	0.00334
19961	TS.triHPacyl.COelim.mtppptmpu	6.571e+43	5.35	5.35	8.374e+39	0.00333
19962	TS.triHPacyl.COelim.tpmtmpu	2.106e+45	7.41	7.41	8.356e+39	0.00332
19963	TS.triHPacyl.COelim.pppmpmpu	1.846e+44	5.97	5.97	8.318e+39	0.00331
19964	TS.triHPacyl.COelim.mmtmmmpu	1.836e+45	7.34	7.34	8.231e+39	0.00327
19965	TS.triHPacyl.COelim.pptmtmpu	8.813e+43	5.53	5.53	8.198e+39	0.00326
19966	TS.triHPacyl.COelim.pmtptmpu	1.450e+44	5.83	5.83	8.162e+39	0.00325
19967	TS.triHPacyl.COelim.ptptmpu	3.507e+44	6.37	6.37	8.093e+39	0.00322
19968	TS.triHPacyl.COelim.pptmtmpu	1.932e+44	6.01	6.01	8.083e+39	0.00321
19969	TS.triHPacyl.COelim.ptptmpu	6.671e+44	6.75	6.75	8.053e+39	0.0032
19970	TS.triHPacyl.COelim.tpmmpmpu	1.787e+44	5.97	5.97	8.041e+39	0.0032
19971	TS.triHPacyl.COelim.pmtmmmpu	3.361e+44	6.34	6.34	8.029e+39	0.00319
19972	TS.triHPacyl.COelim.tmtpmmpu	5.809e+44	6.67	6.67	7.997e+39	0.00318
19973	TS.triHPacyl.COelim.ptppmpu	1.529e+44	5.88	5.88	7.991e+39	0.00318
19974	TS.triHPacyl.COelim.tptmmmpu	8.109e+44	6.88	6.88	7.950e+39	0.00316
19975	TS.triHPacyl.COelim.tmtmmpu	1.713e+45	7.32	7.32	7.937e+39	0.00316
19976	TS.triHPacyl.COelim.pttmmmpu	6.805e+44	6.77	6.77	7.918e+39	0.00315
19977	TS.triHPacyl.COelim.tttmmpu	6.180e+44	6.73	6.73	7.785e+39	0.0031
19978	TS.triHPacyl.COelim.tppmtmpu	2.451e+44	6.18	6.18	7.702e+39	0.00306
19979	TS.triHPacyl.COelim.pmpmtmpu	1.966e+44	6.05	6.05	7.690e+39	0.00306
19980	TS.triHPacyl.COelim.pmtmpmpu	4.577e+44	6.56	6.56	7.673e+39	0.00305
19981	TS.triHPacyl.COelim.ptppmpu	1.445e+44	5.87	5.87	7.656e+39	0.00304
19982	TS.triHPacyl.COelim.pptmpmpu	1.430e+44	5.87	5.87	7.624e+39	0.00303
19983	TS.triHPacyl.COelim.mpppmpu	5.196e+44	6.64	6.64	7.592e+39	0.00302
19984	TS.triHPacyl.COelim.mmtmmppu	6.937e+44	6.81	6.81	7.575e+39	0.00301
19985	TS.triHPacyl.COelim.pmtppmpu	1.991e+44	6.07	6.07	7.494e+39	0.00298
19986	TS.triHPacyl.COelim.pppptmpu	1.302e+45	7.20	7.20	7.463e+39	0.00297
19987	TS.triHPacyl.COelim.tppmpmpu	1.170e+44	5.76	5.76	7.462e+39	0.00297
19988	TS.triHPacyl.COelim.pppmtmpu	1.829e+44	6.03	6.03	7.446e+39	0.00296
19989	TS.triHPacyl.COelim.ptmtmpu	3.434e+44	6.41	6.41	7.408e+39	0.00295
19990	TS.triHPacyl.COelim.pptpmpu	6.479e+44	6.79	6.79	7.301e+39	0.0029
19991	TS.triHPacyl.COelim.pmpmtmpu	5.331e+44	6.68	6.68	7.263e+39	0.00289

19992	TS.triHPacyl.COelim.pmmppptmmu	4.518e+43	5.21	5.21	7.256e+39	0.00289
19993	TS.triHPacyl.COelim.ptptpppmu	4.444e+44	6.57	6.57	7.231e+39	0.00288
19994	TS.triHPacyl.COelim.mmtpmtpmpu	2.262e+45	7.54	7.54	7.222e+39	0.00287
19995	TS.triHPacyl.COelim.ptppptpppu	5.494e+44	6.70	6.70	7.214e+39	0.00287
19996	TS.triHPacyl.COelim.ptttmpmpu	4.408e+44	6.57	6.57	7.169e+39	0.00285
19997	TS.triHPacyl.COelim.ttpmpppmu	3.553e+44	6.45	6.45	7.163e+39	0.00285
19998	TS.triHPacyl.COelim.mpmtpmpmpu	2.993e+44	6.35	6.35	7.131e+39	0.00284
19999	TS.triHPacyl.COelim.pmpmmpmpu	2.436e+44	6.22	6.22	7.113e+39	0.00283
20000	TS.triHPacyl.COelim.ptttptpmu	3.463e+44	6.44	6.44	7.094e+39	0.00282
20001	TS.triHPacyl.COelim.mppptmpu	1.681e+44	6.01	6.01	7.092e+39	0.00282
20002	TS.triHPacyl.COelim.ptttptppu	3.321e+44	6.41	6.41	7.061e+39	0.00281
20003	TS.triHPacyl.COelim.mmtmpmpmpu	2.501e+44	6.25	6.25	7.006e+39	0.00279
20004	TS.triHPacyl.COelim.mptppppmu	9.512e+43	5.67	5.67	7.004e+39	0.00279
20005	TS.triHPacyl.COelim.mmtpmtpmu	1.958e+45	7.48	7.48	6.997e+39	0.00278
20006	TS.triHPacyl.COelim.pmpmmpmpu	4.701e+43	5.25	5.25	6.995e+39	0.00278
20007	TS.triHPacyl.COelim.mptmptppu	8.915e+43	5.64	5.64	6.963e+39	0.00277
20008	TS.triHPacyl.COelim.tttmpmpmu	1.072e+45	7.12	7.12	6.961e+39	0.00277
20009	TS.triHPacyl.COelim.pppmptppu	2.911e+44	6.35	6.35	6.934e+39	0.00276
20010	TS.triHPacyl.COelim.ptttmpppu	3.014e+44	6.37	6.37	6.870e+39	0.00273
20011	TS.triHPacyl.COelim.mttmpmpmu	1.470e+44	5.94	5.94	6.862e+39	0.00273
20012	TS.triHPacyl.COelim.mmpptmpu	1.220e+44	5.83	5.83	6.860e+39	0.00273
20013	TS.triHPacyl.COelim.tmmmpmpmpu	7.969e+43	5.58	5.58	6.851e+39	0.00272
20014	TS.triHPacyl.COelim.pmpmmpmpu	2.616e+43	4.92	4.92	6.845e+39	0.00272
20015	TS.triHPacyl.COelim.mttptpmu	2.815e+44	6.34	6.34	6.822e+39	0.00271
20016	TS.triHPacyl.COelim.pmmppptmmu	5.025e+43	5.31	5.31	6.791e+39	0.0027
20017	TS.triHPacyl.COelim.tmtptmmu	4.868e+44	6.67	6.67	6.758e+39	0.00269
20018	TS.triHPacyl.COelim.ptmtpppmu	2.476e+44	6.27	6.27	6.750e+39	0.00268
20019	TS.triHPacyl.COelim.pttmtmpu	4.508e+44	6.62	6.62	6.750e+39	0.00268
20020	TS.triHPacyl.COelim.mmpptmtmmu	8.090e+44	6.97	6.97	6.735e+39	0.00268
20021	TS.triHPacyl.COelim.tppmmmpmu	5.712e+44	6.77	6.77	6.731e+39	0.00268
20022	TS.triHPacyl.COelim.mtppppmpu	1.318e+44	5.89	5.89	6.719e+39	0.00267
20023	TS.triHPacyl.COelim.ptptptmmu	3.523e+44	6.48	6.48	6.687e+39	0.00266
20024	TS.triHPacyl.COelim.ptptmmmpmu	3.012e+44	6.39	6.39	6.651e+39	0.00264
20025	TS.triHPacyl.COelim.pmtmpmpmu	5.353e+43	5.36	5.36	6.647e+39	0.00264
20026	TS.triHPacyl.COelim.tppptmpu	4.517e+44	6.64	6.64	6.568e+39	0.00261
20027	TS.triHPacyl.COelim.ptmmmpmmu	5.185e+44	6.72	6.72	6.558e+39	0.00261
20028	TS.triHPacyl.COelim.ttmmpmmmpu	3.380e+44	6.47	6.47	6.499e+39	0.00258
20029	TS.triHPacyl.COelim.ppptptpmu	5.196e+44	6.73	6.73	6.487e+39	0.00258
20030	TS.triHPacyl.COelim.ptmpmpmpu	1.911e+44	6.14	6.14	6.472e+39	0.00257
20031	TS.triHPacyl.COelim.ptmtptppmu	2.145e+44	6.21	6.21	6.442e+39	0.00256
20032	TS.triHPacyl.COelim.tptmtpmu	8.002e+44	7.00	7.00	6.387e+39	0.00254
20033	TS.triHPacyl.COelim.pmtptmmmpu	1.865e+44	6.14	6.14	6.305e+39	0.00251
20034	TS.triHPacyl.COelim.ppptmtmpu	2.349e+44	6.28	6.28	6.299e+39	0.0025
20035	TS.triHPacyl.COelim.ttptmtpmu	5.625e+44	6.80	6.80	6.278e+39	0.0025
20036	TS.triHPacyl.COelim.mtmmppmpu	8.547e+43	5.68	5.68	6.187e+39	0.00246
20037	TS.triHPacyl.COelim.ptmmmtppu	2.916e+44	6.42	6.42	6.185e+39	0.00246
20038	TS.triHPacyl.COelim.tpttptpmu	6.558e+44	6.90	6.90	6.142e+39	0.00244
20039	TS.triHPacyl.COelim.mmpmptmmu	2.883e+44	6.41	6.41	6.136e+39	0.00244
20040	TS.triHPacyl.COelim.tpttpppmu	4.236e+44	6.65	6.65	6.100e+39	0.00243
20041	TS.triHPacyl.COelim.mptmptmpu	6.719e+44	6.92	6.92	6.084e+39	0.00242
20042	TS.triHPacyl.COelim.tmpmmmtmmu	1.612e+44	6.07	6.07	6.069e+39	0.00241
20043	TS.triHPacyl.COelim.ttmppptppu	1.315e+45	7.32	7.32	6.066e+39	0.00241
20044	TS.triHPacyl.COelim.mmpmppppmu	4.289e+43	5.29	5.29	6.025e+39	0.0024
20045	TS.triHPacyl.COelim.pptpmpmpmu	1.497e+44	6.04	6.04	5.995e+39	0.00238
20046	TS.triHPacyl.COelim.pmmpppppmu	4.235e+43	5.29	5.29	5.973e+39	0.00238
20047	TS.triHPacyl.COelim.ptmpptmmu	5.213e+43	5.41	5.41	5.972e+39	0.00237
20048	TS.triHPacyl.COelim.mtppmtmpu	4.801e+44	6.74	6.74	5.947e+39	0.00236
20049	TS.triHPacyl.COelim.tttmmpppu	3.474e+44	6.55	6.55	5.926e+39	0.00236
20050	TS.triHPacyl.COelim.ptttpppmu	5.060e+44	6.77	6.77	5.911e+39	0.00235
20051	TS.triHPacyl.COelim.tppmmmmmu	1.792e+44	6.16	6.16	5.877e+39	0.00234
20052	TS.triHPacyl.COelim.ptpmpmpu	5.798e+43	5.49	5.49	5.835e+39	0.00232
20053	TS.triHPacyl.COelim.mttmptmpu	2.321e+44	6.32	6.32	5.769e+39	0.00229
20054	TS.triHPacyl.COelim.tpptptmpu	6.243e+44	6.92	6.92	5.711e+39	0.00227
20055	TS.triHPacyl.COelim.mppppppmu	1.866e+44	6.20	6.20	5.696e+39	0.00226
20056	TS.triHPacyl.COelim.pmtmpmmmu	5.522e+44	6.85	6.85	5.695e+39	0.00226
20057	TS.triHPacyl.COelim.tppmtmmu	3.447e+44	6.57	6.57	5.659e+39	0.00225
20058	TS.triHPacyl.COelim.ppptppmpu	3.590e+44	6.59	6.59	5.655e+39	0.00225
20059	TS.triHPacyl.COelim.pppppppmu	1.779e+44	6.18	6.18	5.639e+39	0.00224
20060	TS.triHPacyl.COelim.mmpptmtmpu	6.897e+44	6.98	6.98	5.637e+39	0.00224
20061	TS.triHPacyl.COelim.mttpppppu	1.719e+44	6.16	6.16	5.617e+39	0.00223
20062	TS.triHPacyl.COelim.tpptpppmu	5.194e+44	6.82	6.82	5.611e+39	0.00223
20063	TS.triHPacyl.COelim.pmmppptppu	2.879e+44	6.47	6.47	5.610e+39	0.00223

20064	TS.triHPacyl.COelim.ttpmmtmmu	2.548e+44	6.40	6.40	5.543e+39	0.0022
20065	TS.triHPacyl.COelim.mmmmmtppmu	2.586e+44	6.41	6.41	5.530e+39	0.0022
20066	TS.triHPacyl.COelim.tptmmtmpu	1.700e+45	7.53	7.53	5.523e+39	0.0022
20067	TS.triHPacyl.COelim.tttpttpmu	2.238e+45	7.70	7.70	5.522e+39	0.0022
20068	TS.triHPacyl.COelim.mmpmpptmpu	2.861e+44	6.47	6.47	5.490e+39	0.00218
20069	TS.triHPacyl.COelim.mmmppmpmmu	1.420e+43	4.69	4.69	5.481e+39	0.00218
20070	TS.triHPacyl.COelim.tpmtmtpmu	2.290e+44	6.35	6.35	5.453e+39	0.00217
20071	TS.triHPacyl.COelim.ptmtmmmmmu	1.017e+45	7.24	7.24	5.449e+39	0.00217
20072	TS.triHPacyl.COelim.ttpmptpmu	3.118e+44	6.53	6.53	5.434e+39	0.00216
20073	TS.triHPacyl.COelim.pptmmpmpu	6.208e+43	5.57	5.57	5.420e+39	0.00216
20074	TS.triHPacyl.COelim.tmttpmppmu	2.346e+45	7.74	7.74	5.390e+39	0.00214
20075	TS.triHPacyl.COelim.mtppmpmpmu	7.010e+43	5.65	5.65	5.371e+39	0.00214
20076	TS.triHPacyl.COelim.pmpptmpu	7.930e+43	5.72	5.72	5.357e+39	0.00213
20077	TS.triHPacyl.COelim.mtppmmpmpu	1.902e+44	6.25	6.25	5.357e+39	0.00213
20078	TS.triHPacyl.COelim.mmtmpmtmpu	4.812e+44	6.80	6.80	5.338e+39	0.00212
20079	TS.triHPacyl.COelim.tmmmpmtmpmu	2.398e+44	6.39	6.39	5.310e+39	0.00211
20080	TS.triHPacyl.COelim.ppptpmpu	5.254e+44	6.86	6.86	5.295e+39	0.00211
20081	TS.triHPacyl.COelim.tpmmpmtppu	8.608e+44	7.15	7.15	5.289e+39	0.0021
20082	TS.triHPacyl.COelim.pttpmtpmu	1.033e+45	7.26	7.26	5.283e+39	0.0021
20083	TS.triHPacyl.COelim.mmpmpppppu	7.508e+43	5.70	5.70	5.260e+39	0.00209
20084	TS.triHPacyl.COelim.ppptpmpu	6.861e+44	7.02	7.02	5.239e+39	0.00208
20085	TS.triHPacyl.COelim.mttpmmmmpu	3.322e+44	6.59	6.59	5.232e+39	0.00208
20086	TS.triHPacyl.COelim.tmttmtppmu	5.837e+44	6.93	6.93	5.204e+39	0.00207
20087	TS.triHPacyl.COelim.tmmmpmtmmu	3.954e+44	6.70	6.70	5.183e+39	0.00206
20088	TS.triHPacyl.COelim.tmpmmtmpu	1.453e+44	6.11	6.11	5.176e+39	0.00206
20089	TS.triHPacyl.COelim.pmmmpptmmu	9.287e+43	5.84	5.84	5.150e+39	0.00205
20090	TS.triHPacyl.COelim.ppptpmpu	7.462e+44	7.09	7.09	5.102e+39	0.00203
20091	TS.triHPacyl.COelim.ptmpmtppmu	6.441e+43	5.63	5.63	5.069e+39	0.00202
20092	TS.triHPacyl.COelim.tpptmtmmu	2.365e+45	7.78	7.78	5.066e+39	0.00201
20093	TS.triHPacyl.COelim.tmmmtpppu	1.125e+44	5.97	5.97	5.065e+39	0.00201
20094	TS.triHPacyl.COelim.pptmmtmmu	4.727e+44	6.83	6.83	5.015e+39	0.00199
20095	TS.triHPacyl.COelim.tmppmpmpu	1.968e+44	6.31	6.31	4.991e+39	0.00198
20096	TS.triHPacyl.COelim.ptmmpmtmpu	1.606e+45	7.56	7.56	4.987e+39	0.00198
20097	TS.triHPacyl.COelim.tptmmmmppu	7.725e+43	5.75	5.75	4.982e+39	0.00198
20098	TS.triHPacyl.COelim.mtmmppmtmmu	2.980e+44	6.56	6.56	4.981e+39	0.00198
20099	TS.triHPacyl.COelim.ptmtmmpmpu	3.137e+44	6.59	6.59	4.967e+39	0.00197
20100	TS.triHPacyl.COelim.pptpmtmpu	1.014e+45	7.29	7.29	4.966e+39	0.00197
20101	TS.triHPacyl.COelim.tmmmpmpmu	4.335e+44	6.78	6.78	4.966e+39	0.00197
20102	TS.triHPacyl.COelim.pttptmpu	5.967e+44	6.97	6.97	4.961e+39	0.00197
20103	TS.triHPacyl.COelim.tmttptmmu	6.422e+44	7.02	7.02	4.944e+39	0.00197
20104	TS.triHPacyl.COelim.ttpmmtmpu	9.197e+43	5.86	5.86	4.940e+39	0.00196
20105	TS.triHPacyl.COelim.pmttptmpu	3.064e+44	6.58	6.58	4.901e+39	0.00195
20106	TS.triHPacyl.COelim.tmttppppu	2.504e+44	6.46	6.46	4.889e+39	0.00194
20107	TS.triHPacyl.COelim.mptppmmpmu	6.289e+43	5.64	5.64	4.880e+39	0.00194
20108	TS.triHPacyl.COelim.tmtmpmmmmu	1.771e+45	7.63	7.63	4.877e+39	0.00194
20109	TS.triHPacyl.COelim.pttppmpmu	6.234e+44	7.01	7.01	4.875e+39	0.00194
20110	TS.triHPacyl.COelim.pttpmmpu	5.912e+44	6.98	6.98	4.840e+39	0.00192
20111	TS.triHPacyl.COelim.ptptmmpmu	4.048e+44	6.76	6.76	4.824e+39	0.00192
20112	TS.triHPacyl.COelim.mttmpppppu	1.512e+44	6.17	6.17	4.811e+39	0.00191
20113	TS.triHPacyl.COelim.tmtptmpu	2.331e+44	6.43	6.43	4.799e+39	0.00191
20114	TS.triHPacyl.COelim.mmmmpmpmu	1.699e+44	6.25	6.25	4.785e+39	0.00191
20115	TS.triHPacyl.COelim.tmpmmtpppu	4.486e+43	5.46	5.46	4.751e+39	0.00189
20116	TS.triHPacyl.COelim.ptmtmpmpu	3.889e+44	6.74	6.74	4.745e+39	0.00189
20117	TS.triHPacyl.COelim.ptppmmmmu	1.269e+44	6.08	6.08	4.729e+39	0.00188
20118	TS.triHPacyl.COelim.tpmtmtpmu	1.601e+45	7.59	7.59	4.719e+39	0.00188
20119	TS.triHPacyl.COelim.mptmtpmpu	8.142e+44	7.19	7.19	4.714e+39	0.00187
20120	TS.triHPacyl.COelim.tttmmmpmu	6.322e+44	7.04	7.04	4.703e+39	0.00187
20121	TS.triHPacyl.COelim.pmpppptmpu	1.185e+44	6.04	6.04	4.690e+39	0.00186
20122	TS.triHPacyl.COelim.pptptmpu	2.827e+44	6.56	6.56	4.676e+39	0.00186
20123	TS.triHPacyl.COelim.mmmppppmpu	1.843e+43	4.94	4.94	4.674e+39	0.00186
20124	TS.triHPacyl.COelim.pmpmpmpu	7.108e+43	5.75	5.75	4.640e+39	0.00185
20125	TS.triHPacyl.COelim.mtmmpmpmu	9.307e+43	5.91	5.91	4.634e+39	0.00184
20126	TS.triHPacyl.COelim.pmtmpmtmpu	1.133e+45	7.40	7.40	4.629e+39	0.00184
20127	TS.triHPacyl.COelim.tttptmpu	1.719e+45	7.65	7.65	4.625e+39	0.00184
20128	TS.triHPacyl.COelim.pttptmpu	4.242e+44	6.81	6.81	4.618e+39	0.00184
20129	TS.triHPacyl.COelim.ptmtptmpu	6.229e+44	7.05	7.05	4.574e+39	0.00182
20130	TS.triHPacyl.COelim.pmtppmpmu	9.587e+43	5.93	5.93	4.573e+39	0.00182
20131	TS.triHPacyl.COelim.pttpmtmpu	6.405e+44	7.07	7.07	4.531e+39	0.0018
20132	TS.triHPacyl.COelim.pptmmtpu	3.388e+44	6.69	6.69	4.512e+39	0.00179
20133	TS.triHPacyl.COelim.tptmmpmmu	1.607e+45	7.62	7.62	4.491e+39	0.00179
20134	TS.triHPacyl.COelim.pppppppmu	2.032e+44	6.39	6.39	4.464e+39	0.00178
20135	TS.triHPacyl.COelim.pttmtmmmu	8.984e+44	7.28	7.28	4.461e+39	0.00177

20136	TS.triHPacyl.COelim.pmttptppmu	6.956e+44	7.13	7.13	4.445e+39	0.00177
20137	TS.triHPacyl.COelim.ttmmmtppmu	1.358e+44	6.16	6.16	4.442e+39	0.00177
20138	TS.triHPacyl.COelim.pmttpppppu	3.358e+44	6.70	6.70	4.437e+39	0.00176
20139	TS.triHPacyl.COelim.ppmtmppmpu	8.428e+43	5.88	5.88	4.420e+39	0.00176
20140	TS.triHPacyl.COelim.mppppppmpu	2.489e+44	6.52	6.52	4.419e+39	0.00176
20141	TS.triHPacyl.COelim.pptmppppmu	9.958e+43	5.98	5.98	4.401e+39	0.00175
20142	TS.triHPacyl.COelim.ppmpmpmpu	4.295e+43	5.48	5.48	4.390e+39	0.00175
20143	TS.triHPacyl.COelim.pppmmtppu	5.791e+44	7.04	7.04	4.334e+39	0.00172
20144	TS.triHPacyl.COelim.tpmtmmpmpu	2.997e+44	6.64	6.64	4.324e+39	0.00172
20145	TS.triHPacyl.COelim.tpmtmtmpu	1.720e+44	6.32	6.32	4.317e+39	0.00172
20146	TS.triHPacyl.COelim.mptpptppu	1.100e+44	6.05	6.05	4.314e+39	0.00172
20147	TS.triHPacyl.COelim.ptmtmtmpu	4.866e+44	6.94	6.94	4.312e+39	0.00171
20148	TS.triHPacyl.COelim.ppttptmmu	4.932e+44	6.95	6.95	4.287e+39	0.0017
20149	TS.triHPacyl.COelim.ttpmmmtppu	1.425e+44	6.21	6.21	4.273e+39	0.0017
20150	TS.triHPacyl.COelim.mpmtptmpu	2.608e+44	6.57	6.57	4.261e+39	0.00169
20151	TS.triHPacyl.COelim.pptmmmtmmu	3.458e+44	6.74	6.74	4.261e+39	0.00169
20152	TS.triHPacyl.COelim.tpppmtmmu	7.555e+44	7.21	7.21	4.249e+39	0.00169
20153	TS.triHPacyl.COelim.tmtmpppmpu	1.346e+45	7.56	7.56	4.211e+39	0.00167
20154	TS.triHPacyl.COelim.pttpmmpmpu	4.766e+44	6.94	6.94	4.177e+39	0.00166
20155	TS.triHPacyl.COelim.tttmtmpmu	8.762e+44	7.31	7.31	4.173e+39	0.00166
20156	TS.triHPacyl.COelim.tptmptpmu	3.634e+44	6.78	6.78	4.170e+39	0.00166
20157	TS.triHPacyl.COelim.ptmtmtmpu	2.335e+44	6.52	6.52	4.166e+39	0.00166
20158	TS.triHPacyl.COelim.tmtpppppu	1.897e+45	7.77	7.77	4.150e+39	0.00165
20159	TS.triHPacyl.COelim.mttmpmpmpu	5.629e+44	7.05	7.05	4.132e+39	0.00164
20160	TS.triHPacyl.COelim.tpptptpu	1.258e+45	7.53	7.53	4.123e+39	0.00164
20161	TS.triHPacyl.COelim.ttmtmtmpu	6.678e+44	7.15	7.15	4.110e+39	0.00163
20162	TS.triHPacyl.COelim.pttptmpu	6.558e+44	7.14	7.14	4.100e+39	0.00163
20163	TS.triHPacyl.COelim.ptmmmtmmu	2.915e+44	6.67	6.67	4.067e+39	0.00162
20164	TS.triHPacyl.COelim.ppttptpmu	5.976e+44	7.10	7.10	4.012e+39	0.0016
20165	TS.triHPacyl.COelim.mmpmpppmpu	1.698e+44	6.35	6.35	4.006e+39	0.00159
20166	TS.triHPacyl.COelim.ttpmmpppu	1.363e+44	6.22	6.22	3.990e+39	0.00159
20167	TS.triHPacyl.COelim.tppmpmpmpu	3.335e+44	6.76	6.76	3.986e+39	0.00158
20168	TS.triHPacyl.COelim.ppmmtmpu	1.071e+45	7.46	7.46	3.946e+39	0.00157
20169	TS.triHPacyl.COelim.ptmmpmmu	3.025e+44	6.71	6.71	3.943e+39	0.00157
20170	TS.triHPacyl.COelim.mmtmpmmmu	6.010e+44	7.12	7.12	3.940e+39	0.00157
20171	TS.triHPacyl.COelim.ppmptmpu	1.428e+44	6.26	6.26	3.932e+39	0.00156
20172	TS.triHPacyl.COelim.ttpmtmpmu	6.750e+44	7.19	7.19	3.923e+39	0.00156
20173	TS.triHPacyl.COelim.ptptptmpu	7.500e+43	5.88	5.88	3.920e+39	0.00156
20174	TS.triHPacyl.COelim.pmtmppmpu	1.717e+44	6.37	6.37	3.918e+39	0.00156
20175	TS.triHPacyl.COelim.ttptmmmu	2.363e+44	6.56	6.56	3.911e+39	0.00156
20176	TS.triHPacyl.COelim.ppmtpmpmu	3.150e+44	6.74	6.74	3.890e+39	0.00155
20177	TS.triHPacyl.COelim.ppmppppmu	3.365e+43	5.41	5.41	3.853e+39	0.00153
20178	TS.triHPacyl.COelim.tmmppmpmpu	5.821e+43	5.74	5.74	3.853e+39	0.00153
20179	TS.triHPacyl.COelim.mmtmpmpmpu	2.326e+44	6.56	6.56	3.843e+39	0.00153
20180	TS.triHPacyl.COelim.mmpmpptpmu	6.571e+44	7.18	7.18	3.838e+39	0.00153
20181	TS.triHPacyl.COelim.ttptmmpmu	5.989e+44	7.13	7.13	3.829e+39	0.00152
20182	TS.triHPacyl.COelim.tmtmmpmu	7.635e+44	7.28	7.28	3.827e+39	0.00152
20183	TS.triHPacyl.COelim.ttmmppppmu	1.020e+45	7.45	7.45	3.808e+39	0.00151
20184	TS.triHPacyl.COelim.ppmmpmtmpu	1.302e+44	6.23	6.23	3.795e+39	0.00151
20185	TS.triHPacyl.COelim.ttppmmmmu	2.929e+44	6.71	6.71	3.790e+39	0.00151
20186	TS.triHPacyl.COelim.ttmmppmpu	6.688e+44	7.21	7.21	3.766e+39	0.0015
20187	TS.triHPacyl.COelim.tppmmmtmpu	5.022e+44	7.04	7.04	3.757e+39	0.00149
20188	TS.triHPacyl.COelim.ptppptmmu	4.063e+44	6.91	6.91	3.729e+39	0.00148
20189	TS.triHPacyl.COelim.tmtmmmmppu	1.560e+45	7.72	7.72	3.722e+39	0.00148
20190	TS.triHPacyl.COelim.tmttptppu	6.711e+44	7.22	7.22	3.707e+39	0.00147
20191	TS.triHPacyl.COelim.ttptmpppu	1.130e+45	7.53	7.53	3.681e+39	0.00146
20192	TS.triHPacyl.COelim.pttptmpu	6.956e+44	7.26	7.26	3.562e+39	0.00142
20193	TS.triHPacyl.COelim.mttmpmmmmu	1.543e+45	7.74	7.74	3.559e+39	0.00142
20194	TS.triHPacyl.COelim.pmmppptpmu	4.885e+43	5.68	5.68	3.553e+39	0.00141
20195	TS.triHPacyl.COelim.ttptmmtppu	1.335e+45	7.65	7.65	3.552e+39	0.00141
20196	TS.triHPacyl.COelim.mmmmmmtmmu	8.641e+44	7.40	7.40	3.538e+39	0.00141
20197	TS.triHPacyl.COelim.mtmppppmpu	1.126e+44	6.18	6.18	3.531e+39	0.0014
20198	TS.triHPacyl.COelim.mmtmptmpu	4.567e+44	7.02	7.02	3.521e+39	0.0014
20199	TS.triHPacyl.COelim.pttptmpu	6.855e+44	7.27	7.27	3.492e+39	0.00139
20200	TS.triHPacyl.COelim.mpppptmpu	2.218e+44	6.60	6.60	3.477e+39	0.00138
20201	TS.triHPacyl.COelim.mmpmptmmu	2.641e+43	5.33	5.33	3.461e+39	0.00138
20202	TS.triHPacyl.COelim.ptmtpmmpu	8.587e+44	7.41	7.41	3.457e+39	0.00137
20203	TS.triHPacyl.COelim.ttptppmpu	6.659e+44	7.26	7.26	3.450e+39	0.00137
20204	TS.triHPacyl.COelim.ptptmpmpu	1.771e+44	6.47	6.47	3.436e+39	0.00137
20205	TS.triHPacyl.COelim.tmtptmmmu	8.625e+43	6.04	6.04	3.423e+39	0.00136
20206	TS.triHPacyl.COelim.ptmmmpmpu	2.933e+44	6.77	6.77	3.418e+39	0.00136
20207	TS.triHPacyl.COelim.tmttptmpmu	8.756e+44	7.43	7.43	3.392e+39	0.00135

20208	TS.triHPacyl.COelim.tmppmtmpu	5.133e+44	7.11	7.11	3.389e+39	0.00135
20209	TS.triHPacyl.COelim.tptmmtmmu	8.266e+44	7.40	7.40	3.387e+39	0.00135
20210	TS.triHPacyl.COelim.mmmmmmmmpu	1.167e+45	7.60	7.60	3.386e+39	0.00135
20211	TS.triHPacyl.COelim.tpptmmmpu	2.570e+44	6.70	6.70	3.374e+39	0.00134
20212	TS.triHPacyl.COelim.mptmppppu	1.821e+44	6.50	6.50	3.371e+39	0.00134
20213	TS.triHPacyl.COelim.tpmmmttmmu	2.355e+44	6.65	6.65	3.359e+39	0.00134
20214	TS.triHPacyl.COelim.tpptmtmpu	3.050e+44	6.81	6.81	3.348e+39	0.00133
20215	TS.triHPacyl.COelim.tmmmpmtmmu	3.736e+44	6.93	6.93	3.340e+39	0.00133
20216	TS.triHPacyl.COelim.pmpmpmtmpu	3.091e+44	6.82	6.82	3.339e+39	0.00133
20217	TS.triHPacyl.COelim.tttmpttpu	9.635e+44	7.50	7.50	3.331e+39	0.00132
20218	TS.triHPacyl.COelim.pmtmptmpu	1.107e+44	6.21	6.21	3.321e+39	0.00132
20219	TS.triHPacyl.COelim.pmpmmppmu	6.282e+43	5.87	5.87	3.314e+39	0.00132
20220	TS.triHPacyl.COelim.pppmptmmu	2.337e+44	6.66	6.66	3.311e+39	0.00132
20221	TS.triHPacyl.COelim.pppmptmmu	9.161e+43	6.10	6.10	3.291e+39	0.00131
20222	TS.triHPacyl.COelim.pppmptmmu	2.212e+43	5.26	5.26	3.283e+39	0.00131
20223	TS.triHPacyl.COelim.pppmptmmu	1.676e+44	6.47	6.47	3.265e+39	0.0013
20224	TS.triHPacyl.COelim.mmmmmmtppu	9.873e+44	7.53	7.53	3.246e+39	0.00129
20225	TS.triHPacyl.COelim.mmpmtmpu	6.492e+44	7.28	7.28	3.234e+39	0.00129
20226	TS.triHPacyl.COelim.mmpmtmpu	2.017e+44	7.28	7.28	3.227e+39	0.00128
20227	TS.triHPacyl.COelim.tpmmtmpu	1.087e+44	6.22	6.22	3.221e+39	0.00128
20228	TS.triHPacyl.COelim.mttmmpmmu	1.698e+44	6.49	6.49	3.186e+39	0.00127
20229	TS.triHPacyl.COelim.mmpmtmpu	7.192e+44	7.35	7.35	3.164e+39	0.00126
20230	TS.triHPacyl.COelim.tttmmtmpu	1.168e+45	7.64	7.64	3.163e+39	0.00126
20231	TS.triHPacyl.COelim.tttmmtmpu	6.321e+44	7.28	7.28	3.153e+39	0.00125
20232	TS.triHPacyl.COelim.mppmptmmu	2.992e+44	6.84	6.84	3.139e+39	0.00125
20233	TS.triHPacyl.COelim.pmpmmmpu	1.368e+45	7.74	7.74	3.134e+39	0.00125
20234	TS.triHPacyl.COelim.tttmmpmmu	3.285e+44	6.89	6.89	3.125e+39	0.00124
20235	TS.triHPacyl.COelim.tttmmtmmu	9.687e+44	7.54	7.54	3.125e+39	0.00124
20236	TS.triHPacyl.COelim.mttppppmmu	1.625e+44	6.48	6.48	3.113e+39	0.00124
20237	TS.triHPacyl.COelim.tmtmtmmu	1.543e+45	7.82	7.82	3.112e+39	0.00124
20238	TS.triHPacyl.COelim.tptmmtmmu	2.017e+44	6.61	6.61	3.109e+39	0.00124
20239	TS.triHPacyl.COelim.pmtppmpu	1.578e+44	6.46	6.46	3.090e+39	0.00123
20240	TS.triHPacyl.COelim.mmpmpptpu	1.995e+44	6.60	6.60	3.085e+39	0.00123
20241	TS.triHPacyl.COelim.ptmptmpu	2.300e+44	6.69	6.69	3.084e+39	0.00123
20242	TS.triHPacyl.COelim.ttmmpmmu	3.868e+45	8.37	8.37	3.066e+39	0.00122
20243	TS.triHPacyl.COelim.mmpmtmpu	1.845e+44	6.57	6.57	3.029e+39	0.0012
20244	TS.triHPacyl.COelim.tttmppmpu	3.866e+45	8.38	8.38	3.016e+39	0.0012
20245	TS.triHPacyl.COelim.mmpmpmmu	1.280e+44	6.35	6.35	3.015e+39	0.0012
20246	TS.triHPacyl.COelim.mptmptmpu	1.626e+44	6.50	6.50	3.008e+39	0.0012
20247	TS.triHPacyl.COelim.mttmptmmu	4.385e+44	7.09	7.09	2.987e+39	0.00119
20248	TS.triHPacyl.COelim.pmtmptmmu	6.111e+44	7.29	7.29	2.982e+39	0.00119
20249	TS.triHPacyl.COelim.tmtppppmu	2.206e+44	6.69	6.69	2.951e+39	0.00117
20250	TS.triHPacyl.COelim.ptmptmpu	2.069e+44	6.81	6.81	2.948e+39	0.00117
20251	TS.triHPacyl.COelim.tmtmtpmpu	2.340e+44	6.73	6.73	2.943e+39	0.00117
20252	TS.triHPacyl.COelim.ttmmpmmu	7.774e+44	7.44	7.44	2.942e+39	0.00117
20253	TS.triHPacyl.COelim.ttptmtpu	6.942e+44	7.38	7.38	2.935e+39	0.00117
20254	TS.triHPacyl.COelim.ptmmpmmu	8.387e+44	7.49	7.49	2.930e+39	0.00116
20255	TS.triHPacyl.COelim.tpmtmmu	1.777e+45	7.94	7.94	2.928e+39	0.00116
20256	TS.triHPacyl.COelim.ptmptmpu	3.807e+44	7.02	7.02	2.923e+39	0.00116
20257	TS.triHPacyl.COelim.pptmptmpu	1.659e+44	6.53	6.53	2.894e+39	0.00115
20258	TS.triHPacyl.COelim.mtppppppu	1.155e+44	6.32	6.32	2.873e+39	0.00114
20259	TS.triHPacyl.COelim.tpmptmpu	6.892e+44	7.39	7.39	2.850e+39	0.00113
20260	TS.triHPacyl.COelim.ptmpttpu	8.888e+44	7.54	7.54	2.836e+39	0.00113
20261	TS.triHPacyl.COelim.pptmmtmpu	3.181e+44	6.93	6.93	2.836e+39	0.00113
20262	TS.triHPacyl.COelim.ptmptmpu	5.442e+44	7.25	7.25	2.834e+39	0.00113
20263	TS.triHPacyl.COelim.tppmmtmmu	6.703e+44	7.38	7.38	2.819e+39	0.00112
20264	TS.triHPacyl.COelim.mttmptmmu	6.549e+44	7.37	7.37	2.817e+39	0.00112
20265	TS.triHPacyl.COelim.mmpmtmpu	1.663e+44	6.55	6.55	2.814e+39	0.00112
20266	TS.triHPacyl.COelim.tttmmtmmu	1.829e+45	7.98	7.98	2.813e+39	0.00112
20267	TS.triHPacyl.COelim.tttmmtmmu	8.601e+44	7.54	7.54	2.786e+39	0.00111
20268	TS.triHPacyl.COelim.pmtmptmpu	7.689e+43	6.10	6.10	2.782e+39	0.00111
20269	TS.triHPacyl.COelim.mtmmpmmu	3.243e+44	6.96	6.96	2.781e+39	0.00111
20270	TS.triHPacyl.COelim.tptpmpu	5.890e+44	7.31	7.31	2.774e+39	0.0011
20271	TS.triHPacyl.COelim.pmtmmmpu	2.930e+44	6.90	6.90	2.772e+39	0.0011
20272	TS.triHPacyl.COelim.pppmmtmpu	5.975e+43	5.95	5.95	2.772e+39	0.0011
20273	TS.triHPacyl.COelim.tptmptmpu	1.197e+45	7.74	7.74	2.763e+39	0.0011
20274	TS.triHPacyl.COelim.mttmmpmpu	3.831e+44	7.06	7.06	2.763e+39	0.0011
20275	TS.triHPacyl.COelim.tpmtmtpu	1.394e+45	7.83	7.83	2.749e+39	0.00109
20276	TS.triHPacyl.COelim.tttmmtmpu	8.242e+44	7.52	7.52	2.746e+39	0.00109
20277	TS.triHPacyl.COelim.ttpmptmpu	1.271e+44	6.41	6.41	2.734e+39	0.00109
20278	TS.triHPacyl.COelim.pmtmmtmpu	7.955e+44	7.51	7.51	2.686e+39	0.00107
20279	TS.triHPacyl.COelim.ptpmtmpu	1.371e+45	7.84	7.84	2.663e+39	0.00106

20280	TS.triHPacyl.COelim.mpttpmtpmu	5.628e+44	7.31	7.31	2.653e+39	0.00106
20281	TS.triHPacyl.COelim.pmpmmmpmu	3.436e+43	5.65	5.65	2.653e+39	0.00105
20282	TS.triHPacyl.COelim.ppmtmtpmu	8.098e+44	7.53	7.53	2.644e+39	0.00105
20283	TS.triHPacyl.COelim.tnmtmppppu	1.871e+44	6.66	6.66	2.624e+39	0.00104
20284	TS.triHPacyl.COelim.tnmtmptmmu	9.869e+43	6.28	6.28	2.620e+39	0.00104
20285	TS.triHPacyl.COelim.mtmtmpppmu	7.641e+44	7.50	7.50	2.612e+39	0.00104
20286	TS.triHPacyl.COelim.ptmmpmpppu	2.192e+44	6.76	6.76	2.607e+39	0.00104
20287	TS.triHPacyl.COelim.tpmtmtpmu	1.520e+45	7.92	7.92	2.593e+39	0.00103
20288	TS.triHPacyl.COelim.pmmtpptppu	1.439e+44	6.51	6.51	2.589e+39	0.00103
20289	TS.triHPacyl.COelim.tptmmpmmpu	1.545e+45	7.93	7.93	2.584e+39	0.00103
20290	TS.triHPacyl.COelim.pmmtppppmu	7.462e+43	6.13	6.13	2.556e+39	0.00102
20291	TS.triHPacyl.COelim.ptmtptppu	2.058e+44	6.74	6.74	2.553e+39	0.00102
20292	TS.triHPacyl.COelim.mptmpmppmu	2.432e+44	6.84	6.84	2.542e+39	0.00101
20293	TS.triHPacyl.COelim.ptptmtmmpu	6.735e+43	6.08	6.08	2.528e+39	0.00101
20294	TS.triHPacyl.COelim.tpptmmpmu	6.554e+45	8.80	8.80	2.527e+39	0.001
20295	TS.triHPacyl.COelim.mmpmtpmmpu	1.531e+45	7.94	7.94	2.519e+39	0.001
20296	TS.triHPacyl.COelim.pmmtpptmpu	1.073e+45	7.73	7.73	2.511e+39	0.000999
20297	TS.triHPacyl.COelim.mptmtpmmpu	4.523e+44	7.21	7.21	2.510e+39	0.000998
20298	TS.triHPacyl.COelim.pptmmpmmpu	6.230e+43	6.03	6.03	2.509e+39	0.000998
20299	TS.triHPacyl.COelim.tttmmpmmpu	7.371e+44	7.51	7.51	2.506e+39	0.000996
20300	TS.triHPacyl.COelim.ptpmpmmpmu	1.309e+44	6.48	6.48	2.505e+39	0.000996
20301	TS.triHPacyl.COelim.mmpmmpmmpmu	2.857e+44	6.95	6.95	2.475e+39	0.000984
20302	TS.triHPacyl.COelim.mtpppmmpmu	1.064e+44	6.36	6.36	2.472e+39	0.000983
20303	TS.triHPacyl.COelim.ttptmmpmmpu	2.479e+44	6.87	6.87	2.469e+39	0.000982
20304	TS.triHPacyl.COelim.ttppmmtppu	4.083e+44	7.16	7.16	2.467e+39	0.000981
20305	TS.triHPacyl.COelim.mptmmpmmpu	1.831e+44	6.69	6.69	2.448e+39	0.000973
20306	TS.triHPacyl.COelim.tmptmmpmmpu	7.160e+44	7.50	7.50	2.444e+39	0.000972
20307	TS.triHPacyl.COelim.mttmmpmmpu	2.317e+44	6.83	6.83	2.435e+39	0.000968
20308	TS.triHPacyl.COelim.mttppptmpu	4.585e+44	7.24	7.24	2.423e+39	0.000963
20309	TS.triHPacyl.COelim.tnmtpppppu	8.328e+43	6.23	6.23	2.417e+39	0.000961
20310	TS.triHPacyl.COelim.ttppmptmmpu	4.712e+44	7.27	7.27	2.395e+39	0.000952
20311	TS.triHPacyl.COelim.pmtppmmpmu	1.118e+44	6.41	6.41	2.395e+39	0.000952
20312	TS.triHPacyl.COelim.mmmmtmtpmu	7.742e+44	7.56	7.56	2.393e+39	0.000952
20313	TS.triHPacyl.COelim.ttppptmmpu	2.066e+44	6.78	6.78	2.376e+39	0.000945
20314	TS.triHPacyl.COelim.ppmtmtpmu	4.452e+44	7.24	7.24	2.365e+39	0.000941
20315	TS.triHPacyl.COelim.tttmtmmpmu	4.916e+44	7.30	7.30	2.359e+39	0.000938
20316	TS.triHPacyl.COelim.tmtmmpmmpu	9.448e+44	7.69	7.69	2.358e+39	0.000938
20317	TS.triHPacyl.COelim.ptmtmtpmu	1.518e+45	7.97	7.97	2.355e+39	0.000937
20318	TS.triHPacyl.COelim.tttmtpptpu	1.332e+45	7.90	7.90	2.353e+39	0.000935
20319	TS.triHPacyl.COelim.mtmtpmmpu	1.310e+44	6.52	6.52	2.337e+39	0.000929
20320	TS.triHPacyl.COelim.ptpmpmtpmu	1.575e+44	6.63	6.63	2.337e+39	0.000929
20321	TS.triHPacyl.COelim.pptptmmpu	3.309e+44	7.07	7.07	2.330e+39	0.000927
20322	TS.triHPacyl.COelim.tttppppmu	5.746e+44	7.40	7.40	2.329e+39	0.000926
20323	TS.triHPacyl.COelim.mptmtpmmpu	8.707e+43	6.28	6.28	2.329e+39	0.000926
20324	TS.triHPacyl.COelim.pttptmtpmu	2.845e+44	6.99	6.99	2.320e+39	0.000922
20325	TS.triHPacyl.COelim.tttmtmmpu	1.116e+45	7.80	7.80	2.313e+39	0.00092
20326	TS.triHPacyl.COelim.tmpmtpppu	1.768e+44	6.71	6.71	2.295e+39	0.000913
20327	TS.triHPacyl.COelim.ptttmmpmmpu	7.194e+44	7.55	7.55	2.282e+39	0.000907
20328	TS.triHPacyl.COelim.tttppptpmu	1.878e+45	8.13	8.13	2.258e+39	0.000898
20329	TS.triHPacyl.COelim.mtmmtmmpmu	2.590e+44	6.95	6.95	2.256e+39	0.000897
20330	TS.triHPacyl.COelim.pmtmtpmmpu	1.369e+44	6.57	6.57	2.245e+39	0.000893
20331	TS.triHPacyl.COelim.pmttptmmpu	3.642e+44	7.16	7.16	2.230e+39	0.000887
20332	TS.triHPacyl.COelim.pppmmpmmpu	3.157e+44	7.07	7.07	2.230e+39	0.000887
20333	TS.triHPacyl.COelim.ptmtptmmpu	4.288e+44	7.25	7.25	2.229e+39	0.000886
20334	TS.triHPacyl.COelim.tpmmmtmmpu	1.165e+44	6.48	6.48	2.225e+39	0.000885
20335	TS.triHPacyl.COelim.mptmmpmmpu	5.158e+44	7.37	7.37	2.220e+39	0.000883
20336	TS.triHPacyl.COelim.mtppmmpmmpu	9.885e+43	6.39	6.39	2.205e+39	0.000877
20337	TS.triHPacyl.COelim.ptmmtptppu	1.657e+44	6.69	6.69	2.201e+39	0.000875
20338	TS.triHPacyl.COelim.mtppmmpmmpu	1.478e+44	6.63	6.63	2.181e+39	0.000867
20339	TS.triHPacyl.COelim.tptmmpmmpu	7.458e+44	7.60	7.60	2.176e+39	0.000865
20340	TS.triHPacyl.COelim.tptmtpmmpu	4.066e+44	7.24	7.24	2.173e+39	0.000864
20341	TS.triHPacyl.COelim.tnmpmtpmmpu	1.479e+44	6.63	6.63	2.171e+39	0.000863
20342	TS.triHPacyl.COelim.ppmtmtpmu	3.862e+44	7.21	7.21	2.170e+39	0.000863
20343	TS.triHPacyl.COelim.pmmptmmpu	8.253e+43	6.29	6.29	2.170e+39	0.000863
20344	TS.triHPacyl.COelim.pptmmpmmpu	2.936e+44	7.04	7.04	2.167e+39	0.000862
20345	TS.triHPacyl.COelim.tmtmtmmpu	1.373e+45	7.96	7.96	2.167e+39	0.000862
20346	TS.triHPacyl.COelim.ptmtmmpmmpu	6.136e+44	7.49	7.49	2.156e+39	0.000857
20347	TS.triHPacyl.COelim.mmpmtpmmpu	3.151e+44	7.09	7.09	2.152e+39	0.000856
20348	TS.triHPacyl.COelim.ttppmtmmpu	1.717e+44	6.73	6.73	2.147e+39	0.000854
20349	TS.triHPacyl.COelim.ptptmtpmmpu	3.076e+44	7.08	7.08	2.126e+39	0.000845
20350	TS.triHPacyl.COelim.mptmtpmmpu	2.019e+44	6.83	6.83	2.119e+39	0.000843
20351	TS.triHPacyl.COelim.tppmmmtmmpu	7.458e+44	7.62	7.62	2.096e+39	0.000834

20352	TS.triHPacyl.COelim.ppmtppmpu	2.987e+44	7.08	7.08	2.091e+39	0.000831
20353	TS.triHPacyl.COelim.tnmtmtmpu	3.447e+44	7.16	7.16	2.089e+39	0.00083
20354	TS.triHPacyl.COelim.ptptmmmmu	5.559e+44	7.45	7.45	2.083e+39	0.000828
20355	TS.triHPacyl.COelim.ttttmmmpu	5.411e+44	7.43	7.43	2.081e+39	0.000828
20356	TS.triHPacyl.COelim.tppptppmu	4.262e+44	7.29	7.29	2.081e+39	0.000827
20357	TS.triHPacyl.COelim.tmtmptmpu	3.106e+44	7.10	7.10	2.073e+39	0.000824
20358	TS.triHPacyl.COelim.mmtppmtmmu	3.101e+44	7.10	7.10	2.070e+39	0.000823
20359	TS.triHPacyl.COelim.ptppmtmpu	4.338e+44	7.31	7.31	2.068e+39	0.000822
20360	TS.triHPacyl.COelim.ppptptmpu	3.581e+44	7.19	7.19	2.064e+39	0.000821
20361	TS.triHPacyl.COelim.mmttmmtmpu	1.007e+45	7.81	7.81	2.060e+39	0.000819
20362	TS.triHPacyl.COelim.mtppmtmpu	7.537e+43	6.27	6.27	2.044e+39	0.000813
20363	TS.triHPacyl.COelim.ttttmtppu	4.892e+44	7.39	7.39	2.032e+39	0.000808
20364	TS.triHPacyl.COelim.ttttptmpu	3.756e+45	8.60	8.60	2.031e+39	0.000808
20365	TS.triHPacyl.COelim.pmmmtmtmpu	2.899e+44	7.08	7.08	2.030e+39	0.000807
20366	TS.triHPacyl.COelim.tpptmmmpu	2.974e+44	7.06	7.06	2.027e+39	0.000806
20367	TS.triHPacyl.COelim.ttptmmmpu	6.873e+44	7.59	7.59	2.020e+39	0.000803
20368	TS.triHPacyl.COelim.ptmmpmmmu	4.499e+44	7.35	7.35	2.001e+39	0.000796
20369	TS.triHPacyl.COelim.mmtptmpmu	2.455e+44	6.99	6.99	1.999e+39	0.000795
20370	TS.triHPacyl.COelim.pppmtppu	3.240e+44	7.16	7.16	1.976e+39	0.000786
20371	TS.triHPacyl.COelim.mmtptmpmu	7.114e+44	7.63	7.63	1.972e+39	0.000784
20372	TS.triHPacyl.COelim.pppmmmpu	3.045e+44	7.12	7.12	1.971e+39	0.000784
20373	TS.triHPacyl.COelim.tmttptmpu	7.744e+44	7.68	7.68	1.958e+39	0.000779
20374	TS.triHPacyl.COelim.pttmtptmpu	5.172e+44	7.45	7.45	1.949e+39	0.000775
20375	TS.triHPacyl.COelim.pppmmtppu	3.365e+44	7.20	7.20	1.928e+39	0.000766
20376	TS.triHPacyl.COelim.tpmmpmpu	1.532e+44	6.73	6.73	1.928e+39	0.000766
20377	TS.triHPacyl.COelim.pttptmpu	1.361e+44	6.66	6.66	1.924e+39	0.000765
20378	TS.triHPacyl.COelim.pmpmptppu	2.494e+44	7.02	7.02	1.912e+39	0.00076
20379	TS.triHPacyl.COelim.tpmmmmpu	1.735e+44	6.81	6.81	1.912e+39	0.00076
20380	TS.triHPacyl.COelim.ttmppmmpu	6.069e+44	7.55	7.55	1.905e+39	0.000758
20381	TS.triHPacyl.COelim.mmtptmpmu	2.453e+44	7.02	7.02	1.890e+39	0.000751
20382	TS.triHPacyl.COelim.mppmptppu	1.928e+44	6.88	6.88	1.890e+39	0.000751
20383	TS.triHPacyl.COelim.tmtmptmpu	5.719e+44	7.52	7.52	1.887e+39	0.00075
20384	TS.triHPacyl.COelim.ttttmtmpu	1.333e+45	8.03	8.03	1.885e+39	0.00075
20385	TS.triHPacyl.COelim.mmtmmpmmpu	4.739e+44	7.41	7.41	1.880e+39	0.000747
20386	TS.triHPacyl.COelim.tptppppmu	3.253e+44	7.19	7.19	1.871e+39	0.000744
20387	TS.triHPacyl.COelim.pmtmtpmpu	4.738e+44	7.42	7.42	1.865e+39	0.000741
20388	TS.triHPacyl.COelim.mmtptmpmu	5.668e+44	7.53	7.53	1.862e+39	0.00074
20389	TS.triHPacyl.COelim.tpmptmpu	1.725e+44	6.82	6.82	1.860e+39	0.00074
20390	TS.triHPacyl.COelim.mtmtmmpmu	7.241e+44	7.67	7.67	1.860e+39	0.00074
20391	TS.triHPacyl.COelim.mpmmmmtmpu	1.756e+44	6.83	6.83	1.849e+39	0.000735
20392	TS.triHPacyl.COelim.mmtmmtmpu	1.872e+45	8.24	8.24	1.847e+39	0.000734
20393	TS.triHPacyl.COelim.ppttptmpu	5.343e+44	7.50	7.50	1.837e+39	0.000731
20394	TS.triHPacyl.COelim.tmtmmmpu	1.603e+45	8.16	8.16	1.835e+39	0.00073
20395	TS.triHPacyl.COelim.tmtmmpmpu	2.984e+44	7.15	7.15	1.835e+39	0.00073
20396	TS.triHPacyl.COelim.ptmtpmmpu	1.151e+44	6.59	6.59	1.814e+39	0.000721
20397	TS.triHPacyl.COelim.pttptmpmu	6.000e+44	7.59	7.59	1.789e+39	0.000711
20398	TS.triHPacyl.COelim.mtmmpmmpu	4.434e+44	7.41	7.41	1.783e+39	0.000709
20399	TS.triHPacyl.COelim.ptmmpmmpu	3.662e+44	7.29	7.29	1.783e+39	0.000709
20400	TS.triHPacyl.COelim.pttptmpmu	4.264e+44	7.39	7.39	1.774e+39	0.000706
20401	TS.triHPacyl.COelim.ppttmtppu	2.860e+44	7.15	7.15	1.770e+39	0.000704
20402	TS.triHPacyl.COelim.tmmpmmtmpu	1.227e+44	6.65	6.65	1.767e+39	0.000702
20403	TS.triHPacyl.COelim.pmpmptmpu	1.015e+44	6.54	6.54	1.748e+39	0.000695
20404	TS.triHPacyl.COelim.tpttmmppu	6.550e+44	7.65	7.65	1.745e+39	0.000694
20405	TS.triHPacyl.COelim.pmtptmpu	7.033e+44	7.70	7.70	1.742e+39	0.000693
20406	TS.triHPacyl.COelim.mmmmttmu	3.391e+44	7.27	7.27	1.729e+39	0.000687
20407	TS.triHPacyl.COelim.pptppmmpu	6.574e+44	7.66	7.66	1.720e+39	0.000684
20408	TS.triHPacyl.COelim.tptmmpmmpu	1.937e+44	6.93	6.93	1.719e+39	0.000683
20409	TS.triHPacyl.COelim.tptmmtmpu	8.864e+44	7.84	7.84	1.717e+39	0.000683
20410	TS.triHPacyl.COelim.mmpmptmpu	2.439e+44	7.07	7.07	1.712e+39	0.000681
20411	TS.triHPacyl.COelim.mppppmpu	5.053e+44	7.51	7.51	1.712e+39	0.000681
20412	TS.triHPacyl.COelim.ptmmpmmpu	4.962e+43	6.13	6.13	1.693e+39	0.000673
20413	TS.triHPacyl.COelim.pptmmpmmpu	2.056e+44	6.98	6.98	1.678e+39	0.000667
20414	TS.triHPacyl.COelim.ptmmpptppu	1.182e+44	6.66	6.66	1.673e+39	0.000665
20415	TS.triHPacyl.COelim.pmtmmtmpu	7.570e+44	7.77	7.77	1.668e+39	0.000663
20416	TS.triHPacyl.COelim.mmtptmpmu	8.183e+44	7.81	7.81	1.661e+39	0.00066
20417	TS.triHPacyl.COelim.tmmpmmpmu	5.501e+43	6.21	6.21	1.651e+39	0.000657
20418	TS.triHPacyl.COelim.pptmmpmmpu	9.044e+43	6.51	6.51	1.645e+39	0.000654
20419	TS.triHPacyl.COelim.ptmmtmmpu	7.759e+44	7.79	7.79	1.640e+39	0.000652
20420	TS.triHPacyl.COelim.pptmtmpmu	4.111e+44	7.41	7.41	1.637e+39	0.000651
20421	TS.triHPacyl.COelim.pmpmmtmmpu	2.118e+44	7.02	7.02	1.636e+39	0.00065
20422	TS.triHPacyl.COelim.mppmptppu	3.394e+43	5.94	5.94	1.610e+39	0.00064
20423	TS.triHPacyl.COelim.pptppmmpu	1.159e+44	6.67	6.67	1.602e+39	0.000637

20424	TS.triHPacyl.COelim.pttpptmpu	3.646e+44	7.36	7.36	1.586e+39	0.000631
20425	TS.triHPacyl.COelim.ttpmmmtmpu	1.842e+44	6.96	6.96	1.578e+39	0.000628
20426	TS.triHPacyl.COelim.mpmtptmpu	2.404e+44	7.12	7.12	1.576e+39	0.000627
20427	TS.triHPacyl.COelim.mmpmpmmmmu	2.942e+44	7.24	7.24	1.566e+39	0.000623
20428	TS.triHPacyl.COelim.pttppmpmpu	4.829e+44	7.54	7.54	1.555e+39	0.000618
20429	TS.triHPacyl.COelim.mttmptmpu	7.579e+44	7.81	7.81	1.552e+39	0.000617
20430	TS.triHPacyl.COelim.pttpptmpu	3.835e+44	7.40	7.40	1.547e+39	0.000615
20431	TS.triHPacyl.COelim.pmpmpmpmpu	2.698e+43	5.83	5.83	1.524e+39	0.000606
20432	TS.triHPacyl.COelim.ttmtmmtmpu	1.051e+45	8.02	8.02	1.515e+39	0.000602
20433	TS.triHPacyl.COelim.ptptptppu	7.318e+43	6.43	6.43	1.505e+39	0.000598
20434	TS.triHPacyl.COelim.tmmmpptppu	5.883e+43	6.30	6.30	1.505e+39	0.000598
20435	TS.triHPacyl.COelim.ttmmmmmmmu	2.600e+44	7.19	7.19	1.496e+39	0.000595
20436	TS.triHPacyl.COelim.ttmmmmpppu	2.128e+44	7.07	7.07	1.495e+39	0.000595
20437	TS.triHPacyl.COelim.ppttptppu	1.376e+44	6.82	6.82	1.490e+39	0.000593
20438	TS.triHPacyl.COelim.ptmtmtmpu	1.014e+44	6.63	6.63	1.489e+39	0.000592
20439	TS.triHPacyl.COelim.tmpmmmtmpu	1.397e+44	6.83	6.83	1.482e+39	0.000589
20440	TS.triHPacyl.COelim.ptmpmmmpu	1.083e+44	6.68	6.68	1.480e+39	0.000589
20441	TS.triHPacyl.COelim.tmtptmpu	4.968e+44	7.59	7.59	1.471e+39	0.000585
20442	TS.triHPacyl.COelim.pttpmtmpu	4.968e+44	7.57	7.57	1.468e+39	0.000584
20443	TS.triHPacyl.COelim.mmpptptmpu	2.439e+44	7.17	7.17	1.463e+39	0.000582
20444	TS.triHPacyl.COelim.ppptppmpu	2.107e+44	7.08	7.08	1.462e+39	0.000581
20445	TS.triHPacyl.COelim.tptptmpu	5.426e+44	7.65	7.65	1.447e+39	0.000575
20446	TS.triHPacyl.COelim.mmpmpmmmpu	1.535e+44	6.90	6.90	1.445e+39	0.000574
20447	TS.triHPacyl.COelim.pmpmpmpmpu	2.185e+44	7.11	7.11	1.434e+39	0.00057
20448	TS.triHPacyl.COelim.pmpptppmu	3.143e+43	5.96	5.96	1.430e+39	0.000568
20449	TS.triHPacyl.COelim.mmpptppmpu	2.799e+44	7.26	7.26	1.429e+39	0.000568
20450	TS.triHPacyl.COelim.mptpmtmpu	3.121e+44	7.33	7.33	1.421e+39	0.000565
20451	TS.triHPacyl.COelim.tmmmpptppu	2.911e+44	7.29	7.29	1.413e+39	0.000562
20452	TS.triHPacyl.COelim.pttppppmpu	5.336e+44	7.66	7.66	1.401e+39	0.000557
20453	TS.triHPacyl.COelim.mttmptmpu	9.409e+44	8.00	8.00	1.391e+39	0.000553
20454	TS.triHPacyl.COelim.ptppmtmpu	1.755e+44	7.01	7.01	1.380e+39	0.000549
20455	TS.triHPacyl.COelim.tmpmpmpmpu	9.311e+44	8.00	8.00	1.378e+39	0.000548
20456	TS.triHPacyl.COelim.tmmmpppppu	1.072e+44	6.72	6.72	1.372e+39	0.000546
20457	TS.triHPacyl.COelim.mpmmpptppu	4.187e+43	6.16	6.16	1.371e+39	0.000545
20458	TS.triHPacyl.COelim.mtpmtmmu	1.343e+45	8.23	8.23	1.369e+39	0.000544
20459	TS.triHPacyl.COelim.tpppmtppu	2.254e+45	8.54	8.54	1.362e+39	0.000542
20460	TS.triHPacyl.COelim.ptmtmpmmu	7.372e+44	7.87	7.87	1.360e+39	0.000541
20461	TS.triHPacyl.COelim.ppptmpmpu	1.874e+44	7.06	7.06	1.352e+39	0.000538
20462	TS.triHPacyl.COelim.ttmtmmpppu	2.934e+44	7.33	7.33	1.340e+39	0.000533
20463	TS.triHPacyl.COelim.mtpmpmpmpu	1.635e+44	6.98	6.98	1.340e+39	0.000533
20464	TS.triHPacyl.COelim.tmttmmpmpu	1.124e+45	8.13	8.13	1.338e+39	0.000532
20465	TS.triHPacyl.COelim.ptpmmmtmpu	1.128e+44	6.76	6.76	1.336e+39	0.000531
20466	TS.triHPacyl.COelim.ptpmpmpmpu	3.217e+44	7.39	7.39	1.336e+39	0.000531
20467	TS.triHPacyl.COelim.pppmmmpmpu	7.766e+43	6.54	6.54	1.334e+39	0.00053
20468	TS.triHPacyl.COelim.mmtmpmtppu	8.670e+44	7.98	7.98	1.330e+39	0.000529
20469	TS.triHPacyl.COelim.tppmpmpmpu	7.959e+43	6.56	6.56	1.321e+39	0.000525
20470	TS.triHPacyl.COelim.pmttpptmpu	2.943e+44	7.34	7.34	1.319e+39	0.000524
20471	TS.triHPacyl.COelim.pppmttppu	1.850e+44	7.07	7.07	1.318e+39	0.000524
20472	TS.triHPacyl.COelim.ttmttppmu	2.752e+44	7.31	7.31	1.305e+39	0.000519
20473	TS.triHPacyl.COelim.pptpmpmpu	8.125e+43	6.58	6.58	1.300e+39	0.000517
20474	TS.triHPacyl.COelim.ttmtptmmu	2.789e+45	8.69	8.69	1.293e+39	0.000514
20475	TS.triHPacyl.COelim.tttmmtmmu	1.832e+45	8.44	8.44	1.293e+39	0.000514
20476	TS.triHPacyl.COelim.ptptptmmu	2.219e+44	7.19	7.19	1.290e+39	0.000513
20477	TS.triHPacyl.COelim.ttptmmmpu	1.522e+44	6.96	6.96	1.290e+39	0.000513
20478	TS.triHPacyl.COelim.ttptmpmpu	4.224e+44	7.57	7.57	1.289e+39	0.000513
20479	TS.triHPacyl.COelim.mpmtmpmpu	2.957e+44	7.36	7.36	1.285e+39	0.000511
20480	TS.triHPacyl.COelim.ttptmtmpu	8.483e+43	6.62	6.62	1.285e+39	0.000511
20481	TS.triHPacyl.COelim.ttmtmpmpu	8.523e+44	7.99	7.99	1.279e+39	0.000508
20482	TS.triHPacyl.COelim.pmpptppmpu	1.242e+44	6.85	6.85	1.277e+39	0.000508
20483	TS.triHPacyl.COelim.tpppmpmpu	2.728e+44	7.32	7.32	1.276e+39	0.000507
20484	TS.triHPacyl.COelim.mptmmtmpu	3.603e+44	7.48	7.48	1.275e+39	0.000507
20485	TS.triHPacyl.COelim.mpmmpmtmmu	2.362e+44	7.23	7.23	1.271e+39	0.000506
20486	TS.triHPacyl.COelim.mttmpmmmpu	1.801e+45	8.45	8.45	1.269e+39	0.000504
20487	TS.triHPacyl.COelim.tptmpmpmpu	3.085e+44	7.40	7.40	1.259e+39	0.000501
20488	TS.triHPacyl.COelim.ttpmpppppu	3.701e+44	7.51	7.51	1.253e+39	0.000498
20489	TS.triHPacyl.COelim.mmtmpmpmpu	8.912e+44	8.03	8.03	1.252e+39	0.000498
20490	TS.triHPacyl.COelim.tmmmmmpmpu	1.227e+44	6.85	6.85	1.251e+39	0.000498
20491	TS.triHPacyl.COelim.mmpptppmpu	5.029e+44	7.69	7.69	1.251e+39	0.000497
20492	TS.triHPacyl.COelim.tttmtmpmpu	6.380e+44	7.84	7.84	1.249e+39	0.000497
20493	TS.triHPacyl.COelim.ttpmmmpmpu	6.315e+44	7.83	7.83	1.247e+39	0.000496
20494	TS.triHPacyl.COelim.mttmpppppu	3.342e+44	7.45	7.45	1.242e+39	0.000494
20495	TS.triHPacyl.COelim.ttmtmmtmmu	1.108e+44	6.80	6.80	1.240e+39	0.000493

20496	TS.triHPacyl.COelim.tmtpptmmmu	6.810e+44	7.88	7.88	1.238e+39	0.000492
20497	TS.triHPacyl.COelim.mtptpmpmmu	2.030e+44	7.16	7.16	1.235e+39	0.000491
20498	TS.triHPacyl.COelim.mptmmmpmpu	7.706e+44	7.96	7.96	1.234e+39	0.000491
20499	TS.triHPacyl.COelim.pptpptppu	3.692e+44	7.52	7.52	1.232e+39	0.00049
20500	TS.triHPacyl.COelim.ptptppmpu	7.140e+44	7.91	7.91	1.230e+39	0.000489
20501	TS.triHPacyl.COelim.pttppmmmu	1.436e+45	8.33	8.33	1.225e+39	0.000487
20502	TS.triHPacyl.COelim.mpmmpptpmu	7.669e+43	6.59	6.59	1.218e+39	0.000484
20503	TS.triHPacyl.COelim.pmtmptpmu	8.085e+44	7.99	7.99	1.215e+39	0.000483
20504	TS.triHPacyl.COelim.tmtmtmpmu	8.760e+44	8.04	8.04	1.214e+39	0.000483
20505	TS.triHPacyl.COelim.mtppmmmpu	2.959e+44	7.40	7.40	1.212e+39	0.000482
20506	TS.triHPacyl.COelim.pptmmmpmu	3.377e+44	7.48	7.48	1.208e+39	0.00048
20507	TS.triHPacyl.COelim.pttppmpmu	9.474e+44	8.09	8.09	1.207e+39	0.00048
20508	TS.triHPacyl.COelim.tpmmpmmmpu	1.746e+44	7.09	7.09	1.193e+39	0.000474
20509	TS.triHPacyl.COelim.ppptmtpmu	4.985e+44	7.72	7.72	1.192e+39	0.000474
20510	TS.triHPacyl.COelim.tttppmmmu	1.066e+45	8.17	8.17	1.191e+39	0.000473
20511	TS.triHPacyl.COelim.tttppmpu	1.435e+45	8.35	8.35	1.190e+39	0.000473
20512	TS.triHPacyl.COelim.tmtmtmpmu	7.661e+43	6.60	6.60	1.189e+39	0.000473
20513	TS.triHPacyl.COelim.ppptmmmpu	3.365e+44	7.49	7.49	1.187e+39	0.000472
20514	TS.triHPacyl.COelim.tpppmtmpu	1.438e+45	9.01	9.01	1.182e+39	0.00047
20515	TS.triHPacyl.COelim.tmtmmpmmu	6.012e+44	7.83	7.83	1.179e+39	0.000469
20516	TS.triHPacyl.COelim.mmtmmppmu	3.193e+44	7.46	7.46	1.178e+39	0.000468
20517	TS.triHPacyl.COelim.tmmppmtmu	3.616e+44	7.53	7.53	1.178e+39	0.000468
20518	TS.triHPacyl.COelim.pmptmmppmu	7.373e+44	7.96	7.96	1.177e+39	0.000468
20519	TS.triHPacyl.COelim.tpptmtppu	1.474e+45	8.37	8.37	1.174e+39	0.000467
20520	TS.triHPacyl.COelim.tppmmtmpu	4.421e+44	7.66	7.66	1.163e+39	0.000462
20521	TS.triHPacyl.COelim.mtptmmmmu	4.293e+44	7.64	7.64	1.162e+39	0.000462
20522	TS.triHPacyl.COelim.ptpmtmmu	1.758e+44	7.11	7.11	1.162e+39	0.000462
20523	TS.triHPacyl.COelim.tmtmmmmmpu	5.404e+44	7.78	7.78	1.161e+39	0.000462
20524	TS.triHPacyl.COelim.ppmmttmmu	2.727e+44	7.37	7.37	1.160e+39	0.000461
20525	TS.triHPacyl.COelim.tpppmtmpu	4.254e+45	9.01	9.01	1.159e+39	0.000461
20526	TS.triHPacyl.COelim.mmtmppmmmu	9.258e+44	8.10	8.10	1.156e+39	0.00046
20527	TS.triHPacyl.COelim.ptmtmmpmu	4.949e+44	7.73	7.73	1.155e+39	0.000459
20528	TS.triHPacyl.COelim.ptmtptpmu	1.666e+44	7.08	7.08	1.154e+39	0.000459
20529	TS.triHPacyl.COelim.tmtptpmu	6.476e+44	7.89	7.89	1.154e+39	0.000459
20530	TS.triHPacyl.COelim.tptmtppu	3.259e+44	7.78	7.78	1.151e+39	0.000457
20531	TS.triHPacyl.COelim.pmmppmpu	5.874e+43	6.47	6.47	1.145e+39	0.000455
20532	TS.triHPacyl.COelim.tttmmmmmpu	1.729e+44	7.11	7.11	1.139e+39	0.000453
20533	TS.triHPacyl.COelim.pmpmmtpmu	2.160e+44	7.25	7.25	1.135e+39	0.000451
20534	TS.triHPacyl.COelim.tppppmmmu	1.742e+44	7.12	7.12	1.134e+39	0.000451
20535	TS.triHPacyl.COelim.tmtmtpmu	1.205e+45	8.28	8.28	1.129e+39	0.000449
20536	TS.triHPacyl.COelim.pmppppppu	1.600e+44	7.07	7.07	1.129e+39	0.000449
20537	TS.triHPacyl.COelim.ptptmtpmu	5.612e+44	7.82	7.82	1.123e+39	0.000446
20538	TS.triHPacyl.COelim.mmpmpmpmu	3.257e+44	7.50	7.50	1.113e+39	0.000443
20539	TS.triHPacyl.COelim.tmmppppmu	1.110e+44	6.86	6.86	1.110e+39	0.000441
20540	TS.triHPacyl.COelim.mtptmpppu	7.917e+44	8.04	8.04	1.108e+39	0.000441
20541	TS.triHPacyl.COelim.mpmmpmtmu	2.037e+44	7.23	7.23	1.105e+39	0.000439
20542	TS.triHPacyl.COelim.tpmppmmmpu	8.706e+43	6.72	6.72	1.104e+39	0.000439
20543	TS.triHPacyl.COelim.pptptppmu	2.769e+44	7.41	7.41	1.103e+39	0.000439
20544	TS.triHPacyl.COelim.mpmmpmpmu	1.296e+44	6.96	6.96	1.098e+39	0.000437
20545	TS.triHPacyl.COelim.ttpmpmpu	1.505e+44	7.05	7.05	1.096e+39	0.000436
20546	TS.triHPacyl.COelim.mmpptmpu	6.644e+44	7.94	7.94	1.093e+39	0.000435
20547	TS.triHPacyl.COelim.mtpmmppmu	5.307e+44	7.81	7.81	1.091e+39	0.000434
20548	TS.triHPacyl.COelim.ppptmpmpu	2.816e+44	7.43	7.43	1.087e+39	0.000432
20549	TS.triHPacyl.COelim.tmtmmmmmu	1.123e+44	6.89	6.89	1.068e+39	0.000425
20550	TS.triHPacyl.COelim.mptmptpmu	1.642e+44	7.12	7.12	1.067e+39	0.000424
20551	TS.triHPacyl.COelim.pmtptmmu	6.742e+44	7.96	7.96	1.065e+39	0.000423
20552	TS.triHPacyl.COelim.ppmptmpu	1.930e+44	7.22	7.22	1.063e+39	0.000423
20553	TS.triHPacyl.COelim.mtmtmpmpu	2.353e+44	7.34	7.34	1.058e+39	0.000421
20554	TS.triHPacyl.COelim.pptmmpmpu	5.654e+44	7.86	7.86	1.056e+39	0.00042
20555	TS.triHPacyl.COelim.pmtptmmu	7.941e+44	8.07	8.07	1.051e+39	0.000418
20556	TS.triHPacyl.COelim.tmpmpmpu	3.231e+44	7.53	7.53	1.050e+39	0.000417
20557	TS.triHPacyl.COelim.mptmmpmpu	3.854e+45	9.01	9.01	1.047e+39	0.000416
20558	TS.triHPacyl.COelim.tpptmtppu	2.850e+45	8.83	8.83	1.046e+39	0.000416
20559	TS.triHPacyl.COelim.ptpmpmpu	4.862e+44	7.78	7.78	1.046e+39	0.000416
20560	TS.triHPacyl.COelim.ptmptmpmu	3.540e+44	7.59	7.59	1.043e+39	0.000415
20561	TS.triHPacyl.COelim.pmtptpmu	2.203e+44	7.31	7.31	1.041e+39	0.000414
20562	TS.triHPacyl.COelim.pmpmpmpu	6.221e+43	6.56	6.56	1.041e+39	0.000414
20563	TS.triHPacyl.COelim.tpmmpmpu	2.163e+44	7.30	7.30	1.037e+39	0.000412
20564	TS.triHPacyl.COelim.ptmmpmpu	5.997e+44	7.91	7.91	1.033e+39	0.000411
20565	TS.triHPacyl.COelim.ptmptmpu	2.758e+44	7.45	7.45	1.032e+39	0.00041
20566	TS.triHPacyl.COelim.tmtmtmpu	3.351e+44	7.57	7.57	1.032e+39	0.00041
20567	TS.triHPacyl.COelim.mpppmpmpu	8.779e+44	8.14	8.14	1.029e+39	0.000409

20568	TS.triHPacyl.COelim.pppmpmmmu	3.547e+44	7.60	7.60	1.026e+39	0.000408
20569	TS.triHPacyl.COelim.tttmptmmmu	3.860e+45	9.03	9.03	1.021e+39	0.000406
20570	TS.triHPacyl.COelim.tmtmtmpmu	9.542e+43	6.83	6.83	1.015e+39	0.000403
20571	TS.triHPacyl.COelim.ttttmmpmpu	6.932e+44	8.01	8.01	1.014e+39	0.000403
20572	TS.triHPacyl.COelim.mtptppmmu	2.022e+44	7.28	7.28	1.011e+39	0.000402
20573	TS.triHPacyl.COelim.mppmmmtmpu	1.282e+44	7.01	7.01	9.988e+38	0.000397
20574	TS.triHPacyl.COelim.mtttptmpu	6.542e+44	7.99	7.99	9.961e+38	0.000396
20575	TS.triHPacyl.COelim.tmtppmmu	6.242e+44	7.96	7.96	9.949e+38	0.000396
20576	TS.triHPacyl.COelim.ptmptmpu	5.023e+44	7.83	7.83	9.941e+38	0.000395
20577	TS.triHPacyl.COelim.pmpmpmpu	7.410e+44	8.06	8.06	9.921e+38	0.000394
20578	TS.triHPacyl.COelim.ttmmttppu	1.321e+44	7.04	7.04	9.889e+38	0.000393
20579	TS.triHPacyl.COelim.mmptmpmpu	2.871e+44	7.50	7.50	9.883e+38	0.000393
20580	TS.triHPacyl.COelim.ttmmtmpmu	3.593e+44	7.63	7.63	9.855e+38	0.000392
20581	TS.triHPacyl.COelim.ptptppppu	1.832e+44	7.23	7.23	9.846e+38	0.000391
20582	TS.triHPacyl.COelim.tttptmpu	5.956e+44	7.94	7.94	9.799e+38	0.00039
20583	TS.triHPacyl.COelim.ppmmtmpu	5.306e+44	7.87	7.87	9.773e+38	0.000389
20584	TS.triHPacyl.COelim.pptppmmu	3.640e+44	7.65	7.65	9.683e+38	0.000385
20585	TS.triHPacyl.COelim.pmpmtmpmu	3.427e+43	6.25	6.25	9.672e+38	0.000385
20586	TS.triHPacyl.COelim.pptptppu	3.696e+44	7.67	7.67	9.608e+38	0.000382
20587	TS.triHPacyl.COelim.pttptppmu	2.981e+44	7.54	7.54	9.585e+38	0.000381
20588	TS.triHPacyl.COelim.ppmmtmmu	2.396e+44	7.41	7.41	9.529e+38	0.000379
20589	TS.triHPacyl.COelim.tmmmmmpmu	1.183e+45	8.37	8.37	9.523e+38	0.000379
20590	TS.triHPacyl.COelim.ttpmtmpu	2.303e+44	7.39	7.39	9.514e+38	0.000378
20591	TS.triHPacyl.COelim.mtppptppu	1.820e+44	7.25	7.25	9.471e+38	0.000377
20592	TS.triHPacyl.COelim.pttmtmpu	1.340e+44	7.07	7.07	9.414e+38	0.000374
20593	TS.triHPacyl.COelim.tmpmmmtmpu	9.005e+43	6.84	6.84	9.379e+38	0.000373
20594	TS.triHPacyl.COelim.tmpmtmpu	2.399e+44	7.43	7.43	9.249e+38	0.000367
20595	TS.triHPacyl.COelim.tmpmttppu	9.229e+44	8.24	8.24	9.237e+38	0.000367
20596	TS.triHPacyl.COelim.tpmmmmpmu	1.081e+44	6.96	6.96	9.175e+38	0.000365
20597	TS.triHPacyl.COelim.tmttptppu	7.017e+44	8.08	8.08	9.068e+38	0.000361
20598	TS.triHPacyl.COelim.mmmmtppu	8.688e+43	6.84	6.84	9.067e+38	0.000361
20599	TS.triHPacyl.COelim.pttmtppu	4.503e+44	7.82	7.82	9.062e+38	0.00036
20600	TS.triHPacyl.COelim.pmpptmmu	3.795e+43	6.34	6.34	9.059e+38	0.00036
20601	TS.triHPacyl.COelim.tmtmtmpu	7.171e+44	8.10	8.10	9.031e+38	0.000359
20602	TS.triHPacyl.COelim.tmmmtmpu	2.024e+44	7.35	7.35	9.002e+38	0.000358
20603	TS.triHPacyl.COelim.pptppmmu	5.884e+44	7.99	7.99	8.960e+38	0.000356
20604	TS.triHPacyl.COelim.ptptmpmmu	2.934e+44	7.57	7.57	8.958e+38	0.000356
20605	TS.triHPacyl.COelim.pmtmptmmu	3.904e+44	7.74	7.74	8.956e+38	0.000356
20606	TS.triHPacyl.COelim.mtppmtmmu	1.938e+44	7.33	7.33	8.920e+38	0.000355
20607	TS.triHPacyl.COelim.pmttppmmu	7.293e+44	8.12	8.12	8.912e+38	0.000354
20608	TS.triHPacyl.COelim.tpptmpmu	8.146e+44	8.18	8.18	8.895e+38	0.000354
20609	TS.triHPacyl.COelim.mmtmmtpu	6.875e+44	8.08	8.08	8.884e+38	0.000353
20610	TS.triHPacyl.COelim.mmmmtppu	1.786e+44	7.28	7.28	8.883e+38	0.000353
20611	TS.triHPacyl.COelim.tmpmtmpu	1.168e+44	7.03	7.03	8.815e+38	0.00035
20612	TS.triHPacyl.COelim.tmpmtmpu	8.669e+43	6.86	6.86	8.761e+38	0.000348
20613	TS.triHPacyl.COelim.tmpmtmpu	1.515e+44	7.20	7.20	8.660e+38	0.000344
20614	TS.triHPacyl.COelim.mmmmtppu	1.349e+44	7.13	7.13	8.646e+38	0.000344
20615	TS.triHPacyl.COelim.ptmtptmmu	8.535e+43	6.86	6.86	8.547e+38	0.00034
20616	TS.triHPacyl.COelim.pttptmpu	1.630e+45	8.62	8.62	8.527e+38	0.000339
20617	TS.triHPacyl.COelim.mppmtmpu	2.891e+44	7.59	7.59	8.520e+38	0.000339
20618	TS.triHPacyl.COelim.tmtppmmu	2.528e+45	8.89	8.89	8.441e+38	0.000336
20619	TS.triHPacyl.COelim.ptmpmtppu	1.219e+45	8.46	8.46	8.433e+38	0.000335
20620	TS.triHPacyl.COelim.pmpmtmmu	1.097e+44	7.02	7.02	8.417e+38	0.000335
20621	TS.triHPacyl.COelim.mptptmpu	2.707e+44	7.56	7.56	8.388e+38	0.000334
20622	TS.triHPacyl.COelim.pmtppmmu	7.101e+44	8.14	8.14	8.368e+38	0.000333
20623	TS.triHPacyl.COelim.ptmpmpmpu	9.509e+43	6.94	6.94	8.336e+38	0.000331
20624	TS.triHPacyl.COelim.tppmmppu	3.351e+44	7.70	7.70	8.244e+38	0.000328
20625	TS.triHPacyl.COelim.pmmppmmu	1.379e+44	7.17	7.17	8.242e+38	0.000328
20626	TS.triHPacyl.COelim.tpmptmpu	6.623e+43	6.73	6.73	8.237e+38	0.000328
20627	TS.triHPacyl.COelim.tmmmtmpu	1.501e+44	7.22	7.22	8.215e+38	0.000327
20628	TS.triHPacyl.COelim.mppppptmmu	1.831e+44	7.34	7.34	8.194e+38	0.000326
20629	TS.triHPacyl.COelim.tpppttppu	1.718e+45	8.68	8.68	8.187e+38	0.000326
20630	TS.triHPacyl.COelim.mmtmmmmu	9.562e+44	8.33	8.33	8.137e+38	0.000324
20631	TS.triHPacyl.COelim.tmtppmmu	4.999e+45	9.32	9.32	8.134e+38	0.000323
20632	TS.triHPacyl.COelim.tptmtmpu	3.083e+44	7.66	7.66	8.131e+38	0.000323
20633	TS.triHPacyl.COelim.tmpmmppu	5.856e+44	8.04	8.04	8.117e+38	0.000323
20634	TS.triHPacyl.COelim.tmtmmmpu	3.989e+44	7.82	7.82	7.968e+38	0.000317
20635	TS.triHPacyl.COelim.pppmtmpu	1.912e+45	8.76	8.76	7.935e+38	0.000316
20636	TS.triHPacyl.COelim.mttppmmu	1.316e+45	8.54	8.54	7.909e+38	0.000314
20637	TS.triHPacyl.COelim.tmtppmmu	1.708e+45	8.70	8.70	7.908e+38	0.000314
20638	TS.triHPacyl.COelim.mtmppmmu	1.549e+44	7.27	7.27	7.812e+38	0.000311
20639	TS.triHPacyl.COelim.tpmptmpu	3.978e+44	7.83	7.83	7.804e+38	0.00031

20640	TS.triHPacyl.COelim.ptmpmpmpmu	5.352e+44	8.01	8.01	7.785e+38	0.00031
20641	TS.triHPacyl.COelim.pmpmtmpmu	5.168e+44	7.99	7.99	7.778e+38	0.000309
20642	TS.triHPacyl.COelim.tmtmtmmu	5.357e+44	8.02	8.02	7.702e+38	0.000306
20643	TS.triHPacyl.COelim.mmmmmppppu	1.418e+44	7.23	7.23	7.660e+38	0.000305
20644	TS.triHPacyl.COelim.tmpmtmpu	1.647e+44	7.32	7.32	7.654e+38	0.000304
20645	TS.triHPacyl.COelim.mptpptompu	6.241e+44	8.12	8.12	7.598e+38	0.000302
20646	TS.triHPacyl.COelim.mptmtpmpu	3.919e+44	7.84	7.84	7.566e+38	0.000301
20647	TS.triHPacyl.COelim.pptpmpmu	1.151e+44	7.12	7.12	7.534e+38	0.0003
20648	TS.triHPacyl.COelim.tmpmmmmu	2.866e+44	7.67	7.67	7.386e+38	0.000294
20649	TS.triHPacyl.COelim.tppptommu	6.613e+44	8.17	8.17	7.386e+38	0.000294
20650	TS.triHPacyl.COelim.pptppmpmu	6.487e+44	8.16	8.16	7.379e+38	0.000293
20651	TS.triHPacyl.COelim.tmpmtmpu	2.732e+44	7.64	7.64	7.375e+38	0.000293
20652	TS.triHPacyl.COelim.tmpppppmu	1.502e+44	7.29	7.29	7.373e+38	0.000293
20653	TS.triHPacyl.COelim.tptmtppu	1.517e+44	7.29	7.29	7.362e+38	0.000293
20654	TS.triHPacyl.COelim.mppmtmpmu	1.541e+45	8.68	8.68	7.311e+38	0.000291
20655	TS.triHPacyl.COelim.tmpmpppu	3.771e+44	7.85	7.85	7.241e+38	0.000288
20656	TS.triHPacyl.COelim.tmmmpppu	6.586e+44	8.18	8.18	7.204e+38	0.000286
20657	TS.triHPacyl.COelim.ptpptompu	1.861e+44	7.43	7.43	7.181e+38	0.000286
20658	TS.triHPacyl.COelim.tmtmtpmpu	1.047e+45	8.46	8.46	7.174e+38	0.000285
20659	TS.triHPacyl.COelim.tttmpmpmu	3.789e+45	9.23	9.23	7.155e+38	0.000285
20660	TS.triHPacyl.COelim.tpmmtmpmu	2.802e+44	7.68	7.68	7.129e+38	0.000283
20661	TS.triHPacyl.COelim.tppmpmpu	3.600e+44	7.83	7.83	7.098e+38	0.000282
20662	TS.triHPacyl.COelim.mmtmpmpmu	9.013e+44	8.38	8.38	7.085e+38	0.000282
20663	TS.triHPacyl.COelim.pmtmpppu	4.083e+44	7.91	7.91	7.050e+38	0.00028
20664	TS.triHPacyl.COelim.mptmpmpu	6.577e+43	6.82	6.82	7.048e+38	0.00028
20665	TS.triHPacyl.COelim.pptmtmpu	7.239e+44	8.25	8.25	7.034e+38	0.00028
20666	TS.triHPacyl.COelim.tppppmpu	5.903e+44	8.13	8.13	7.010e+38	0.000279
20667	TS.triHPacyl.COelim.mmmpppmu	5.474e+43	6.72	6.72	6.988e+38	0.000278
20668	TS.triHPacyl.COelim.ptppmtmmu	1.194e+44	7.18	7.18	6.970e+38	0.000277
20669	TS.triHPacyl.COelim.ptpptompu	3.363e+44	7.80	7.80	6.945e+38	0.000276
20670	TS.triHPacyl.COelim.tmtmtpmpu	2.039e+44	7.75	7.75	6.911e+38	0.000275
20671	TS.triHPacyl.COelim.pptppmpu	2.487e+44	7.63	7.63	6.891e+38	0.000274
20672	TS.triHPacyl.COelim.ptmpmtmpu	9.165e+44	8.41	8.41	6.831e+38	0.000272
20673	TS.triHPacyl.COelim.mptmpppu	7.133e+43	6.89	6.89	6.828e+38	0.000272
20674	TS.triHPacyl.COelim.tmpmtppu	6.943e+43	6.87	6.87	6.825e+38	0.000271
20675	TS.triHPacyl.COelim.mmtmpmpu	1.370e+45	8.65	8.65	6.818e+38	0.000271
20676	TS.triHPacyl.COelim.tmmmtmpu	3.560e+44	7.85	7.85	6.811e+38	0.000271
20677	TS.triHPacyl.COelim.mppmmmpmu	1.093e+44	7.15	7.15	6.784e+38	0.00027
20678	TS.triHPacyl.COelim.pmtpppmu	2.200e+44	7.57	7.57	6.780e+38	0.00027
20679	TS.triHPacyl.COelim.tppmtmpu	1.053e+45	8.50	8.50	6.740e+38	0.000268
20680	TS.triHPacyl.COelim.tmtmpmmu	3.196e+45	9.17	9.17	6.702e+38	0.000266
20681	TS.triHPacyl.COelim.mmtmtppu	7.803e+44	8.33	8.33	6.660e+38	0.000265
20682	TS.triHPacyl.COelim.tppmtmmu	5.801e+44	8.15	8.15	6.649e+38	0.000264
20683	TS.triHPacyl.COelim.ptmtpmpu	7.917e+43	6.97	6.97	6.608e+38	0.000263
20684	TS.triHPacyl.COelim.pptpptomu	5.798e+44	8.16	8.16	6.557e+38	0.000261
20685	TS.triHPacyl.COelim.pttptmmu	1.013e+45	8.50	8.50	6.545e+38	0.00026
20686	TS.triHPacyl.COelim.pttmmtpu	1.213e+45	8.60	8.60	6.538e+38	0.00026
20687	TS.triHPacyl.COelim.tmtmmtpu	1.313e+45	8.66	8.66	6.416e+38	0.000255
20688	TS.triHPacyl.COelim.mtpmpmpu	8.008e+43	7.00	7.00	6.404e+38	0.000255
20689	TS.triHPacyl.COelim.mmmmtppu	2.653e+44	7.71	7.71	6.379e+38	0.000254
20690	TS.triHPacyl.COelim.mptpmpmu	1.580e+44	7.41	7.41	6.369e+38	0.000253
20691	TS.triHPacyl.COelim.mppmmtpu	9.215e+43	7.08	7.08	6.366e+38	0.000253
20692	TS.triHPacyl.COelim.tmmmtppu	6.291e+44	8.23	8.23	6.345e+38	0.000252
20693	TS.triHPacyl.COelim.pmtppmpu	7.954e+44	8.37	8.37	6.341e+38	0.000252
20694	TS.triHPacyl.COelim.pppmtmpu	9.964e+43	7.13	7.13	6.338e+38	0.000252
20695	TS.triHPacyl.COelim.mppmtmmu	2.361e+44	7.65	7.65	6.331e+38	0.000252
20696	TS.triHPacyl.COelim.pmtmmmmu	3.050e+44	7.81	7.81	6.262e+38	0.000249
20697	TS.triHPacyl.COelim.tppppppu	1.253e+45	8.65	8.65	6.255e+38	0.000249
20698	TS.triHPacyl.COelim.ppmmtmpu	3.924e+44	7.96	7.96	6.221e+38	0.000247
20699	TS.triHPacyl.COelim.mppppmpu	7.918e+44	8.38	8.38	6.192e+38	0.000246
20700	TS.triHPacyl.COelim.mmpmmmpu	1.975e+44	7.56	7.56	6.184e+38	0.000246
20701	TS.triHPacyl.COelim.ptmmmtmpu	1.720e+45	8.85	8.85	6.163e+38	0.000245
20702	TS.triHPacyl.COelim.mtppmmmu	3.768e+44	7.95	7.95	6.130e+38	0.000244
20703	TS.triHPacyl.COelim.ptmpmpmu	9.518e+43	7.13	7.13	6.129e+38	0.000244
20704	TS.triHPacyl.COelim.mppmmmmu	7.098e+43	6.95	6.95	6.121e+38	0.000243
20705	TS.triHPacyl.COelim.mtppmtmpu	3.102e+44	7.84	7.84	6.063e+38	0.000241
20706	TS.triHPacyl.COelim.tpppmpu	1.796e+45	8.88	8.88	6.052e+38	0.000241
20707	TS.triHPacyl.COelim.tmmppmmu	3.688e+44	7.94	7.94	6.048e+38	0.00024
20708	TS.triHPacyl.COelim.pmmptmpu	2.728e+44	7.76	7.76	6.040e+38	0.00024
20709	TS.triHPacyl.COelim.mmtmmmmu	2.715e+45	9.13	9.13	6.017e+38	0.000239
20710	TS.triHPacyl.COelim.pmtmpmpu	6.785e+44	8.31	8.31	6.005e+38	0.000239
20711	TS.triHPacyl.COelim.mppppmpu	5.430e+44	8.18	8.18	5.980e+38	0.000238

20712	TS.triHPacyl.COelim.ptmtmtpu	1.801e+45	8.89	8.89	5.980e+38	0.000238
20713	TS.triHPacyl.COelim.ttmtmtpu	3.091e+44	7.84	7.84	5.965e+38	0.000237
20714	TS.triHPacyl.COelim.mpttpmmpu	4.457e+44	8.06	8.06	5.951e+38	0.000237
20715	TS.triHPacyl.COelim.ttmtmtpu	1.578e+45	8.82	8.82	5.927e+38	0.000236
20716	TS.triHPacyl.COelim.tptmpmmpu	2.823e+44	7.79	7.79	5.920e+38	0.000235
20717	TS.triHPacyl.COelim.mtttmmmpu	2.025e+45	8.98	8.98	5.857e+38	0.000233
20718	TS.triHPacyl.COelim.tpttmmmpu	3.553e+44	7.94	7.94	5.849e+38	0.000233
20719	TS.triHPacyl.COelim.mpptmtpu	1.199e+45	8.67	8.67	5.834e+38	0.000232
20720	TS.triHPacyl.COelim.mtttptmpu	6.161e+44	8.28	8.28	5.760e+38	0.000229
20721	TS.triHPacyl.COelim.mtmtppmpu	2.482e+44	7.74	7.74	5.737e+38	0.000228
20722	TS.triHPacyl.COelim.mtmtppmpu	9.934e+44	8.56	8.56	5.725e+38	0.000228
20723	TS.triHPacyl.COelim.mttppmmpu	1.747e+45	8.90	8.90	5.723e+38	0.000228
20724	TS.triHPacyl.COelim.ttmptmmpu	2.029e+44	7.62	7.62	5.717e+38	0.000227
20725	TS.triHPacyl.COelim.tmmppmmpu	1.518e+44	7.45	7.45	5.652e+38	0.000225
20726	TS.triHPacyl.COelim.pttptmmpu	9.213e+44	8.44	8.44	5.638e+38	0.000224
20727	TS.triHPacyl.COelim.mttmmmpu	6.579e+44	8.33	8.33	5.618e+38	0.000223
20728	TS.triHPacyl.COelim.tpmppmpu	2.924e+44	7.85	7.85	5.571e+38	0.000222
20729	TS.triHPacyl.COelim.tpmmpmtpu	1.800e+44	7.56	7.56	5.562e+38	0.000221
20730	TS.triHPacyl.COelim.ppmppmmpu	8.718e+43	7.13	7.13	5.561e+38	0.000221
20731	TS.triHPacyl.COelim.mmpptmmpu	4.051e+44	8.05	8.05	5.550e+38	0.000221
20732	TS.triHPacyl.COelim.pptptmmpu	2.596e+44	7.79	7.79	5.527e+38	0.00022
20733	TS.triHPacyl.COelim.tttmmpmpu	6.026e+44	8.29	8.29	5.504e+38	0.000219
20734	TS.triHPacyl.COelim.pptmmpu	5.211e+44	8.20	8.20	5.497e+38	0.000219
20735	TS.triHPacyl.COelim.tpttmmmpu	1.176e+45	8.69	8.69	5.471e+38	0.000218
20736	TS.triHPacyl.COelim.pptmmpmpu	1.806e+44	7.58	7.58	5.450e+38	0.000217
20737	TS.triHPacyl.COelim.ttmppmmpu	6.425e+44	8.33	8.33	5.447e+38	0.000217
20738	TS.triHPacyl.COelim.mmpptmmpu	3.929e+44	8.04	8.04	5.430e+38	0.000216
20739	TS.triHPacyl.COelim.mtptmmpu	2.913e+44	7.87	7.87	5.364e+38	0.000213
20740	TS.triHPacyl.COelim.mpttptmmpu	8.631e+44	8.52	8.52	5.351e+38	0.000213
20741	TS.triHPacyl.COelim.mpptmmpu	3.094e+44	7.92	7.92	5.272e+38	0.00021
20742	TS.triHPacyl.COelim.tpttmmmpu	6.927e+44	8.40	8.40	5.263e+38	0.000209
20743	TS.triHPacyl.COelim.mtppmmpu	1.278e+44	7.40	7.40	5.237e+38	0.000208
20744	TS.triHPacyl.COelim.tmtppmpu	1.072e+44	7.29	7.29	5.234e+38	0.000208
20745	TS.triHPacyl.COelim.mtppmmpu	8.005e+43	7.12	7.12	5.217e+38	0.000207
20746	TS.triHPacyl.COelim.mtptmmpu	2.750e+44	7.86	7.86	5.209e+38	0.000207
20747	TS.triHPacyl.COelim.mpptmmpu	2.991e+45	9.28	9.28	5.204e+38	0.000207
20748	TS.triHPacyl.COelim.pmtptmmpu	1.057e+44	7.29	7.29	5.167e+38	0.000205
20749	TS.triHPacyl.COelim.ttmppmmpu	2.536e+44	7.81	7.81	5.157e+38	0.000205
20750	TS.triHPacyl.COelim.ptmptmmpu	6.328e+43	6.99	6.99	5.139e+38	0.000204
20751	TS.triHPacyl.COelim.pppmmpu	1.119e+45	8.70	8.70	5.129e+38	0.000204
20752	TS.triHPacyl.COelim.tmtmtpu	4.102e+45	9.48	9.48	5.063e+38	0.000201
20753	TS.triHPacyl.COelim.tmtmtpu	2.686e+45	9.23	9.23	5.062e+38	0.000201
20754	TS.triHPacyl.COelim.pptmmpu	1.077e+45	8.69	8.69	5.061e+38	0.000201
20755	TS.triHPacyl.COelim.tmtmtpu	5.134e+44	8.25	8.25	5.042e+38	0.0002
20756	TS.triHPacyl.COelim.mtmmmpu	3.787e+44	8.07	8.07	5.030e+38	0.0002
20757	TS.triHPacyl.COelim.tttmmmpu	8.314e+44	8.54	8.54	4.998e+38	0.000199
20758	TS.triHPacyl.COelim.tmmppmmpu	2.584e+44	7.84	7.84	4.998e+38	0.000199
20759	TS.triHPacyl.COelim.mtppmmpu	1.493e+44	7.52	7.52	4.978e+38	0.000198
20760	TS.triHPacyl.COelim.ttptmmpu	2.317e+44	7.78	7.78	4.977e+38	0.000198
20761	TS.triHPacyl.COelim.pmpmmpu	5.985e+43	6.97	6.97	4.975e+38	0.000198
20762	TS.triHPacyl.COelim.mmpmmpu	2.435e+44	7.81	7.81	4.966e+38	0.000197
20763	TS.triHPacyl.COelim.pttptmmpu	1.982e+45	9.07	9.07	4.934e+38	0.000196
20764	TS.triHPacyl.COelim.mtmmmpu	5.240e+44	8.27	8.27	4.912e+38	0.000195
20765	TS.triHPacyl.COelim.tmtmmpu	7.432e+44	8.49	8.49	4.875e+38	0.000194
20766	TS.triHPacyl.COelim.tpmmpu	2.475e+44	7.83	7.83	4.870e+38	0.000194
20767	TS.triHPacyl.COelim.mtppmmpu	2.259e+44	7.78	7.78	4.861e+38	0.000193
20768	TS.triHPacyl.COelim.tmppmmpu	2.263e+44	7.78	7.78	4.849e+38	0.000193
20769	TS.triHPacyl.COelim.tmpmmpu	2.398e+45	9.20	9.20	4.791e+38	0.000191
20770	TS.triHPacyl.COelim.tmtmmpu	4.076e+44	8.14	8.14	4.767e+38	0.00019
20771	TS.triHPacyl.COelim.tptmmpu	6.044e+44	8.38	8.38	4.747e+38	0.000189
20772	TS.triHPacyl.COelim.mptmmpu	2.621e+45	9.26	9.26	4.745e+38	0.000189
20773	TS.triHPacyl.COelim.ptmtmmpu	2.199e+44	7.79	7.79	4.678e+38	0.000186
20774	TS.triHPacyl.COelim.pmtmmpu	1.709e+44	7.64	7.64	4.663e+38	0.000185
20775	TS.triHPacyl.COelim.mmpmmpu	1.534e+44	7.58	7.58	4.641e+38	0.000185
20776	TS.triHPacyl.COelim.ptptmmpu	4.979e+44	8.28	8.28	4.640e+38	0.000185
20777	TS.triHPacyl.COelim.mmtmmpu	1.170e+45	8.79	8.79	4.626e+38	0.000184
20778	TS.triHPacyl.COelim.tpmmpu	5.038e+43	6.91	6.91	4.624e+38	0.000184
20779	TS.triHPacyl.COelim.tmmmpu	2.246e+44	7.81	7.81	4.617e+38	0.000184
20780	TS.triHPacyl.COelim.pmtmmpu	3.189e+44	8.02	8.02	4.613e+38	0.000183
20781	TS.triHPacyl.COelim.mtppmmpu	1.758e+44	7.66	7.66	4.609e+38	0.000183
20782	TS.triHPacyl.COelim.mttmmpu	1.937e+45	9.09	9.09	4.590e+38	0.000183
20783	TS.triHPacyl.COelim.pptmmpu	1.209e+45	8.82	8.82	4.575e+38	0.000182

20784	TS.triHPacyl.COelim.tppmpttmmu	5.208e+44	8.31	8.31	4.571e+38	0.000182
20785	TS.triHPacyl.COelim.mtmmpmmmmu	4.366e+44	8.21	8.21	4.561e+38	0.000181
20786	TS.triHPacyl.COelim.pmmtpttppu	4.731e+44	8.26	8.26	4.534e+38	0.00018
20787	TS.triHPacyl.COelim.ttptmmpppu	1.794e+44	7.68	7.68	4.531e+38	0.00018
20788	TS.triHPacyl.COelim.mptmmmtmmu	1.874e+45	9.09	9.09	4.496e+38	0.000179
20789	TS.triHPacyl.COelim.mppppptppu	3.068e+44	8.01	8.01	4.492e+38	0.000179
20790	TS.triHPacyl.COelim.tmtmpmpmu	2.683e+45	9.30	9.30	4.490e+38	0.000179
20791	TS.triHPacyl.COelim.tmpppppmmu	2.267e+44	7.83	7.83	4.486e+38	0.000178
20792	TS.triHPacyl.COelim.mttmmmtpmu	4.783e+44	8.28	8.28	4.473e+38	0.000178
20793	TS.triHPacyl.COelim.pmptmmmpmu	1.584e+45	8.99	8.99	4.462e+38	0.000177
20794	TS.triHPacyl.COelim.pptptmpmu	4.113e+44	8.19	8.19	4.462e+38	0.000177
20795	TS.triHPacyl.COelim.tpmtmtmmu	4.700e+44	8.27	8.27	4.451e+38	0.000177
20796	TS.triHPacyl.COelim.tmmpttppu	1.943e+44	7.74	7.74	4.441e+38	0.000177
20797	TS.triHPacyl.COelim.mmpppptpmu	1.435e+44	7.56	7.56	4.427e+38	0.000176
20798	TS.triHPacyl.COelim.pptmmmpmu	5.565e+44	8.37	8.37	4.426e+38	0.000176
20799	TS.triHPacyl.COelim.ppppmtmmu	3.201e+44	8.05	8.05	4.398e+38	0.000175
20800	TS.triHPacyl.COelim.tttptmpmu	4.081e+44	8.19	8.19	4.392e+38	0.000175
20801	TS.triHPacyl.COelim.tpttmmppmu	5.972e+44	8.42	8.42	4.383e+38	0.000174
20802	TS.triHPacyl.COelim.pmmmpmmmu	2.107e+44	7.80	7.80	4.368e+38	0.000174
20803	TS.triHPacyl.COelim.tptmttppu	1.874e+45	9.11	9.11	4.357e+38	0.000173
20804	TS.triHPacyl.COelim.ttptmtppu	1.035e+44	7.38	7.38	4.354e+38	0.000173
20805	TS.triHPacyl.COelim.mmtmmtpmu	7.019e+44	8.53	8.53	4.321e+38	0.000172
20806	TS.triHPacyl.COelim.tttmppmmu	3.771e+44	9.53	9.53	4.312e+38	0.000171
20807	TS.triHPacyl.COelim.mttmppppmu	1.899e+44	7.75	7.75	4.294e+38	0.000171
20808	TS.triHPacyl.COelim.pmpptpmu	9.946e+43	7.37	7.37	4.242e+38	0.000169
20809	TS.triHPacyl.COelim.mtptmppmu	2.214e+44	7.85	7.85	4.236e+38	0.000168
20810	TS.triHPacyl.COelim.mmtptmpmu	2.287e+44	7.87	7.87	4.226e+38	0.000168
20811	TS.triHPacyl.COelim.tmmmpmmmu	3.904e+43	6.82	6.82	4.207e+38	0.000167
20812	TS.triHPacyl.COelim.tmpmmtpu	1.612e+44	7.67	7.67	4.194e+38	0.000167
20813	TS.triHPacyl.COelim.tmtmttppu	2.561e+45	9.32	9.32	4.175e+38	0.000166
20814	TS.triHPacyl.COelim.pptptmppu	5.597e+44	8.42	8.42	4.143e+38	0.000165
20815	TS.triHPacyl.COelim.ttptmmmmu	3.644e+44	8.16	8.16	4.134e+38	0.000164
20816	TS.triHPacyl.COelim.tmpmtmpmu	8.777e+44	8.69	8.69	4.131e+38	0.000164
20817	TS.triHPacyl.COelim.mpptmpmu	2.465e+45	9.30	9.30	4.119e+38	0.000164
20818	TS.triHPacyl.COelim.tpptmppu	1.231e+45	8.89	8.89	4.112e+38	0.000164
20819	TS.triHPacyl.COelim.ttpmmtppu	1.927e+44	7.79	7.79	4.106e+38	0.000163
20820	TS.triHPacyl.COelim.mppppptppu	4.798e+44	8.33	8.33	4.105e+38	0.000163
20821	TS.triHPacyl.COelim.tmmpptpmu	4.358e+43	6.90	6.90	4.086e+38	0.000162
20822	TS.triHPacyl.COelim.mmpmmpppu	2.617e+44	7.97	7.97	4.072e+38	0.000162
20823	TS.triHPacyl.COelim.mtmppppmu	8.469e+43	7.30	7.30	4.067e+38	0.000162
20824	TS.triHPacyl.COelim.mpptpppmu	1.036e+45	8.79	8.79	4.064e+38	0.000162
20825	TS.triHPacyl.COelim.ptppmtpu	3.239e+44	8.10	8.10	4.062e+38	0.000162
20826	TS.triHPacyl.COelim.tmpmpptppu	1.089e+45	8.83	8.83	4.054e+38	0.000161
20827	TS.triHPacyl.COelim.pmtppmpmu	5.017e+44	8.37	8.37	4.043e+38	0.000161
20828	TS.triHPacyl.COelim.mtptmtppu	2.265e+45	9.26	9.26	4.039e+38	0.000161
20829	TS.triHPacyl.COelim.mmpptmmmu	7.679e+44	8.62	8.62	4.028e+38	0.00016
20830	TS.triHPacyl.COelim.tttmmtpmu	3.419e+45	9.51	9.51	4.024e+38	0.00016
20831	TS.triHPacyl.COelim.tpmppmtpu	3.797e+43	6.83	6.83	4.005e+38	0.000159
20832	TS.triHPacyl.COelim.ppmtpmppu	1.700e+44	7.73	7.73	3.996e+38	0.000159
20833	TS.triHPacyl.COelim.tpmtptmpu	7.740e+44	8.63	8.63	3.984e+38	0.000158
20834	TS.triHPacyl.COelim.mmttmtmpu	6.588e+44	8.54	8.54	3.983e+38	0.000158
20835	TS.triHPacyl.COelim.pmmppppmu	4.527e+43	6.94	6.94	3.979e+38	0.000158
20836	TS.triHPacyl.COelim.tpttmmmmu	8.604e+44	8.70	8.70	3.952e+38	0.000157
20837	TS.triHPacyl.COelim.pptppmmmu	6.947e+44	8.57	8.57	3.944e+38	0.000157
20838	TS.triHPacyl.COelim.mmtptmppmu	2.208e+45	9.27	9.27	3.926e+38	0.000156
20839	TS.triHPacyl.COelim.mmtptmpmu	4.562e+44	8.33	8.33	3.907e+38	0.000155
20840	TS.triHPacyl.COelim.tttmtppmu	5.065e+44	8.40	8.40	3.877e+38	0.000154
20841	TS.triHPacyl.COelim.tttmttmmu	7.207e+44	8.61	8.61	3.869e+38	0.000154
20842	TS.triHPacyl.COelim.pppmmpmmu	1.024e+45	8.82	8.82	3.867e+38	0.000154
20843	TS.triHPacyl.COelim.mptppptpmu	9.932e+43	7.43	7.43	3.853e+38	0.000153
20844	TS.triHPacyl.COelim.mtpppppppu	4.163e+44	8.29	8.29	3.813e+38	0.000152
20845	TS.triHPacyl.COelim.mtttpppppu	5.788e+44	8.49	8.49	3.769e+38	0.00015
20846	TS.triHPacyl.COelim.tmmtpptmmu	1.208e+44	7.56	7.56	3.760e+38	0.000149
20847	TS.triHPacyl.COelim.tptmttppu	9.945e+44	8.82	8.82	3.751e+38	0.000149
20848	TS.triHPacyl.COelim.pptmmtppu	1.477e+45	9.06	9.06	3.738e+38	0.000149
20849	TS.triHPacyl.COelim.mmpptpppmu	3.661e+44	8.23	8.23	3.706e+38	0.000147
20850	TS.triHPacyl.COelim.mmtptmpppu	2.363e+45	9.33	9.33	3.705e+38	0.000147
20851	TS.triHPacyl.COelim.tmpmmmmmu	8.333e+43	7.35	7.35	3.702e+38	0.000147
20852	TS.triHPacyl.COelim.pptmtppmu	4.043e+44	8.29	8.29	3.686e+38	0.000147
20853	TS.triHPacyl.COelim.pmtmpmmpmu	3.962e+44	8.28	8.28	3.675e+38	0.000146
20854	TS.triHPacyl.COelim.pppmmtppu	1.295e+45	8.99	8.99	3.646e+38	0.000145
20855	TS.triHPacyl.COelim.tpttmmmpu	2.197e+45	9.31	9.31	3.638e+38	0.000145

20856	TS.triHPacyl.COelim.ttmtmtpmu	2.188e+44	7.94	7.94	3.609e+38	0.000143
20857	TS.triHPacyl.COelim.mmmmmmtmmpu	2.266e+44	7.96	7.96	3.609e+38	0.000143
20858	TS.triHPacyl.COelim.tpmtmmtmmu	4.497e+44	8.37	8.37	3.607e+38	0.000143
20859	TS.triHPacyl.COelim.mptmmtmmpu	2.682e+44	8.06	8.06	3.600e+38	0.000143
20860	TS.triHPacyl.COelim.tmpptmmpu	3.958e+45	9.67	9.67	3.600e+38	0.000143
20861	TS.triHPacyl.COelim.ppttpptpmu	5.042e+44	8.44	8.44	3.578e+38	0.000142
20862	TS.triHPacyl.COelim.tpmmmpmmu	1.213e+44	7.59	7.59	3.567e+38	0.000142
20863	TS.triHPacyl.COelim.mmmmpmtmmu	2.970e+44	8.13	8.13	3.565e+38	0.000142
20864	TS.triHPacyl.COelim.ppptmmtpmu	1.268e+45	9.00	9.00	3.542e+38	0.000141
20865	TS.triHPacyl.COelim.ttptpmmpmu	7.487e+44	8.69	8.69	3.490e+38	0.000139
20866	TS.triHPacyl.COelim.tmtmmtmmu	6.143e+45	9.95	9.95	3.489e+38	0.000139
20867	TS.triHPacyl.COelim.ttmppmpmu	1.684e+45	9.18	9.18	3.478e+38	0.000138
20868	TS.triHPacyl.COelim.tmtpmnmpu	2.081e+45	9.30	9.30	3.473e+38	0.000138
20869	TS.triHPacyl.COelim.mtmmpmpppu	1.675e+44	7.80	7.80	3.470e+38	0.000138
20870	TS.triHPacyl.COelim.mptpmnmpu	1.726e+44	7.82	7.82	3.465e+38	0.000138
20871	TS.triHPacyl.COelim.mtmprmtmmu	9.266e+43	7.45	7.45	3.456e+38	0.000137
20872	TS.triHPacyl.COelim.tttmmtmmpu	1.753e+44	7.83	7.83	3.440e+38	0.000137
20873	TS.triHPacyl.COelim.pppmmnmpu	5.114e+44	8.48	8.48	3.422e+38	0.000136
20874	TS.triHPacyl.COelim.pmtpmtpmu	2.653e+45	8.09	8.09	3.408e+38	0.000135
20875	TS.triHPacyl.COelim.ttpmtpmpu	1.365e+44	7.69	7.69	3.400e+38	0.000135
20876	TS.triHPacyl.COelim.mmtpmnmmu	1.245e+45	9.01	9.01	3.396e+38	0.000135
20877	TS.triHPacyl.COelim.mmpptppmpu	2.190e+44	7.98	7.98	3.387e+38	0.000135
20878	TS.triHPacyl.COelim.tmmmmmtpmu	4.117e+44	8.35	8.35	3.380e+38	0.000134
20879	TS.triHPacyl.COelim.ttptmpppu	4.672e+45	9.80	9.80	3.377e+38	0.000134
20880	TS.triHPacyl.COelim.pttptmmpu	9.660e+44	8.86	8.86	3.372e+38	0.000134
20881	TS.triHPacyl.COelim.ttpmmmmnmpu	1.878e+44	7.89	7.89	3.347e+38	0.000133
20882	TS.triHPacyl.COelim.mtmtpmpppu	1.953e+44	7.92	7.92	3.344e+38	0.000133
20883	TS.triHPacyl.COelim.pmtmmmtpmu	7.979e+44	8.76	8.76	3.340e+38	0.000133
20884	TS.triHPacyl.COelim.ptmmmpmmu	2.323e+44	8.02	8.02	3.318e+38	0.000132
20885	TS.triHPacyl.COelim.ptpmtmmpu	1.238e+44	7.65	7.65	3.304e+38	0.000131
20886	TS.triHPacyl.COelim.mmttmppmu	1.532e+45	9.15	9.15	3.301e+38	0.000131
20887	TS.triHPacyl.COelim.ttmtpmmmu	3.365e+44	8.25	8.25	3.300e+38	0.000131
20888	TS.triHPacyl.COelim.pmtmmnmpu	2.149e+44	7.98	7.98	3.299e+38	0.000131
20889	TS.triHPacyl.COelim.mptmmtpmu	1.629e+45	9.19	9.19	3.286e+38	0.000131
20890	TS.triHPacyl.COelim.ppmmtmmmu	1.173e+44	7.62	7.62	3.284e+38	0.000131
20891	TS.triHPacyl.COelim.mmtmmtmmu	7.289e+45	10.08	10.08	3.282e+38	0.000131
20892	TS.triHPacyl.COelim.ttmppmpmpu	1.128e+44	7.60	7.60	3.282e+38	0.000131
20893	TS.triHPacyl.COelim.pttmmtpmu	6.298e+44	8.63	8.63	3.281e+38	0.00013
20894	TS.triHPacyl.COelim.mpppmnmpu	2.761e+44	8.14	8.14	3.273e+38	0.00013
20895	TS.triHPacyl.COelim.pptmmtmmu	6.392e+44	8.64	8.64	3.264e+38	0.00013
20896	TS.triHPacyl.COelim.ttmmpmtpu	1.791e+44	7.88	7.88	3.262e+38	0.00013
20897	TS.triHPacyl.COelim.pptppmpmpu	2.009e+44	7.95	7.95	3.262e+38	0.00013
20898	TS.triHPacyl.COelim.pmtmpppmu	4.372e+44	8.41	8.41	3.259e+38	0.00013
20899	TS.triHPacyl.COelim.mtptmtpmu	5.915e+44	8.59	8.59	3.251e+38	0.000129
20900	TS.triHPacyl.COelim.mptpmmtmpu	2.020e+45	9.33	9.33	3.246e+38	0.000129
20901	TS.triHPacyl.COelim.ttmptpmmpu	5.344e+43	7.16	7.16	3.242e+38	0.000129
20902	TS.triHPacyl.COelim.mmpmtmmpu	7.112e+44	8.71	8.71	3.231e+38	0.000128
20903	TS.triHPacyl.COelim.tmppppppmu	1.458e+44	7.77	7.77	3.209e+38	0.000128
20904	TS.triHPacyl.COelim.mptmmpmpu	6.223e+44	8.63	8.63	3.206e+38	0.000127
20905	TS.triHPacyl.COelim.mmmmmtpmpu	2.523e+44	8.10	8.10	3.189e+38	0.000127
20906	TS.triHPacyl.COelim.pptpppppmu	1.837e+44	7.91	7.91	3.181e+38	0.000126
20907	TS.triHPacyl.COelim.ptpmmtpmu	1.660e+44	7.85	7.85	3.177e+38	0.000126
20908	TS.triHPacyl.COelim.tmpmtpmpu	9.252e+44	8.88	8.88	3.167e+38	0.000126
20909	TS.triHPacyl.COelim.tmmmpmtpmu	1.483e+44	7.79	7.79	3.131e+38	0.000124
20910	TS.triHPacyl.COelim.ppmppmpmpu	7.246e+43	7.37	7.37	3.111e+38	0.000124
20911	TS.triHPacyl.COelim.mpmtmmpmu	3.111e+44	8.24	8.24	3.111e+38	0.000124
20912	TS.triHPacyl.COelim.tmmmpmmpmu	3.137e+43	6.87	6.87	3.089e+38	0.000123
20913	TS.triHPacyl.COelim.mpttptmpmu	3.112e+44	8.24	8.24	3.081e+38	0.000123
20914	TS.triHPacyl.COelim.ptmppmmmpu	2.842e+44	8.19	8.19	3.080e+38	0.000122
20915	TS.triHPacyl.COelim.mpptptpmu	6.554e+44	8.69	8.69	3.078e+38	0.000122
20916	TS.triHPacyl.COelim.tpptmmtmpu	6.564e+44	8.69	8.69	3.073e+38	0.000122
20917	TS.triHPacyl.COelim.pptmmpmpu	3.301e+44	8.28	8.28	3.067e+38	0.000122
20918	TS.triHPacyl.COelim.ptptmmtpmu	9.490e+44	8.91	8.91	3.054e+38	0.000121
20919	TS.triHPacyl.COelim.tmmmtmtpu	6.089e+44	8.65	8.65	3.045e+38	0.000121
20920	TS.triHPacyl.COelim.pmttptmpmu	1.370e+44	7.76	7.76	3.035e+38	0.000121
20921	TS.triHPacyl.COelim.ttpmtpmpu	2.430e+44	8.11	8.11	3.022e+38	0.00012
20922	TS.triHPacyl.COelim.ppptptpmu	4.356e+44	8.46	8.46	3.014e+38	0.00012
20923	TS.triHPacyl.COelim.pttptmtpu	3.564e+44	8.34	8.34	3.004e+38	0.000119
20924	TS.triHPacyl.COelim.ttmtpmmpu	7.705e+44	8.80	8.80	2.997e+38	0.000119
20925	TS.triHPacyl.COelim.ttmtmmtmpu	5.697e+44	8.62	8.62	2.989e+38	0.000119
20926	TS.triHPacyl.COelim.pptmtpmpu	7.182e+44	8.76	8.76	2.986e+38	0.000119
20927	TS.triHPacyl.COelim.tmmmtmtpmu	4.359e+44	8.46	8.46	2.981e+38	0.000119

20928	TS.triHPacyl.COelim.pmmmpmtmpu	2.481e+44	8.13	8.13	2.975e+38	0.000118
20929	TS.triHPacyl.COelim.tttmtmmmu	1.112e+45	9.03	9.03	2.959e+38	0.000118
20930	TS.triHPacyl.COelim.mtppppptpmu	1.382e+44	7.78	7.78	2.954e+38	0.000117
20931	TS.triHPacyl.COelim.ttptmtmpu	2.032e+44	8.02	8.02	2.940e+38	0.000117
20932	TS.triHPacyl.COelim.ttttppmmmpu	1.318e+46	10.50	10.50	2.939e+38	0.000117
20933	TS.triHPacyl.COelim.tpmtmtppu	1.370e+45	9.15	9.15	2.935e+38	0.000117
20934	TS.triHPacyl.COelim.mttmmpmpu	5.184e+44	8.58	8.58	2.925e+38	0.000116
20935	TS.triHPacyl.COelim.ttmppmmpu	2.570e+44	8.16	8.16	2.921e+38	0.000116
20936	TS.triHPacyl.COelim.ptptmptpmu	8.098e+44	8.84	8.84	2.920e+38	0.000116
20937	TS.triHPacyl.COelim.ttmtmtppu	1.592e+44	7.88	7.88	2.902e+38	0.000115
20938	TS.triHPacyl.COelim.tppmmmpmpu	1.927e+44	7.99	7.99	2.901e+38	0.000115
20939	TS.triHPacyl.COelim.mmmppptpmu	5.053e+43	7.19	7.19	2.899e+38	0.000115
20940	TS.triHPacyl.COelim.tttppmmmpu	7.952e+44	8.84	8.84	2.896e+38	0.000115
20941	TS.triHPacyl.COelim.tpmtppmpu	6.121e+44	8.68	8.68	2.895e+38	0.000115
20942	TS.triHPacyl.COelim.mptpmtppu	2.565e+44	8.17	8.17	2.871e+38	0.000114
20943	TS.triHPacyl.COelim.mptpmtppu	1.452e+44	7.83	7.83	2.857e+38	0.000114
20944	TS.triHPacyl.COelim.mptpmtppu	3.184e+44	8.30	8.30	2.856e+38	0.000114
20945	TS.triHPacyl.COelim.ppmptttmmu	3.636e+44	8.39	8.39	2.833e+38	0.000113
20946	TS.triHPacyl.COelim.mtmppmmmpu	2.218e+44	8.09	8.09	2.832e+38	0.000113
20947	TS.triHPacyl.COelim.tpmtppmpu	2.414e+44	8.14	8.14	2.820e+38	0.000112
20948	TS.triHPacyl.COelim.tttmptmmpu	8.265e+44	8.88	8.88	2.804e+38	0.000111
20949	TS.triHPacyl.COelim.pptmmtmmpu	8.174e+44	8.87	8.87	2.804e+38	0.000111
20950	TS.triHPacyl.COelim.pptpmtppu	2.598e+44	8.19	8.19	2.790e+38	0.000111
20951	TS.triHPacyl.COelim.tmtmtppu	2.153e+45	9.46	9.46	2.769e+38	0.00011
20952	TS.triHPacyl.COelim.tmtmtppu	9.295e+44	8.96	8.96	2.766e+38	0.00011
20953	TS.triHPacyl.COelim.tppmtmmmu	5.125e+44	8.60	8.60	2.766e+38	0.00011
20954	TS.triHPacyl.COelim.mmtmmpmmu	4.553e+45	9.91	9.91	2.749e+38	0.000109
20955	TS.triHPacyl.COelim.tmpmtppu	1.212e+45	9.12	9.12	2.740e+38	0.000109
20956	TS.triHPacyl.COelim.pppmmtpmu	1.347e+45	9.19	9.19	2.728e+38	0.000108
20957	TS.triHPacyl.COelim.ptmptmtpmu	1.864e+44	8.01	8.01	2.718e+38	0.000108
20958	TS.triHPacyl.COelim.mmtmmpmpu	1.214e+44	7.76	7.76	2.705e+38	0.000108
20959	TS.triHPacyl.COelim.tppmmmpu	4.449e+45	9.92	9.92	2.657e+38	0.000106
20960	TS.triHPacyl.COelim.ptmppppppu	1.326e+44	7.82	7.82	2.653e+38	0.000105
20961	TS.triHPacyl.COelim.mtpmmmpu	1.087e+44	7.70	7.70	2.652e+38	0.000105
20962	TS.triHPacyl.COelim.tppmtmmpu	2.745e+45	9.63	9.63	2.647e+38	0.000105
20963	TS.triHPacyl.COelim.ppppmtmpu	4.310e+43	7.16	7.16	2.642e+38	0.000105
20964	TS.triHPacyl.COelim.mmpptmmpu	1.737e+44	7.99	7.99	2.642e+38	0.000105
20965	TS.triHPacyl.COelim.mtmppptppu	3.851e+44	8.46	8.46	2.635e+38	0.000105
20966	TS.triHPacyl.COelim.tmmppmmmpu	2.290e+44	8.15	8.15	2.626e+38	0.000104
20967	TS.triHPacyl.COelim.pttmtmtpu	2.935e+45	9.68	9.68	2.625e+38	0.000104
20968	TS.triHPacyl.COelim.mtpmmpmpu	1.597e+44	7.94	7.94	2.620e+38	0.000104
20969	TS.triHPacyl.COelim.tptmmpmpu	2.338e+45	9.54	9.54	2.616e+38	0.000104
20970	TS.triHPacyl.COelim.ttttmmmpu	1.098e+45	9.09	9.09	2.611e+38	0.000104
20971	TS.triHPacyl.COelim.tppmtpppu	5.171e+44	8.64	8.64	2.608e+38	0.000104
20972	TS.triHPacyl.COelim.ppmtpppmu	1.953e+44	8.07	8.07	2.575e+38	0.000102
20973	TS.triHPacyl.COelim.pmpmtmmpu	6.516e+44	8.80	8.80	2.527e+38	0.0001
20974	TS.triHPacyl.COelim.pppmmpmpu	2.774e+44	8.29	8.29	2.527e+38	0.0001
20975	TS.triHPacyl.COelim.tppmtpmpu	4.132e+44	8.53	8.53	2.515e+38	0.0001
20976	TS.triHPacyl.COelim.mtmmtmmpu	1.072e+45	9.10	9.10	2.508e+38	9.97e-05
20977	TS.triHPacyl.COelim.ttmtptmmpu	6.940e+45	10.22	10.22	2.503e+38	9.95e-05
20978	TS.triHPacyl.COelim.mpppmtmmpu	4.781e+45	10.00	10.00	2.500e+38	9.94e-05
20979	TS.triHPacyl.COelim.tmtmmpmpu	1.644e+45	9.36	9.36	2.492e+38	9.91e-05
20980	TS.triHPacyl.COelim.mtttppmmpu	4.799e+44	8.63	8.63	2.487e+38	9.89e-05
20981	TS.triHPacyl.COelim.pmmmpmpmu	6.686e+43	7.46	7.46	2.472e+38	9.83e-05
20982	TS.triHPacyl.COelim.pmtmmtmmpu	1.086e+45	9.12	9.12	2.454e+38	9.76e-05
20983	TS.triHPacyl.COelim.tppmppppu	1.631e+44	8.00	8.00	2.441e+38	9.71e-05
20984	TS.triHPacyl.COelim.mpmtpmmpu	4.806e+44	8.64	8.64	2.441e+38	9.71e-05
20985	TS.triHPacyl.COelim.ttmppmtpmu	6.480e+44	8.82	8.82	2.419e+38	9.62e-05
20986	TS.triHPacyl.COelim.mttmmpmpu	2.493e+44	8.26	8.26	2.404e+38	9.56e-05
20987	TS.triHPacyl.COelim.mmtmtppmu	1.352e+45	9.27	9.27	2.399e+38	9.54e-05
20988	TS.triHPacyl.COelim.mtttppmtmmpu	7.078e+44	8.88	8.88	2.398e+38	9.53e-05
20989	TS.triHPacyl.COelim.pmpmmpmmpu	1.034e+44	7.74	7.74	2.395e+38	9.52e-05
20990	TS.triHPacyl.COelim.mpttppmmpu	1.646e+44	8.02	8.02	2.374e+38	9.44e-05
20991	TS.triHPacyl.COelim.tpttmmmpu	8.789e+44	9.02	9.02	2.372e+38	9.43e-05
20992	TS.triHPacyl.COelim.tmmppmmpu	9.034e+43	7.66	7.66	2.370e+38	9.42e-05
20993	TS.triHPacyl.COelim.pmmtpptmmpu	5.925e+43	7.41	7.41	2.365e+38	9.4e-05
20994	TS.triHPacyl.COelim.pptmmpmpu	2.749e+44	8.33	8.33	2.364e+38	9.4e-05
20995	TS.triHPacyl.COelim.pmtmmtmmpu	3.054e+44	8.39	8.39	2.362e+38	9.39e-05
20996	TS.triHPacyl.COelim.mtpmmpmmpu	1.111e+44	7.79	7.79	2.357e+38	9.37e-05
20997	TS.triHPacyl.COelim.pmmmtmmpu	5.243e+44	8.72	8.72	2.348e+38	9.33e-05
20998	TS.triHPacyl.COelim.mmppppmpu	2.618e+44	8.30	8.30	2.347e+38	9.33e-05
20999	TS.triHPacyl.COelim.tppmmpmmpu	1.466e+44	7.96	7.96	2.339e+38	9.3e-05

21000	TS.triHPacyl.COelim.mmtmptmmu	7.385e+44	8.92	8.92	2.337e+38	9.29e-05
21001	TS.triHPacyl.COelim.tmpmpppppu	2.337e+44	8.24	8.24	2.314e+38	9.2e-05
21002	TS.triHPacyl.COelim.ptmmtpmmu	1.941e+44	8.13	8.13	2.309e+38	9.18e-05
21003	TS.triHPacyl.COelim.mmtmptmpu	4.340e+44	8.61	8.61	2.305e+38	9.16e-05
21004	TS.triHPacyl.COelim.mmtmpmpmpu	3.492e+44	8.48	8.48	2.304e+38	9.16e-05
21005	TS.triHPacyl.COelim.ttptmttppu	4.976e+44	8.70	8.70	2.300e+38	9.15e-05
21006	TS.triHPacyl.COelim.tmmmtmmmu	2.052e+44	8.18	8.18	2.273e+38	9.04e-05
21007	TS.triHPacyl.COelim.tmmmtmmmu	7.394e+44	8.94	8.94	2.267e+38	9.02e-05
21008	TS.triHPacyl.COelim.tmpptmpmpu	1.994e+45	9.53	9.53	2.264e+38	9e-05
21009	TS.triHPacyl.COelim.ttptmppppu	4.084e+45	9.96	9.96	2.249e+38	8.94e-05
21010	TS.triHPacyl.COelim.tmpmpmpmpu	1.175e+44	7.85	7.85	2.228e+38	8.86e-05
21011	TS.triHPacyl.COelim.tpptptmmu	1.379e+46	10.70	10.70	2.219e+38	8.82e-05
21012	TS.triHPacyl.COelim.tpmmtmtpu	1.399e+45	9.34	9.34	2.214e+38	8.8e-05
21013	TS.triHPacyl.COelim.mpptpmmpmu	1.846e+44	8.13	8.13	2.198e+38	8.74e-05
21014	TS.triHPacyl.COelim.mtptmpmpu	3.458e+44	8.51	8.51	2.191e+38	8.71e-05
21015	TS.triHPacyl.COelim.mpmmmpppmu	3.051e+44	8.43	8.43	2.188e+38	8.7e-05
21016	TS.triHPacyl.COelim.ttptmtppmu	1.425e+45	9.35	9.35	2.188e+38	8.7e-05
21017	TS.triHPacyl.COelim.tpmmpmtmpu	4.462e+44	8.66	8.66	2.184e+38	8.68e-05
21018	TS.triHPacyl.COelim.ptmmtpmpu	1.015e+45	9.15	9.15	2.182e+38	8.68e-05
21019	TS.triHPacyl.COelim.mpptptmpu	7.626e+44	8.98	8.98	2.174e+38	8.64e-05
21020	TS.triHPacyl.COelim.tmtppmpppu	3.147e+45	9.83	9.83	2.169e+38	8.62e-05
21021	TS.triHPacyl.COelim.tmpmtmmmpmu	3.553e+44	8.53	8.53	2.168e+38	8.62e-05
21022	TS.triHPacyl.COelim.ppmtmmpmpu	1.796e+44	8.13	8.13	2.147e+38	8.54e-05
21023	TS.triHPacyl.COelim.ttptmmtmpu	3.046e+44	8.45	8.45	2.146e+38	8.53e-05
21024	TS.triHPacyl.COelim.mpmtpmtppu	8.867e+44	9.08	9.08	2.145e+38	8.53e-05
21025	TS.triHPacyl.COelim.tpmmpmpmpu	1.642e+44	8.08	8.08	2.135e+38	8.49e-05
21026	TS.triHPacyl.COelim.mptpmtppu	1.534e+45	9.41	9.41	2.134e+38	8.49e-05
21027	TS.triHPacyl.COelim.tmpmpmtmpu	3.197e+44	8.48	8.48	2.123e+38	8.44e-05
21028	TS.triHPacyl.COelim.ttpmpmtppu	9.282e+44	9.12	9.12	2.117e+38	8.42e-05
21029	TS.triHPacyl.COelim.mpttptmpu	1.000e+45	9.16	9.16	2.114e+38	8.41e-05
21030	TS.triHPacyl.COelim.ppttpptppu	1.012e+45	9.18	9.18	2.092e+38	8.32e-05
21031	TS.triHPacyl.COelim.tmmmtmmppu	1.114e+45	9.24	9.24	2.078e+38	8.26e-05
21032	TS.triHPacyl.COelim.pmmtppmtmpu	6.565e+44	8.92	8.92	2.072e+38	8.24e-05
21033	TS.triHPacyl.COelim.ttttptmpu	2.803e+45	9.80	9.80	2.039e+38	8.11e-05
21034	TS.triHPacyl.COelim.mmtmmpmpmu	1.474e+45	9.42	9.42	2.037e+38	8.1e-05
21035	TS.triHPacyl.COelim.tmmmtmmpu	6.205e+44	8.90	8.90	2.022e+38	8.04e-05
21036	TS.triHPacyl.COelim.ttpmptppu	7.725e+44	9.04	9.04	2.017e+38	8.02e-05
21037	TS.triHPacyl.COelim.tpmmtmmpmu	2.765e+44	8.43	8.43	2.014e+38	8.01e-05
21038	TS.triHPacyl.COelim.pptmttmmu	5.201e+44	8.80	8.80	2.009e+38	7.99e-05
21039	TS.triHPacyl.COelim.mtttppmmmu	1.207e+45	9.31	9.31	2.000e+38	7.95e-05
21040	TS.triHPacyl.COelim.tpmmtppmu	2.148e+44	8.28	8.28	1.998e+38	7.94e-05
21041	TS.triHPacyl.COelim.mmpmtmmtmpu	6.292e+44	8.92	8.92	1.996e+38	7.94e-05
21042	TS.triHPacyl.COelim.tmmmpmtmpu	4.986e+43	7.41	7.41	1.978e+38	7.86e-05
21043	TS.triHPacyl.COelim.mmtmmpmpmu	5.184e+44	8.81	8.81	1.978e+38	7.86e-05
21044	TS.triHPacyl.COelim.ttpmmtppu	3.426e+44	8.56	8.56	1.976e+38	7.86e-05
21045	TS.triHPacyl.COelim.pmmppttppu	8.201e+43	7.71	7.71	1.975e+38	7.85e-05
21046	TS.triHPacyl.COelim.tmpmttmmu	2.590e+45	9.77	9.77	1.969e+38	7.83e-05
21047	TS.triHPacyl.COelim.mmmmpmmtmmu	3.259e+44	8.54	8.54	1.959e+38	7.79e-05
21048	TS.triHPacyl.COelim.tmpmpttppu	4.096e+44	8.68	8.68	1.952e+38	7.76e-05
21049	TS.triHPacyl.COelim.tmmpptppu	6.127e+44	8.92	8.92	1.950e+38	7.75e-05
21050	TS.triHPacyl.COelim.mptmpmmmpu	8.719e+44	9.13	9.13	1.947e+38	7.74e-05
21051	TS.triHPacyl.COelim.mttppmtppu	4.854e+44	8.78	8.78	1.942e+38	7.72e-05
21052	TS.triHPacyl.COelim.tpttptmmpu	1.238e+45	9.34	9.34	1.936e+38	7.7e-05
21053	TS.triHPacyl.COelim.tptmmmmmpu	2.346e+44	8.35	8.35	1.930e+38	7.67e-05
21054	TS.triHPacyl.COelim.mtmtppmtmmu	7.964e+44	9.08	9.08	1.920e+38	7.63e-05
21055	TS.triHPacyl.COelim.pptppppmpu	9.831e+43	7.84	7.84	1.917e+38	7.62e-05
21056	TS.triHPacyl.COelim.tpptpmmpmu	4.470e+44	8.74	8.74	1.905e+38	7.58e-05
21057	TS.triHPacyl.COelim.mpmmpmpppu	7.248e+43	7.66	7.66	1.901e+38	7.56e-05
21058	TS.triHPacyl.COelim.tppmpmtppu	2.620e+44	8.43	8.43	1.901e+38	7.56e-05
21059	TS.triHPacyl.COelim.mttmmpmpmu	1.232e+45	9.36	9.36	1.878e+38	7.47e-05
21060	TS.triHPacyl.COelim.tpttppmmpu	3.500e+45	9.98	9.98	1.869e+38	7.43e-05
21061	TS.triHPacyl.COelim.ppmppppmpu	1.875e+44	8.24	8.24	1.863e+38	7.41e-05
21062	TS.triHPacyl.COelim.ptmppptmpu	3.658e+43	7.27	7.27	1.863e+38	7.41e-05
21063	TS.triHPacyl.COelim.tpmppppmpu	1.500e+44	8.11	8.11	1.855e+38	7.38e-05
21064	TS.triHPacyl.COelim.pmptmmtmpu	7.627e+44	9.08	9.08	1.854e+38	7.37e-05
21065	TS.triHPacyl.COelim.mmtmpmtppu	6.606e+44	8.99	8.99	1.851e+38	7.36e-05
21066	TS.triHPacyl.COelim.ttmppmtmpu	5.923e+44	8.93	8.93	1.846e+38	7.34e-05
21067	TS.triHPacyl.COelim.ppmmmmmmmmu	9.590e+43	7.85	7.85	1.830e+38	7.28e-05
21068	TS.triHPacyl.COelim.ppmmmmpmpu	1.283e+44	8.03	8.03	1.808e+38	7.19e-05
21069	TS.triHPacyl.COelim.ppmmmtpmpu	1.208e+44	8.00	8.00	1.799e+38	7.15e-05
21070	TS.triHPacyl.COelim.pmptmpmpu	5.962e+43	7.58	7.58	1.798e+38	7.15e-05
21071	TS.triHPacyl.COelim.mpmmmmtmmpu	1.904e+44	8.27	8.27	1.788e+38	7.11e-05

21072	TS.triHPacyl.COelim.tmtpmmtppu	6.564e+44	9.01	9.01	1.783e+38	7.09e-05
21073	TS.triHPacyl.COelim.tmtpmmtppu	4.858e+44	8.83	8.83	1.783e+38	7.09e-05
21074	TS.triHPacyl.COelim.mttmmmpmmu	6.258e+44	8.99	8.99	1.782e+38	7.09e-05
21075	TS.triHPacyl.COelim.tmtpmmtppu	2.538e+44	8.45	8.45	1.779e+38	7.07e-05
21076	TS.triHPacyl.COelim.mmttmppppu	5.247e+44	8.88	8.88	1.773e+38	7.05e-05
21077	TS.triHPacyl.COelim.mmtmmptppu	4.185e+44	8.75	8.75	1.763e+38	7.01e-05
21078	TS.triHPacyl.COelim.tmppppmtppu	9.234e+44	9.23	9.23	1.749e+38	6.95e-05
21079	TS.triHPacyl.COelim.tmtppmpmpu	9.875e+45	10.64	10.64	1.748e+38	6.95e-05
21080	TS.triHPacyl.COelim.mmtmtttmmu	1.071e+45	9.32	9.32	1.748e+38	6.95e-05
21081	TS.triHPacyl.COelim.ptmpmtppmu	1.415e+44	8.11	8.11	1.746e+38	6.94e-05
21082	TS.triHPacyl.COelim.pptpmtmmu	1.723e+44	8.23	8.23	1.746e+38	6.94e-05
21083	TS.triHPacyl.COelim.ptttppppu	2.295e+45	9.77	9.77	1.738e+38	6.91e-05
21084	TS.triHPacyl.COelim.pmtptmmpu	3.892e+44	8.72	8.72	1.737e+38	6.91e-05
21085	TS.triHPacyl.COelim.tpptmmmmu	5.047e+44	8.87	8.87	1.735e+38	6.9e-05
21086	TS.triHPacyl.COelim.tmpmptmpu	4.198e+44	8.76	8.76	1.734e+38	6.9e-05
21087	TS.triHPacyl.COelim.ptmmpppmu	2.249e+44	8.39	8.39	1.734e+38	6.89e-05
21088	TS.triHPacyl.COelim.tpptpmtppu	6.114e+45	10.36	10.36	1.732e+38	6.89e-05
21089	TS.triHPacyl.COelim.tmttmmtppu	1.764e+45	9.62	9.62	1.727e+38	6.87e-05
21090	TS.triHPacyl.COelim.pmpmpmtppu	6.375e+43	7.64	7.64	1.724e+38	6.86e-05
21091	TS.triHPacyl.COelim.mttppppmu	6.165e+44	9.00	9.00	1.723e+38	6.85e-05
21092	TS.triHPacyl.COelim.pmttptmmpu	1.694e+44	8.23	8.23	1.716e+38	6.82e-05
21093	TS.triHPacyl.COelim.mttmmppmmu	8.614e+44	9.20	9.20	1.713e+38	6.81e-05
21094	TS.triHPacyl.COelim.mttmpmtppu	5.678e+44	8.96	8.96	1.701e+38	6.77e-05
21095	TS.triHPacyl.COelim.ptmtmptppu	1.053e+45	9.32	9.32	1.698e+38	6.75e-05
21096	TS.triHPacyl.COelim.tmtptmtpu	1.384e+45	9.49	9.49	1.694e+38	6.74e-05
21097	TS.triHPacyl.COelim.mtmtmptmpu	5.593e+43	7.58	7.58	1.691e+38	6.73e-05
21098	TS.triHPacyl.COelim.mptppppmpu	9.023e+43	7.86	7.86	1.689e+38	6.71e-05
21099	TS.triHPacyl.COelim.tmtptmmpmu	8.747e+43	7.85	7.85	1.683e+38	6.69e-05
21100	TS.triHPacyl.COelim.mtptmmmpmu	3.311e+44	8.64	8.64	1.679e+38	6.67e-05
21101	TS.triHPacyl.COelim.mptpmttppu	1.493e+45	9.54	9.54	1.671e+38	6.65e-05
21102	TS.triHPacyl.COelim.mptmpmmmu	5.740e+44	8.97	8.97	1.668e+38	6.63e-05
21103	TS.triHPacyl.COelim.ptmtmmtppu	2.551e+45	9.86	9.86	1.662e+38	6.61e-05
21104	TS.triHPacyl.COelim.tptpmmppu	4.028e+44	8.76	8.76	1.660e+38	6.6e-05
21105	TS.triHPacyl.COelim.mpttmtppu	1.578e+45	9.58	9.58	1.658e+38	6.59e-05
21106	TS.triHPacyl.COelim.mttmmmpmu	1.005e+45	9.31	9.31	1.651e+38	6.57e-05
21107	TS.triHPacyl.COelim.tpmmpmtppu	4.635e+44	8.85	8.85	1.646e+38	6.55e-05
21108	TS.triHPacyl.COelim.tmppttppu	2.734e+45	9.92	9.92	1.633e+38	6.49e-05
21109	TS.triHPacyl.COelim.pptmmmmmu	7.392e+44	9.14	9.14	1.632e+38	6.49e-05
21110	TS.triHPacyl.COelim.pmttptmmpu	1.097e+44	8.00	8.00	1.628e+38	6.47e-05
21111	TS.triHPacyl.COelim.pmttppmpmu	5.423e+43	7.59	7.59	1.616e+38	6.43e-05
21112	TS.triHPacyl.COelim.ttptmmpmu	1.904e+45	9.72	9.72	1.591e+38	6.33e-05
21113	TS.triHPacyl.COelim.pmpmmtppu	1.773e+44	8.31	8.31	1.580e+38	6.28e-05
21114	TS.triHPacyl.COelim.mptmmmtmmu	9.758e+44	9.32	9.32	1.576e+38	6.27e-05
21115	TS.triHPacyl.COelim.pptmmpmmpu	1.082e+45	9.39	9.39	1.570e+38	6.24e-05
21116	TS.triHPacyl.COelim.ptpmmtppu	1.273e+44	8.12	8.12	1.561e+38	6.21e-05
21117	TS.triHPacyl.COelim.pptppmpmu	3.061e+44	8.64	8.64	1.560e+38	6.2e-05
21118	TS.triHPacyl.COelim.tmtppmtppu	8.987e+44	9.28	9.28	1.555e+38	6.18e-05
21119	TS.triHPacyl.COelim.pmpmtmmpmu	1.032e+45	9.37	9.37	1.552e+38	6.17e-05
21120	TS.triHPacyl.COelim.tppmpmpmu	1.478e+44	8.21	8.21	1.533e+38	6.1e-05
21121	TS.triHPacyl.COelim.tppmptppu	1.309e+44	8.14	8.14	1.530e+38	6.08e-05
21122	TS.triHPacyl.COelim.mttmmtppu	2.573e+44	8.55	8.55	1.508e+38	6e-05
21123	TS.triHPacyl.COelim.ttptppmpmu	7.605e+44	9.20	9.20	1.498e+38	5.96e-05
21124	TS.triHPacyl.COelim.ptmmpmmpmu	2.018e+44	8.42	8.42	1.492e+38	5.93e-05
21125	TS.triHPacyl.COelim.mppppmmpu	3.230e+44	8.70	8.70	1.479e+38	5.88e-05
21126	TS.triHPacyl.COelim.tttppmpmu	3.589e+45	10.14	10.14	1.477e+38	5.87e-05
21127	TS.triHPacyl.COelim.mpttptmmpu	1.087e+45	9.43	9.43	1.476e+38	5.87e-05
21128	TS.triHPacyl.COelim.mtttppmmpu	1.038e+45	9.40	9.40	1.463e+38	5.82e-05
21129	TS.triHPacyl.COelim.mttmmtpmmu	6.090e+44	9.09	9.09	1.460e+38	5.8e-05
21130	TS.triHPacyl.COelim.mtttppmpmu	6.587e+44	9.14	9.14	1.441e+38	5.73e-05
21131	TS.triHPacyl.COelim.mtmtmmpmmpu	8.135e+44	9.27	9.27	1.440e+38	5.73e-05
21132	TS.triHPacyl.COelim.mmpptppmmpu	1.062e+45	9.43	9.43	1.428e+38	5.68e-05
21133	TS.triHPacyl.COelim.mtmppppppu	1.308e+44	8.19	8.19	1.425e+38	5.66e-05
21134	TS.triHPacyl.COelim.pmpptmmpu	3.615e+43	7.42	7.42	1.423e+38	5.66e-05
21135	TS.triHPacyl.COelim.tmtmmmmmpu	9.250e+44	9.36	9.36	1.416e+38	5.63e-05
21136	TS.triHPacyl.COelim.mmpptppmmpu	8.924e+43	7.96	7.96	1.412e+38	5.62e-05
21137	TS.triHPacyl.COelim.mpmmmtpmpu	1.383e+44	8.23	8.23	1.405e+38	5.59e-05
21138	TS.triHPacyl.COelim.pmpmtmmpmu	1.076e+44	8.08	8.08	1.398e+38	5.56e-05
21139	TS.triHPacyl.COelim.mttmmpmmpu	2.273e+44	8.53	8.53	1.397e+38	5.55e-05
21140	TS.triHPacyl.COelim.ttptptmmpu	2.430e+44	8.57	8.57	1.381e+38	5.49e-05
21141	TS.triHPacyl.COelim.tmttmmtppu	3.034e+45	10.09	10.09	1.364e+38	5.42e-05
21142	TS.triHPacyl.COelim.tpttmtppu	3.023e+45	10.09	10.09	1.357e+38	5.4e-05
21143	TS.triHPacyl.COelim.mpmmpmtppu	2.698e+44	8.65	8.65	1.353e+38	5.38e-05

21144	TS.triHPacyl.COelim.mtptmpppmu	7.377e+44	9.25	9.25	1.345e+38	5.35e-05
21145	TS.triHPacyl.COelim.mptmmtmppu	2.157e+44	8.52	8.52	1.343e+38	5.34e-05
21146	TS.triHPacyl.COelim.ppptmmmpmu	4.850e+44	9.00	9.00	1.342e+38	5.34e-05
21147	TS.triHPacyl.COelim.ppptmtppmu	5.699e+44	9.10	9.10	1.338e+38	5.32e-05
21148	TS.triHPacyl.COelim.mmpmmtppmu	4.344e+44	8.94	8.94	1.337e+38	5.32e-05
21149	TS.triHPacyl.COelim.tmtmpptpmu	4.052e+45	10.28	10.28	1.319e+38	5.24e-05
21150	TS.triHPacyl.COelim.mmtmmmtppmu	7.369e+45	10.64	10.64	1.302e+38	5.18e-05
21151	TS.triHPacyl.COelim.mmpmmtppmu	2.867e+44	8.71	8.71	1.301e+38	5.17e-05
21152	TS.triHPacyl.COelim.mmtmpptppu	3.525e+44	8.83	8.83	1.299e+38	5.17e-05
21153	TS.triHPacyl.COelim.tmpmmmpmmu	1.299e+44	8.24	8.24	1.293e+38	5.14e-05
21154	TS.triHPacyl.COelim.mptmptmmpu	4.804e+44	9.02	9.02	1.291e+38	5.13e-05
21155	TS.triHPacyl.COelim.pmptptppmu	6.542e+43	7.83	7.83	1.290e+38	5.13e-05
21156	TS.triHPacyl.COelim.mmpptppmmu	9.906e+44	9.45	9.45	1.284e+38	5.1e-05
21157	TS.triHPacyl.COelim.tmtptmmmmu	3.407e+44	8.82	8.82	1.282e+38	5.1e-05
21158	TS.triHPacyl.COelim.mppptmmpmu	1.892e+44	8.47	8.47	1.280e+38	5.09e-05
21159	TS.triHPacyl.COelim.mppppmmmpmu	3.442e+44	8.83	8.83	1.276e+38	5.07e-05
21160	TS.triHPacyl.COelim.tppmmmtmmu	6.989e+44	9.25	9.25	1.266e+38	5.03e-05
21161	TS.triHPacyl.COelim.tpmmmmtppmu	1.038e+45	9.49	9.49	1.263e+38	5.02e-05
21162	TS.triHPacyl.COelim.mptmptmmpu	4.125e+44	8.94	8.94	1.261e+38	5.01e-05
21163	TS.triHPacyl.COelim.pptppppmu	2.474e+44	8.64	8.64	1.257e+38	5e-05
21164	TS.triHPacyl.COelim.tpptpmtmmu	8.669e+45	10.76	10.76	1.253e+38	4.98e-05
21165	TS.triHPacyl.COelim.ttpmmmmmpmu	2.703e+44	8.70	8.70	1.247e+38	4.96e-05
21166	TS.triHPacyl.COelim.tmtmttppu	2.001e+45	9.89	9.89	1.246e+38	4.95e-05
21167	TS.triHPacyl.COelim.ttmppmmmpmu	1.323e+44	8.27	8.27	1.246e+38	4.95e-05
21168	TS.triHPacyl.COelim.ttmppptmpu	7.700e+44	9.33	9.33	1.235e+38	4.91e-05
21169	TS.triHPacyl.COelim.tpttptmpmu	1.282e+45	9.63	9.63	1.235e+38	4.91e-05
21170	TS.triHPacyl.COelim.tmmmtmmmmu	9.072e+44	9.43	9.43	1.226e+38	4.87e-05
21171	TS.triHPacyl.COelim.ttttptmmpu	3.239e+45	10.19	10.19	1.212e+38	4.82e-05
21172	TS.triHPacyl.COelim.ptmppmtppmu	2.372e+44	8.64	8.64	1.211e+38	4.82e-05
21173	TS.triHPacyl.COelim.mpttmmppmu	3.022e+45	10.16	10.16	1.198e+38	4.77e-05
21174	TS.triHPacyl.COelim.tmpppmtmmu	5.578e+44	9.16	9.16	1.186e+38	4.71e-05
21175	TS.triHPacyl.COelim.pmpmmpppu	4.840e+43	7.71	7.71	1.179e+38	4.69e-05
21176	TS.triHPacyl.COelim.pmpmpmpppu	4.430e+43	7.66	7.66	1.174e+38	4.67e-05
21177	TS.triHPacyl.COelim.pmpmtmtpu	6.804e+44	9.28	9.28	1.172e+38	4.66e-05
21178	TS.triHPacyl.COelim.mptmptmmpu	9.243e+44	9.47	9.47	1.170e+38	4.65e-05
21179	TS.triHPacyl.COelim.pmpmtmtpu	5.442e+44	9.16	9.16	1.164e+38	4.63e-05
21180	TS.triHPacyl.COelim.mtpppmtmmu	3.612e+44	8.91	8.91	1.163e+38	4.63e-05
21181	TS.triHPacyl.COelim.tmmmpmpppmu	3.128e+43	7.46	7.46	1.160e+38	4.61e-05
21182	TS.triHPacyl.COelim.tmtmptppu	1.960e+45	9.92	9.92	1.155e+38	4.59e-05
21183	TS.triHPacyl.COelim.pptmmtppmu	6.833e+44	9.30	9.30	1.151e+38	4.57e-05
21184	TS.triHPacyl.COelim.mtmmmpmpmu	3.530e+44	8.91	8.91	1.143e+38	4.55e-05
21185	TS.triHPacyl.COelim.tmpmpmtmpu	2.413e+44	8.68	8.68	1.143e+38	4.54e-05
21186	TS.triHPacyl.COelim.pmpmptppmu	3.311e+43	7.50	7.50	1.141e+38	4.54e-05
21187	TS.triHPacyl.COelim.pmpmtmtpu	2.985e+44	8.81	8.81	1.139e+38	4.53e-05
21188	TS.triHPacyl.COelim.pmmptmtpmu	4.924e+43	7.74	7.74	1.139e+38	4.53e-05
21189	TS.triHPacyl.COelim.ttpmmmtppmu	5.004e+44	9.12	9.12	1.133e+38	4.51e-05
21190	TS.triHPacyl.COelim.mtpppmtppu	4.113e+44	9.01	9.01	1.131e+38	4.5e-05
21191	TS.triHPacyl.COelim.pmpmtpppu	5.107e+43	7.76	7.76	1.128e+38	4.49e-05
21192	TS.triHPacyl.COelim.tmttppppmu	4.062e+44	9.00	9.00	1.121e+38	4.46e-05
21193	TS.triHPacyl.COelim.mpttpttppu	1.660e+45	9.85	9.85	1.103e+38	4.38e-05
21194	TS.triHPacyl.COelim.mmttppppmu	1.126e+45	9.63	9.63	1.096e+38	4.36e-05
21195	TS.triHPacyl.COelim.tppmmmmmpu	1.910e+44	8.57	8.57	1.093e+38	4.35e-05
21196	TS.triHPacyl.COelim.mmpmtmtpu	5.778e+44	9.23	9.23	1.090e+38	4.33e-05
21197	TS.triHPacyl.COelim.ppptmppmpu	2.284e+44	8.68	8.68	1.080e+38	4.29e-05
21198	TS.triHPacyl.COelim.tmpmpmtppu	1.883e+44	8.57	8.57	1.079e+38	4.29e-05
21199	TS.triHPacyl.COelim.pmpmtmtpu	1.128e+44	8.27	8.27	1.073e+38	4.27e-05
21200	TS.triHPacyl.COelim.mtmtmmpmpu	7.413e+44	9.39	9.39	1.070e+38	4.26e-05
21201	TS.triHPacyl.COelim.pmpptppppu	4.152e+43	7.67	7.67	1.069e+38	4.25e-05
21202	TS.triHPacyl.COelim.tptpmtppu	5.608e+44	9.23	9.23	1.060e+38	4.22e-05
21203	TS.triHPacyl.COelim.tmpmmtppmu	6.319e+43	7.94	7.94	1.045e+38	4.15e-05
21204	TS.triHPacyl.COelim.ttmppmtppu	3.714e+44	8.99	8.99	1.043e+38	4.15e-05
21205	TS.triHPacyl.COelim.mppptppppmu	3.616e+43	7.61	7.61	1.043e+38	4.15e-05
21206	TS.triHPacyl.COelim.tmptmtpmu	4.375e+44	9.10	9.10	1.026e+38	4.08e-05
21207	TS.triHPacyl.COelim.mptmmtppu	3.008e+44	8.88	8.88	1.024e+38	4.07e-05
21208	TS.triHPacyl.COelim.mppmmppppu	6.462e+43	7.96	7.96	1.020e+38	4.06e-05
21209	TS.triHPacyl.COelim.mttmmmmmpu	1.462e+45	9.83	9.83	1.011e+38	4.02e-05
21210	TS.triHPacyl.COelim.tmptmtpmu	1.654e+45	9.90	9.90	1.008e+38	4.01e-05
21211	TS.triHPacyl.COelim.tttmmtppu	1.361e+45	9.79	9.79	1.005e+38	4e-05
21212	TS.triHPacyl.COelim.tmpmtppppu	1.118e+45	9.67	9.67	1.002e+38	3.99e-05
21213	TS.triHPacyl.COelim.ptmpmmtmmu	6.056e+44	9.31	9.31	1.002e+38	3.98e-05
21214	TS.triHPacyl.COelim.mmpmttppu	5.184e+44	9.22	9.22	9.919e+37	3.94e-05
21215	TS.triHPacyl.COelim.tttmmtppu	2.343e+45	10.12	10.12	9.889e+37	3.93e-05

21216	TS.triHPacyl.COelim.ptmppmpmpu	3.574e+44	9.01	9.01	9.829e+37	3.91e-05
21217	TS.triHPacyl.COelim.mmtmtmptmmpu	2.025e+44	8.67	8.67	9.818e+37	3.9e-05
21218	TS.triHPacyl.COelim.ttmppmmtmpu	4.389e+43	7.76	7.76	9.737e+37	3.87e-05
21219	TS.triHPacyl.COelim.ppptmmpppu	4.209e+44	9.11	9.11	9.650e+37	3.84e-05
21220	TS.triHPacyl.COelim.ppttpmpmpu	1.969e+44	8.67	8.67	9.588e+37	3.81e-05
21221	TS.triHPacyl.COelim.tmtptmmpmpu	9.324e+44	9.60	9.60	9.516e+37	3.78e-05
21222	TS.triHPacyl.COelim.mppmpptmpu	1.545e+44	8.53	8.53	9.484e+37	3.77e-05
21223	TS.triHPacyl.COelim.mmtmtmtpmpu	3.076e+44	8.94	8.94	9.417e+37	3.74e-05
21224	TS.triHPacyl.COelim.ppptpppppu	2.350e+44	8.78	8.78	9.393e+37	3.73e-05
21225	TS.triHPacyl.COelim.pmttptmmpu	4.302e+44	9.15	9.15	9.362e+37	3.72e-05
21226	TS.triHPacyl.COelim.pmttptmpmpu	6.934e+44	9.43	9.43	9.355e+37	3.72e-05
21227	TS.triHPacyl.COelim.mmmmmppmpu	3.550e+44	9.03	9.03	9.313e+37	3.7e-05
21228	TS.triHPacyl.COelim.tmtptmtpmpu	3.105e+45	10.33	10.33	9.276e+37	3.69e-05
21229	TS.triHPacyl.COelim.ttttppmpu	4.357e+45	10.53	10.53	9.263e+37	3.68e-05
21230	TS.triHPacyl.COelim.pttpmmtmpu	8.667e+44	9.58	9.58	9.090e+37	3.61e-05
21231	TS.triHPacyl.COelim.ptmmpmmmpu	1.225e+44	8.41	8.41	9.082e+37	3.61e-05
21232	TS.triHPacyl.COelim.ttmppmpmpu	3.818e+44	9.10	9.10	8.952e+37	3.56e-05
21233	TS.triHPacyl.COelim.tpmmpmpmpu	4.248e+44	9.17	9.17	8.935e+37	3.55e-05
21234	TS.triHPacyl.COelim.tmpmpmmmpu	2.684e+44	8.90	8.90	8.890e+37	3.54e-05
21235	TS.triHPacyl.COelim.ttpmptmpu	6.079e+44	9.38	9.38	8.872e+37	3.53e-05
21236	TS.triHPacyl.COelim.mmttppmmmpu	6.181e+45	10.77	10.77	8.817e+37	3.51e-05
21237	TS.triHPacyl.COelim.mpttppmpu	1.693e+44	8.63	8.63	8.809e+37	3.5e-05
21238	TS.triHPacyl.COelim.ppptmmpmpu	3.811e+44	9.11	9.11	8.808e+37	3.5e-05
21239	TS.triHPacyl.COelim.pmtptmmpu	2.168e+44	8.77	8.77	8.787e+37	3.49e-05
21240	TS.triHPacyl.COelim.tpmtpmmmpu	5.265e+44	9.30	9.30	8.786e+37	3.49e-05
21241	TS.triHPacyl.COelim.mtptppppmpu	5.770e+44	9.36	9.36	8.776e+37	3.49e-05
21242	TS.triHPacyl.COelim.tpptmmpmpu	6.091e+44	9.39	9.39	8.727e+37	3.47e-05
21243	TS.triHPacyl.COelim.ptmtmtpmpu	2.159e+45	10.15	10.15	8.715e+37	3.47e-05
21244	TS.triHPacyl.COelim.mtppptmpu	2.293e+44	8.81	8.81	8.706e+37	3.46e-05
21245	TS.triHPacyl.COelim.ppptmtpmpu	4.461e+44	9.21	9.21	8.692e+37	3.46e-05
21246	TS.triHPacyl.COelim.mtppmmpmpu	1.368e+44	8.51	8.51	8.667e+37	3.45e-05
21247	TS.triHPacyl.COelim.mpttppmmmpu	2.247e+44	8.81	8.81	8.566e+37	3.41e-05
21248	TS.triHPacyl.COelim.mtmtmmpmpu	8.790e+44	9.62	9.62	8.560e+37	3.4e-05
21249	TS.triHPacyl.COelim.pmttptmpu	4.637e+44	9.24	9.24	8.557e+37	3.4e-05
21250	TS.triHPacyl.COelim.mppmpmpmpu	2.097e+44	8.77	8.77	8.535e+37	3.39e-05
21251	TS.triHPacyl.COelim.pptmptmmpu	3.226e+44	9.03	9.03	8.531e+37	3.39e-05
21252	TS.triHPacyl.COelim.tpmmtmmpu	3.559e+44	9.09	9.09	8.513e+37	3.39e-05
21253	TS.triHPacyl.COelim.mtmppmmmpu	5.437e+44	9.35	9.35	8.420e+37	3.35e-05
21254	TS.triHPacyl.COelim.tttmptmpu	2.504e+45	10.26	10.26	8.355e+37	3.32e-05
21255	TS.triHPacyl.COelim.pptmmpmmmpu	1.818e+44	8.70	8.70	8.316e+37	3.31e-05
21256	TS.triHPacyl.COelim.tmttppmmmpu	2.505e+45	10.27	10.27	8.297e+37	3.3e-05
21257	TS.triHPacyl.COelim.pmpppppppu	7.253e+43	8.16	8.16	8.277e+37	3.29e-05
21258	TS.triHPacyl.COelim.ttmppmmmpu	2.948e+44	8.99	8.99	8.275e+37	3.29e-05
21259	TS.triHPacyl.COelim.mmpppptmpu	1.411e+44	8.56	8.56	8.253e+37	3.28e-05
21260	TS.triHPacyl.COelim.ttttptmmpu	2.757e+45	10.33	10.33	8.249e+37	3.28e-05
21261	TS.triHPacyl.COelim.ttmppmmmpu	4.230e+44	9.21	9.21	8.237e+37	3.28e-05
21262	TS.triHPacyl.COelim.mttppptmpu	3.242e+44	9.05	9.05	8.222e+37	3.27e-05
21263	TS.triHPacyl.COelim.mttmmpmmmpu	7.636e+44	9.57	9.57	8.210e+37	3.26e-05
21264	TS.triHPacyl.COelim.ttmppptmpu	1.606e+45	10.01	10.01	8.176e+37	3.25e-05
21265	TS.triHPacyl.COelim.ttptmtmmpu	1.876e+45	10.11	10.11	8.126e+37	3.23e-05
21266	TS.triHPacyl.COelim.mptmmmpmpu	2.387e+44	8.88	8.88	8.107e+37	3.22e-05
21267	TS.triHPacyl.COelim.mmpmmmtmpu	3.678e+44	9.14	9.14	8.050e+37	3.2e-05
21268	TS.triHPacyl.COelim.ttttmtmpu	2.313e+45	10.24	10.24	7.994e+37	3.18e-05
21269	TS.triHPacyl.COelim.pmtmmpmmmpu	5.384e+44	9.37	9.37	7.977e+37	3.17e-05
21270	TS.triHPacyl.COelim.ttptmtpmpu	1.971e+45	10.15	10.15	7.925e+37	3.15e-05
21271	TS.triHPacyl.COelim.mtmtmmpmmmpu	4.291e+44	9.24	9.24	7.916e+37	3.15e-05
21272	TS.triHPacyl.COelim.mtppmmpmmmpu	4.704e+44	9.30	9.30	7.860e+37	3.13e-05
21273	TS.triHPacyl.COelim.mtttppmpmpu	7.375e+44	9.58	9.58	7.789e+37	3.1e-05
21274	TS.triHPacyl.COelim.pmttptmmpu	1.961e+44	8.79	8.79	7.736e+37	3.08e-05
21275	TS.triHPacyl.COelim.mmtmmpmmmpu	9.479e+44	9.73	9.73	7.675e+37	3.05e-05
21276	TS.triHPacyl.COelim.mtmppmpmpu	2.120e+44	8.84	8.84	7.643e+37	3.04e-05
21277	TS.triHPacyl.COelim.mttmmpmpmpu	5.547e+45	10.79	10.79	7.639e+37	3.04e-05
21278	TS.triHPacyl.COelim.pptptmmpu	3.708e+44	9.18	9.18	7.635e+37	3.04e-05
21279	TS.triHPacyl.COelim.tmpmmmpmpu	3.017e+44	9.06	9.06	7.624e+37	3.03e-05
21280	TS.triHPacyl.COelim.ttttptmmpu	4.034e+45	10.61	10.61	7.588e+37	3.02e-05
21281	TS.triHPacyl.COelim.ttpmmtmmpu	2.262e+44	8.89	8.89	7.522e+37	2.99e-05
21282	TS.triHPacyl.COelim.ttpmptmpu	2.397e+44	8.93	8.93	7.494e+37	2.98e-05
21283	TS.triHPacyl.COelim.tmpptmmpu	4.324e+44	9.29	9.29	7.395e+37	2.94e-05
21284	TS.triHPacyl.COelim.mmpmmppppu	2.847e+44	9.04	9.04	7.387e+37	2.94e-05
21285	TS.triHPacyl.COelim.ttmtptmpu	1.182e+44	8.52	8.52	7.384e+37	2.94e-05
21286	TS.triHPacyl.COelim.mppmtmmpu	5.240e+44	9.41	9.41	7.373e+37	2.93e-05
21287	TS.triHPacyl.COelim.mttppmpmpu	5.164e+44	9.41	9.41	7.265e+37	2.89e-05

21288	TS.triHPacyl.COelim.pmttppmmmu	4.107e+44	9.27	9.27	7.261e+37	2.89e-05
21289	TS.triHPacyl.COelim.tmttmppppu	4.140e+44	9.28	9.28	7.182e+37	2.86e-05
21290	TS.triHPacyl.COelim.tmttmppmmu	8.563e+43	8.34	8.34	7.161e+37	2.85e-05
21291	TS.triHPacyl.COelim.tpmpttppu	1.098e+44	8.49	8.49	7.156e+37	2.85e-05
21292	TS.triHPacyl.COelim.tmtpttppu	2.348e+45	10.32	10.32	7.154e+37	2.84e-05
21293	TS.triHPacyl.COelim.pppttmmmu	5.726e+44	9.48	9.48	7.138e+37	2.84e-05
21294	TS.triHPacyl.COelim.ttpttppu	4.386e+44	9.32	9.32	7.082e+37	2.82e-05
21295	TS.triHPacyl.COelim.ttptppppu	3.106e+44	9.12	9.12	7.038e+37	2.8e-05
21296	TS.triHPacyl.COelim.ttmpmtmpu	4.433e+43	7.96	7.96	7.000e+37	2.78e-05
21297	TS.triHPacyl.COelim.pmppttmpu	1.777e+44	8.79	8.79	6.987e+37	2.78e-05
21298	TS.triHPacyl.COelim.mtmppmmmu	6.138e+43	8.17	8.17	6.899e+37	2.74e-05
21299	TS.triHPacyl.COelim.mptpmmmu	1.180e+44	8.56	8.56	6.891e+37	2.74e-05
21300	TS.triHPacyl.COelim.pmpmtppppu	4.676e+44	9.38	9.38	6.845e+37	2.72e-05
21301	TS.triHPacyl.COelim.mmmptmmmu	5.357e+44	9.47	9.47	6.804e+37	2.71e-05
21302	TS.triHPacyl.COelim.ptmtpppmmu	8.665e+43	8.39	8.39	6.742e+37	2.68e-05
21303	TS.triHPacyl.COelim.mtmppppmpu	8.559e+44	9.75	9.75	6.728e+37	2.68e-05
21304	TS.triHPacyl.COelim.mmpmmmpmpu	2.755e+44	9.08	9.08	6.720e+37	2.67e-05
21305	TS.triHPacyl.COelim.ppmtpptmmu	2.505e+44	9.02	9.02	6.712e+37	2.67e-05
21306	TS.triHPacyl.COelim.mmpmtmmmu	7.128e+44	9.65	9.65	6.692e+37	2.66e-05
21307	TS.triHPacyl.COelim.tmtmpmpmpu	3.981e+44	9.30	9.30	6.669e+37	2.65e-05
21308	TS.triHPacyl.COelim.pmpmtpppmu	2.244e+44	8.96	8.96	6.661e+37	2.65e-05
21309	TS.triHPacyl.COelim.tmttppmmmu	2.031e+45	10.27	10.27	6.654e+37	2.65e-05
21310	TS.triHPacyl.COelim.mptmmppppu	3.231e+45	10.55	10.55	6.648e+37	2.64e-05
21311	TS.triHPacyl.COelim.mttppppmpu	1.147e+45	9.94	9.94	6.633e+37	2.64e-05
21312	TS.triHPacyl.COelim.ptttmtppu	1.883e+45	10.23	10.23	6.622e+37	2.63e-05
21313	TS.triHPacyl.COelim.mptppmmmu	1.450e+44	8.70	8.70	6.612e+37	2.63e-05
21314	TS.triHPacyl.COelim.mmtmmpmpu	5.264e+44	9.48	9.48	6.574e+37	2.61e-05
21315	TS.triHPacyl.COelim.mtmmpmtmpu	2.664e+45	10.45	10.45	6.549e+37	2.6e-05
21316	TS.triHPacyl.COelim.pmmppptmpu	2.085e+44	8.93	8.93	6.537e+37	2.6e-05
21317	TS.triHPacyl.COelim.ttptmmtpmu	1.516e+45	10.12	10.12	6.482e+37	2.58e-05
21318	TS.triHPacyl.COelim.tmpmntmmu	3.425e+44	9.23	9.23	6.481e+37	2.58e-05
21319	TS.triHPacyl.COelim.pmmtptmpu	1.412e+44	8.71	8.71	6.430e+37	2.56e-05
21320	TS.triHPacyl.COelim.mmpmptmpu	3.962e+44	9.33	9.33	6.360e+37	2.53e-05
21321	TS.triHPacyl.COelim.mpptpmtmpu	1.509e+45	10.13	10.13	6.274e+37	2.49e-05
21322	TS.triHPacyl.COelim.mpttmtmpu	3.517e+45	10.64	10.64	6.246e+37	2.48e-05
21323	TS.triHPacyl.COelim.tpmtptmpu	1.313e+45	10.05	10.05	6.217e+37	2.47e-05
21324	TS.triHPacyl.COelim.tpmmpmpmmu	3.454e+44	9.26	9.26	6.187e+37	2.46e-05
21325	TS.triHPacyl.COelim.mtmtpmmpu	6.688e+44	9.66	9.66	6.167e+37	2.45e-05
21326	TS.triHPacyl.COelim.tmmpmtmpu	1.726e+44	8.86	8.86	6.057e+37	2.41e-05
21327	TS.triHPacyl.COelim.pmptppppu	8.071e+43	8.41	8.41	6.001e+37	2.39e-05
21328	TS.triHPacyl.COelim.mmmptttmpu	1.045e+45	9.94	9.94	5.952e+37	2.37e-05
21329	TS.triHPacyl.COelim.ttptppppmu	1.644e+45	10.22	10.22	5.927e+37	2.36e-05
21330	TS.triHPacyl.COelim.mmttmrmmmu	3.259e+45	10.63	10.63	5.918e+37	2.35e-05
21331	TS.triHPacyl.COelim.ttptpmmmpu	3.828e+44	9.35	9.35	5.914e+37	2.35e-05
21332	TS.triHPacyl.COelim.pmmptpmmu	5.087e+43	8.15	8.15	5.901e+37	2.35e-05
21333	TS.triHPacyl.COelim.pptmmtpmu	1.807e+45	10.28	10.28	5.874e+37	2.34e-05
21334	TS.triHPacyl.COelim.ppptppppmu	3.625e+44	9.32	9.32	5.873e+37	2.34e-05
21335	TS.triHPacyl.COelim.tmpmpmtppu	4.342e+44	9.43	9.43	5.870e+37	2.33e-05
21336	TS.triHPacyl.COelim.ttmppmmmu	3.519e+44	9.31	9.31	5.857e+37	2.33e-05
21337	TS.triHPacyl.COelim.mtttppmpmu	1.225e+45	10.05	10.05	5.842e+37	2.32e-05
21338	TS.triHPacyl.COelim.mmttmrmmmu	3.049e+45	10.60	10.60	5.757e+37	2.29e-05
21339	TS.triHPacyl.COelim.mmpppmmmu	1.711e+44	8.89	8.89	5.730e+37	2.28e-05
21340	TS.triHPacyl.COelim.ptmmpmpppu	4.031e+43	8.04	8.04	5.645e+37	2.24e-05
21341	TS.triHPacyl.COelim.ttmpttppu	1.288e+44	8.73	8.73	5.624e+37	2.24e-05
21342	TS.triHPacyl.COelim.ttptpmtmpu	1.185e+45	10.06	10.06	5.609e+37	2.23e-05
21343	TS.triHPacyl.COelim.tmpppptmpu	4.440e+44	9.47	9.47	5.594e+37	2.22e-05
21344	TS.triHPacyl.COelim.mmmptmpmu	2.218e+44	9.06	9.06	5.580e+37	2.22e-05
21345	TS.triHPacyl.COelim.tmpmtpppmu	1.020e+44	8.60	8.60	5.549e+37	2.21e-05
21346	TS.triHPacyl.COelim.ppmtmppppu	2.173e+44	9.05	9.05	5.520e+37	2.2e-05
21347	TS.triHPacyl.COelim.mtmppppppu	3.150e+44	9.27	9.27	5.519e+37	2.19e-05
21348	TS.triHPacyl.COelim.ppmppppppu	1.967e+44	9.00	9.00	5.442e+37	2.16e-05
21349	TS.triHPacyl.COelim.tttppmmmpu	2.849e+45	10.60	10.60	5.393e+37	2.14e-05
21350	TS.triHPacyl.COelim.ttmmtpmmu	2.035e+44	9.03	9.03	5.389e+37	2.14e-05
21351	TS.triHPacyl.COelim.mmmmmmtmpu	2.268e+44	9.09	9.09	5.378e+37	2.14e-05
21352	TS.triHPacyl.COelim.mpttpmmppu	3.317e+44	9.32	9.32	5.377e+37	2.14e-05
21353	TS.triHPacyl.COelim.mtppmtppmu	1.540e+44	8.87	8.87	5.357e+37	2.13e-05
21354	TS.triHPacyl.COelim.ttptpmtmpu	2.997e+45	10.64	10.64	5.300e+37	2.11e-05
21355	TS.triHPacyl.COelim.mmmmtmpppu	4.254e+44	9.48	9.48	5.295e+37	2.11e-05
21356	TS.triHPacyl.COelim.pmppttppu	1.933e+44	9.01	9.01	5.275e+37	2.1e-05
21357	TS.triHPacyl.COelim.mtppppptppu	3.287e+44	9.33	9.33	5.263e+37	2.09e-05
21358	TS.triHPacyl.COelim.pmtmmtpmpu	2.536e+44	9.18	9.18	5.234e+37	2.08e-05
21359	TS.triHPacyl.COelim.pmpmttppu	1.574e+45	10.28	10.28	5.129e+37	2.04e-05

21360	TS.triHPacyl.COelim.mtppmptmpu	1.826e+44	8.99	8.99	5.127e+37	2.04e-05
21361	TS.triHPacyl.COelim.mpptmpppmu	1.027e+45	10.02	10.02	5.125e+37	2.04e-05
21362	TS.triHPacyl.COelim.tmpmtpppmu	2.922e+44	9.28	9.28	5.051e+37	2.01e-05
21363	TS.triHPacyl.COelim.mmpmtppppu	2.104e+44	9.09	9.09	5.027e+37	2e-05
21364	TS.triHPacyl.COelim.mmmppmmmmu	3.277e+43	7.99	7.99	4.994e+37	1.99e-05
21365	TS.triHPacyl.COelim.tttmttppmu	1.629e+45	10.31	10.31	4.985e+37	1.98e-05
21366	TS.triHPacyl.COelim.mmpmmmmmpu	2.297e+44	9.15	9.15	4.935e+37	1.96e-05
21367	TS.triHPacyl.COelim.mmpmmpppmu	2.436e+44	9.19	9.19	4.913e+37	1.95e-05
21368	TS.triHPacyl.COelim.ttptpmpmu	1.817e+45	10.39	10.39	4.910e+37	1.95e-05
21369	TS.triHPacyl.COelim.tpmmmtpmu	6.672e+44	9.79	9.79	4.899e+37	1.95e-05
21370	TS.triHPacyl.COelim.mtptpmtmpu	1.202e+45	10.14	10.14	4.895e+37	1.95e-05
21371	TS.triHPacyl.COelim.pmmmpmpmu	8.624e+43	8.57	8.57	4.894e+37	1.95e-05
21372	TS.triHPacyl.COelim.pptmpmpmu	1.824e+44	9.02	9.02	4.868e+37	1.94e-05
21373	TS.triHPacyl.COelim.mmmmpmpmu	1.173e+44	8.76	8.76	4.868e+37	1.94e-05
21374	TS.triHPacyl.COelim.tmtptmpmu	6.101e+44	9.74	9.74	4.868e+37	1.94e-05
21375	TS.triHPacyl.COelim.pptmpmpmu	3.801e+44	9.46	9.46	4.865e+37	1.93e-05
21376	TS.triHPacyl.COelim.pmmppmmmu	1.583e+44	8.94	8.94	4.860e+37	1.93e-05
21377	TS.triHPacyl.COelim.tpmmttppmu	2.530e+44	9.22	9.22	4.854e+37	1.93e-05
21378	TS.triHPacyl.COelim.mttmmmpmu	1.456e+45	10.27	10.27	4.841e+37	1.92e-05
21379	TS.triHPacyl.COelim.mmpmmmtppu	3.233e+44	9.37	9.37	4.823e+37	1.92e-05
21380	TS.triHPacyl.COelim.tmpmtppmu	1.661e+45	10.35	10.35	4.800e+37	1.91e-05
21381	TS.triHPacyl.COelim.ppmtmmmpu	1.998e+45	10.46	10.46	4.764e+37	1.89e-05
21382	TS.triHPacyl.COelim.pppmpmpmu	4.027e+43	8.14	8.14	4.737e+37	1.88e-05
21383	TS.triHPacyl.COelim.tmpppmpmu	5.157e+44	9.66	9.66	4.717e+37	1.88e-05
21384	TS.triHPacyl.COelim.mmmmpmtmpu	4.981e+44	9.64	9.64	4.698e+37	1.87e-05
21385	TS.triHPacyl.COelim.tpmmtmmmpu	3.988e+44	9.51	9.51	4.692e+37	1.87e-05
21386	TS.triHPacyl.COelim.pmpmptmpu	2.643e+44	9.27	9.27	4.668e+37	1.86e-05
21387	TS.triHPacyl.COelim.mttmpptppu	2.358e+44	9.20	9.20	4.649e+37	1.85e-05
21388	TS.triHPacyl.COelim.mtppmpptppu	2.177e+44	9.16	9.16	4.632e+37	1.84e-05
21389	TS.triHPacyl.COelim.tpptpmtmpu	7.088e+45	11.25	11.25	4.519e+37	1.8e-05
21390	TS.triHPacyl.COelim.pttmtpppu	1.162e+45	10.18	10.18	4.490e+37	1.79e-05
21391	TS.triHPacyl.COelim.tmpptmpu	1.433e+44	8.93	8.93	4.455e+37	1.77e-05
21392	TS.triHPacyl.COelim.mpptmmmpmu	5.945e+44	9.78	9.78	4.449e+37	1.77e-05
21393	TS.triHPacyl.COelim.mpmtpppmu	6.559e+44	9.84	9.84	4.435e+37	1.76e-05
21394	TS.triHPacyl.COelim.mtptmmmpmu	5.530e+44	9.74	9.74	4.419e+37	1.76e-05
21395	TS.triHPacyl.COelim.tmtptppmu	4.480e+44	9.63	9.63	4.361e+37	1.73e-05
21396	TS.triHPacyl.COelim.mpmtpmpmu	4.850e+44	9.68	9.68	4.339e+37	1.73e-05
21397	TS.triHPacyl.COelim.tptpmpmpu	1.947e+45	10.51	10.51	4.308e+37	1.71e-05
21398	TS.triHPacyl.COelim.pmtmpppu	2.461e+44	9.28	9.28	4.301e+37	1.71e-05
21399	TS.triHPacyl.COelim.mttmpmpmu	1.761e+45	10.46	10.46	4.212e+37	1.67e-05
21400	TS.triHPacyl.COelim.pmmmpmtppu	3.279e+43	8.09	8.09	4.200e+37	1.67e-05
21401	TS.triHPacyl.COelim.mmtmpmpmu	2.546e+45	10.68	10.68	4.196e+37	1.67e-05
21402	TS.triHPacyl.COelim.pmptpmtmpu	4.163e+44	9.61	9.61	4.184e+37	1.66e-05
21403	TS.triHPacyl.COelim.pmmppppmu	2.111e+43	7.84	7.84	4.131e+37	1.64e-05
21404	TS.triHPacyl.COelim.mmpmmmtmpu	2.947e+44	9.41	9.41	4.127e+37	1.64e-05
21405	TS.triHPacyl.COelim.ptpmtppu	6.274e+43	8.49	8.49	4.125e+37	1.64e-05
21406	TS.triHPacyl.COelim.mpmmpptppu	1.242e+44	8.90	8.90	4.102e+37	1.63e-05
21407	TS.triHPacyl.COelim.pptmpmpmu	3.081e+44	9.44	9.44	4.091e+37	1.63e-05
21408	TS.triHPacyl.COelim.tmtppmmmpu	8.684e+44	10.06	10.06	4.070e+37	1.62e-05
21409	TS.triHPacyl.COelim.pptmttppu	2.773e+45	10.76	10.76	4.040e+37	1.61e-05
21410	TS.triHPacyl.COelim.mtmtptmpu	1.333e+45	10.33	10.33	3.976e+37	1.58e-05
21411	TS.triHPacyl.COelim.mttmpmpmu	6.369e+44	9.89	9.89	3.953e+37	1.57e-05
21412	TS.triHPacyl.COelim.mmpmmpppu	2.536e+45	10.72	10.72	3.908e+37	1.55e-05
21413	TS.triHPacyl.COelim.tttppmmmu	2.798e+45	10.78	10.78	3.904e+37	1.55e-05
21414	TS.triHPacyl.COelim.pmmppmpmu	1.223e+44	8.92	8.92	3.854e+37	1.53e-05
21415	TS.triHPacyl.COelim.mtppmtmpu	1.871e+44	9.19	9.19	3.752e+37	1.49e-05
21416	TS.triHPacyl.COelim.tpmmtpppu	2.485e+44	9.37	9.37	3.742e+37	1.49e-05
21417	TS.triHPacyl.COelim.pptpmtppu	4.359e+44	9.70	9.70	3.740e+37	1.49e-05
21418	TS.triHPacyl.COelim.tmmppmmmu	3.337e+44	9.54	9.54	3.737e+37	1.49e-05
21419	TS.triHPacyl.COelim.mtppmpppu	5.255e+43	8.44	8.44	3.731e+37	1.48e-05
21420	TS.triHPacyl.COelim.ppptmmmmu	6.735e+44	9.97	9.97	3.699e+37	1.47e-05
21421	TS.triHPacyl.COelim.tmtptmpu	3.819e+45	11.00	11.00	3.696e+37	1.47e-05
21422	TS.triHPacyl.COelim.pptmmmmmpu	4.319e+44	9.70	9.70	3.689e+37	1.47e-05
21423	TS.triHPacyl.COelim.mttmtppmu	2.396e+45	10.73	10.73	3.684e+37	1.46e-05
21424	TS.triHPacyl.COelim.ppmmtpppu	1.670e+44	9.14	9.14	3.676e+37	1.46e-05
21425	TS.triHPacyl.COelim.pptmtmmmu	6.393e+44	9.94	9.94	3.671e+37	1.46e-05
21426	TS.triHPacyl.COelim.tmpptmpu	1.526e+44	9.09	9.09	3.668e+37	1.46e-05
21427	TS.triHPacyl.COelim.pmptpmtmpu	8.091e+44	10.08	10.08	3.665e+37	1.46e-05
21428	TS.triHPacyl.COelim.mppmmppmu	1.325e+44	9.00	9.00	3.659e+37	1.46e-05
21429	TS.triHPacyl.COelim.tpmtpppmu	9.276e+44	10.16	10.16	3.656e+37	1.45e-05
21430	TS.triHPacyl.COelim.mtppmmppmu	3.512e+44	9.59	9.59	3.639e+37	1.45e-05
21431	TS.triHPacyl.COelim.mttptppmu	5.083e+44	9.81	9.81	3.637e+37	1.45e-05

21432	TS.triHPacyl.COelim.pmppttmpu	3.603e+44	9.61	9.61	3.606e+37	1.43e-05
21433	TS.triHPacyl.COelim.mtttmmpmpu	9.681e+44	10.21	10.21	3.525e+37	1.4e-05
21434	TS.triHPacyl.COelim.ttptmmtmmu	2.734e+45	10.84	10.84	3.494e+37	1.39e-05
21435	TS.triHPacyl.COelim.mptmppppu	3.672e+44	9.64	9.64	3.467e+37	1.38e-05
21436	TS.triHPacyl.COelim.ttttpttpmu	5.364e+45	11.25	11.25	3.438e+37	1.37e-05
21437	TS.triHPacyl.COelim.ptmpmpppmu	4.349e+44	9.76	9.76	3.404e+37	1.35e-05
21438	TS.triHPacyl.COelim.pmmtppmmpu	4.248e+44	9.75	9.75	3.362e+37	1.34e-05
21439	TS.triHPacyl.COelim.mmttmppppu	5.473e+44	9.90	9.90	3.340e+37	1.33e-05
21440	TS.triHPacyl.COelim.mpptmtmpu	7.813e+44	10.12	10.12	3.322e+37	1.32e-05
21441	TS.triHPacyl.COelim.mtptppmmpu	5.170e+44	9.88	9.88	3.299e+37	1.31e-05
21442	TS.triHPacyl.COelim.mmmmtmmpu	1.681e+46	11.95	11.95	3.290e+37	1.31e-05
21443	TS.triHPacyl.COelim.mtmtppmmpu	6.465e+44	10.01	10.01	3.276e+37	1.3e-05
21444	TS.triHPacyl.COelim.mtmtptmpu	2.267e+45	10.76	10.76	3.266e+37	1.3e-05
21445	TS.triHPacyl.COelim.pptmptmpu	7.168e+44	10.08	10.08	3.236e+37	1.29e-05
21446	TS.triHPacyl.COelim.mtptmmpmpu	3.662e+44	9.68	9.68	3.227e+37	1.28e-05
21447	TS.triHPacyl.COelim.mptmppppu	7.021e+44	10.07	10.07	3.221e+37	1.28e-05
21448	TS.triHPacyl.COelim.tpmtmmpppu	2.666e+44	9.50	9.50	3.180e+37	1.26e-05
21449	TS.triHPacyl.COelim.pptmtpmpu	6.719e+44	10.06	10.06	3.156e+37	1.26e-05
21450	TS.triHPacyl.COelim.mtppmptmpu	1.891e+44	9.31	9.31	3.121e+37	1.24e-05
21451	TS.triHPacyl.COelim.mmpmmtppu	3.437e+44	9.68	9.68	3.068e+37	1.22e-05
21452	TS.triHPacyl.COelim.ttmppmmpu	1.032e+44	8.96	8.96	3.065e+37	1.22e-05
21453	TS.triHPacyl.COelim.pmmtppmpu	7.808e+44	10.17	10.17	3.051e+37	1.21e-05
21454	TS.triHPacyl.COelim.ptmppmtmmu	1.562e+44	9.21	9.21	3.034e+37	1.21e-05
21455	TS.triHPacyl.COelim.mtmtmmpmpu	4.783e+44	9.89	9.89	3.001e+37	1.19e-05
21456	TS.triHPacyl.COelim.ppptmmtmpu	1.636e+45	10.62	10.62	2.998e+37	1.19e-05
21457	TS.triHPacyl.COelim.mtppmptmpu	3.850e+44	9.76	9.76	2.986e+37	1.19e-05
21458	TS.triHPacyl.COelim.ppmptppmu	6.619e+43	8.71	8.71	2.979e+37	1.18e-05
21459	TS.triHPacyl.COelim.mptmmtmmu	2.610e+45	10.91	10.91	2.943e+37	1.17e-05
21460	TS.triHPacyl.COelim.pmptmmpmpu	8.317e+44	10.23	10.23	2.931e+37	1.17e-05
21461	TS.triHPacyl.COelim.mmtmmpmpu	1.496e+45	10.59	10.59	2.910e+37	1.16e-05
21462	TS.triHPacyl.COelim.mptmmtppu	7.234e+44	10.15	10.15	2.895e+37	1.15e-05
21463	TS.triHPacyl.COelim.ttmtpptpu	1.957e+45	10.75	10.75	2.877e+37	1.14e-05
21464	TS.triHPacyl.COelim.tttptmpu	8.097e+45	11.61	11.61	2.831e+37	1.13e-05
21465	TS.triHPacyl.COelim.mpmmtmmpu	1.089e+45	10.42	10.42	2.806e+37	1.12e-05
21466	TS.triHPacyl.COelim.ttmpptpu	4.189e+44	9.85	9.85	2.798e+37	1.11e-05
21467	TS.triHPacyl.COelim.ttmppmtpu	2.435e+44	9.54	9.54	2.756e+37	1.1e-05
21468	TS.triHPacyl.COelim.mptpmtmpu	3.793e+44	9.80	9.80	2.744e+37	1.09e-05
21469	TS.triHPacyl.COelim.pptmmtmpu	2.045e+45	10.81	10.81	2.718e+37	1.08e-05
21470	TS.triHPacyl.COelim.mptpmpmpu	8.549e+44	10.31	10.31	2.656e+37	1.06e-05
21471	TS.triHPacyl.COelim.mtmptmpmu	3.757e+44	9.82	9.82	2.655e+37	1.06e-05
21472	TS.triHPacyl.COelim.tpmmmtmmpu	1.926e+44	9.42	9.42	2.645e+37	1.05e-05
21473	TS.triHPacyl.COelim.mptpmtppu	1.089e+45	10.46	10.46	2.620e+37	1.04e-05
21474	TS.triHPacyl.COelim.ppptmmpmpu	8.665e+44	10.32	10.32	2.619e+37	1.04e-05
21475	TS.triHPacyl.COelim.mmpmmtmmpu	1.890e+44	9.42	9.42	2.601e+37	1.03e-05
21476	TS.triHPacyl.COelim.pmpmmpmpu	1.656e+44	9.34	9.34	2.589e+37	1.03e-05
21477	TS.triHPacyl.COelim.ttptmmtmmpu	2.301e+45	10.92	10.92	2.535e+37	1.01e-05
21478	TS.triHPacyl.COelim.ttmppmmpu	1.852e+44	9.42	9.42	2.530e+37	1.01e-05
21479	TS.triHPacyl.COelim.mtmtmpmpmu	1.158e+45	10.52	10.52	2.529e+37	1.01e-05
21480	TS.triHPacyl.COelim.pmmmppppu	4.062e+43	8.53	8.53	2.494e+37	9.92e-06
21481	TS.triHPacyl.COelim.mttmmpmpu	1.277e+45	10.59	10.59	2.448e+37	9.73e-06
21482	TS.triHPacyl.COelim.tmtpppppu	1.609e+45	10.74	10.74	2.432e+37	9.67e-06
21483	TS.triHPacyl.COelim.ttmppmtmpu	3.417e+44	9.82	9.82	2.417e+37	9.61e-06
21484	TS.triHPacyl.COelim.pmtmptmpu	9.508e+44	10.43	10.43	2.412e+37	9.59e-06
21485	TS.triHPacyl.COelim.ttptmmpmpu	4.604e+45	11.37	11.37	2.412e+37	9.59e-06
21486	TS.triHPacyl.COelim.mtptmtpu	1.071e+45	10.50	10.50	2.399e+37	9.54e-06
21487	TS.triHPacyl.COelim.ttmmpmmpu	2.182e+44	9.55	9.55	2.396e+37	9.53e-06
21488	TS.triHPacyl.COelim.tmpmmtmpu	1.713e+44	9.41	9.41	2.395e+37	9.52e-06
21489	TS.triHPacyl.COelim.mptmtpmpu	1.114e+45	10.53	10.53	2.387e+37	9.49e-06
21490	TS.triHPacyl.COelim.pmtmmpmpu	6.080e+44	10.18	10.18	2.351e+37	9.35e-06
21491	TS.triHPacyl.COelim.mptmptmmpu	5.424e+44	10.11	10.11	2.348e+37	9.34e-06
21492	TS.triHPacyl.COelim.ppmtpptppu	1.007e+45	10.48	10.48	2.344e+37	9.32e-06
21493	TS.triHPacyl.COelim.ttmppmmpu	3.569e+44	9.86	9.86	2.332e+37	9.27e-06
21494	TS.triHPacyl.COelim.mmpmmtppu	3.100e+44	9.78	9.78	2.326e+37	9.25e-06
21495	TS.triHPacyl.COelim.mtmtppmmpu	5.959e+44	10.18	10.18	2.288e+37	9.1e-06
21496	TS.triHPacyl.COelim.mptmtpppu	6.889e+44	10.27	10.27	2.273e+37	9.04e-06
21497	TS.triHPacyl.COelim.pptmmtmmpu	4.960e+44	10.08	10.08	2.249e+37	8.94e-06
21498	TS.triHPacyl.COelim.mtmtppmpu	3.330e+44	9.84	9.84	2.245e+37	8.93e-06
21499	TS.triHPacyl.COelim.tpmpmmpu	4.710e+44	10.05	10.05	2.244e+37	8.92e-06
21500	TS.triHPacyl.COelim.tmtptppu	2.664e+45	11.08	11.08	2.244e+37	8.92e-06
21501	TS.triHPacyl.COelim.tmtptmpu	1.697e+45	10.82	10.82	2.216e+37	8.81e-06
21502	TS.triHPacyl.COelim.mptmtpmpu	3.277e+45	11.22	11.22	2.212e+37	8.79e-06
21503	TS.triHPacyl.COelim.pptmmtmmpu	5.455e+44	10.15	10.15	2.198e+37	8.74e-06

21504	TS.triHPacyl.COelim.mttmpmtpmu	1.909e+45	10.90	10.90	2.182e+37	8.68e-06
21505	TS.triHPacyl.COelim.mptpmtpppu	3.655e+44	9.92	9.92	2.167e+37	8.62e-06
21506	TS.triHPacyl.COelim.pptmmmmmu	7.325e+44	10.34	10.34	2.157e+37	8.58e-06
21507	TS.triHPacyl.COelim.pptmtmmpu	8.219e+44	10.41	10.41	2.149e+37	8.55e-06
21508	TS.triHPacyl.COelim.tmpmmtmpmu	1.761e+44	9.49	9.49	2.145e+37	8.53e-06
21509	TS.triHPacyl.COelim.pmtppptpmu	2.209e+44	9.63	9.63	2.130e+37	8.47e-06
21510	TS.triHPacyl.COelim.mtptpptpmu	1.126e+45	10.61	10.61	2.116e+37	8.41e-06
21511	TS.triHPacyl.COelim.mmptmpmmmu	5.384e+45	11.54	11.54	2.104e+37	8.37e-06
21512	TS.triHPacyl.COelim.ppmpmpmpmu	2.157e+43	8.25	8.25	2.100e+37	8.35e-06
21513	TS.triHPacyl.COelim.mtptpmtmu	7.289e+44	10.36	10.36	2.077e+37	8.26e-06
21514	TS.triHPacyl.COelim.ttmpmpmmu	1.003e+44	9.18	9.18	2.077e+37	8.26e-06
21515	TS.triHPacyl.COelim.ppmpptmpu	2.990e+44	9.83	9.83	2.067e+37	8.22e-06
21516	TS.triHPacyl.COelim.mptppmmmpu	3.870e+44	9.99	9.99	2.043e+37	8.12e-06
21517	TS.triHPacyl.COelim.mmtmpmmmu	5.395e+45	11.57	11.57	2.027e+37	8.06e-06
21518	TS.triHPacyl.COelim.mtptpmtpmu	6.620e+44	10.32	10.32	2.025e+37	8.05e-06
21519	TS.triHPacyl.COelim.pptmtpppu	6.004e+44	10.26	10.26	2.017e+37	8.02e-06
21520	TS.triHPacyl.COelim.mmtppmmmu	9.226e+45	11.90	11.90	1.989e+37	7.91e-06
21521	TS.triHPacyl.COelim.pptpmtpmu	7.298e+44	10.39	10.39	1.970e+37	7.83e-06
21522	TS.triHPacyl.COelim.mtppmtpmu	1.741e+44	9.54	9.54	1.963e+37	7.8e-06
21523	TS.triHPacyl.COelim.pptmtmpu	1.495e+45	10.82	10.82	1.953e+37	7.77e-06
21524	TS.triHPacyl.COelim.pmpptmpu	8.244e+44	10.48	10.48	1.902e+37	7.56e-06
21525	TS.triHPacyl.COelim.mtptpmtpmu	6.225e+44	10.33	10.33	1.863e+37	7.41e-06
21526	TS.triHPacyl.COelim.mpppmtmpu	2.128e+45	11.06	11.06	1.851e+37	7.36e-06
21527	TS.triHPacyl.COelim.pmtpmtpmu	5.460e+44	10.26	10.26	1.832e+37	7.28e-06
21528	TS.triHPacyl.COelim.tmpmmmtmu	1.739e+44	9.58	9.58	1.826e+37	7.26e-06
21529	TS.triHPacyl.COelim.mppmtmpmu	1.280e+45	10.78	10.78	1.788e+37	7.11e-06
21530	TS.triHPacyl.COelim.mptmmmpu	7.013e+44	10.42	10.42	1.788e+37	7.11e-06
21531	TS.triHPacyl.COelim.pmmmpmtpmu	7.894e+43	9.12	9.12	1.779e+37	7.07e-06
21532	TS.triHPacyl.COelim.mpptmmtmpu	5.249e+44	10.26	10.26	1.754e+37	6.97e-06
21533	TS.triHPacyl.COelim.mmtmpmpmu	1.259e+44	9.43	9.43	1.699e+37	6.76e-06
21534	TS.triHPacyl.COelim.tmtptmpu	6.219e+44	10.39	10.39	1.687e+37	6.71e-06
21535	TS.triHPacyl.COelim.mmpmtmpu	2.995e+45	11.33	11.33	1.671e+37	6.64e-06
21536	TS.triHPacyl.COelim.mmtmpmpmu	7.203e+44	10.49	10.49	1.648e+37	6.55e-06
21537	TS.triHPacyl.COelim.tmpmmmmmpu	1.716e+44	9.63	9.63	1.644e+37	6.54e-06
21538	TS.triHPacyl.COelim.mmmmmmmmpu	5.713e+45	11.73	11.73	1.629e+37	6.48e-06
21539	TS.triHPacyl.COelim.mpppmtmpu	1.263e+44	9.47	9.47	1.599e+37	6.36e-06
21540	TS.triHPacyl.COelim.pmtppmpu	1.956e+44	9.73	9.73	1.599e+37	6.36e-06
21541	TS.triHPacyl.COelim.mpptmtmpu	5.884e+44	10.40	10.40	1.574e+37	6.26e-06
21542	TS.triHPacyl.COelim.mptmtpppu	1.472e+46	12.32	12.32	1.571e+37	6.25e-06
21543	TS.triHPacyl.COelim.tmpmmmmmmu	1.895e+44	9.73	9.73	1.555e+37	6.18e-06
21544	TS.triHPacyl.COelim.mptpmmmmu	5.509e+44	10.36	10.36	1.552e+37	6.17e-06
21545	TS.triHPacyl.COelim.mmtppppmu	3.129e+45	11.41	11.41	1.531e+37	6.09e-06
21546	TS.triHPacyl.COelim.ttmpmmpmu	1.578e+44	9.63	9.63	1.516e+37	6.03e-06
21547	TS.triHPacyl.COelim.mmtmtmpmu	6.390e+45	11.84	11.84	1.514e+37	6.02e-06
21548	TS.triHPacyl.COelim.mpmtppppu	2.137e+44	9.83	9.83	1.467e+37	5.83e-06
21549	TS.triHPacyl.COelim.pptpmmmpu	9.021e+44	10.69	10.69	1.467e+37	5.83e-06
21550	TS.triHPacyl.COelim.mpptpmtpmu	5.039e+44	10.35	10.35	1.456e+37	5.79e-06
21551	TS.triHPacyl.COelim.mmtmpmpmu	3.803e+45	11.56	11.56	1.437e+37	5.72e-06
21552	TS.triHPacyl.COelim.mtmtppmpu	4.182e+44	10.25	10.25	1.436e+37	5.71e-06
21553	TS.triHPacyl.COelim.tpmmmmmmmu	2.130e+44	9.84	9.84	1.434e+37	5.7e-06
21554	TS.triHPacyl.COelim.tmpptpppu	1.287e+44	9.55	9.55	1.433e+37	5.7e-06
21555	TS.triHPacyl.COelim.mptpmtpmu	1.070e+45	10.81	10.81	1.426e+37	5.67e-06
21556	TS.triHPacyl.COelim.mpptpmtpmu	6.136e+44	10.48	10.48	1.418e+37	5.64e-06
21557	TS.triHPacyl.COelim.pmtmtmpmu	2.567e+44	9.98	9.98	1.369e+37	5.44e-06
21558	TS.triHPacyl.COelim.mtmtppmpmu	1.691e+45	11.11	11.11	1.358e+37	5.4e-06
21559	TS.triHPacyl.COelim.mtmtppmpmu	1.386e+45	11.00	11.00	1.346e+37	5.35e-06
21560	TS.triHPacyl.COelim.mpppmtmpu	2.452e+45	11.34	11.34	1.345e+37	5.35e-06
21561	TS.triHPacyl.COelim.mpppppppu	2.568e+45	11.37	11.37	1.343e+37	5.34e-06
21562	TS.triHPacyl.COelim.mptptmpu	6.884e+44	10.59	10.59	1.333e+37	5.3e-06
21563	TS.triHPacyl.COelim.pptmmmmmmu	5.457e+44	10.46	10.46	1.319e+37	5.24e-06
21564	TS.triHPacyl.COelim.mptptmmpu	4.337e+44	10.32	10.32	1.316e+37	5.23e-06
21565	TS.triHPacyl.COelim.pptmmmmmpu	6.137e+44	10.53	10.53	1.310e+37	5.21e-06
21566	TS.triHPacyl.COelim.mmmmpmmmmmu	3.295e+44	10.16	10.16	1.307e+37	5.2e-06
21567	TS.triHPacyl.COelim.tppmpmmmu	2.135e+44	9.90	9.90	1.302e+37	5.18e-06
21568	TS.triHPacyl.COelim.mtttppmpu	6.864e+44	10.60	10.60	1.291e+37	5.14e-06
21569	TS.triHPacyl.COelim.tpmtpmtpmu	3.301e+45	11.54	11.54	1.284e+37	5.1e-06
21570	TS.triHPacyl.COelim.mpptpmmmmu	6.177e+44	10.55	10.55	1.265e+37	5.03e-06
21571	TS.triHPacyl.COelim.mptpmtpmu	8.727e+44	10.77	10.77	1.250e+37	4.97e-06
21572	TS.triHPacyl.COelim.mtmtppmpu	1.769e+45	11.19	11.19	1.245e+37	4.95e-06
21573	TS.triHPacyl.COelim.pptmmmmmpu	9.605e+44	10.83	10.83	1.238e+37	4.92e-06
21574	TS.triHPacyl.COelim.mtppmmpmu	7.606e+44	10.70	10.70	1.229e+37	4.89e-06
21575	TS.triHPacyl.COelim.mppmpmmmmmu	9.523e+43	9.48	9.48	1.191e+37	4.74e-06

21576	TS.triHPacyl.COelim.mmpmmtppu	2.052e+45	11.31	11.31	1.183e+37	4.7e-06
21577	TS.triHPacyl.COelim.mppmpppmu	3.130e+43	8.82	8.82	1.181e+37	4.7e-06
21578	TS.triHPacyl.COelim.ptmpmtmmu	2.573e+44	10.07	10.07	1.181e+37	4.7e-06
21579	TS.triHPacyl.COelim.mmpmtmmpu	7.799e+43	9.36	9.36	1.179e+37	4.69e-06
21580	TS.triHPacyl.COelim.mmpmpmpmmu	9.141e+43	9.46	9.46	1.169e+37	4.65e-06
21581	TS.triHPacyl.COelim.mptmtmmu	1.511e+45	11.14	11.14	1.168e+37	4.64e-06
21582	TS.triHPacyl.COelim.pmmppmtmpu	4.430e+43	9.04	9.04	1.150e+37	4.57e-06
21583	TS.triHPacyl.COelim.pmpmpmpmmu	3.037e+44	10.19	10.19	1.148e+37	4.56e-06
21584	TS.triHPacyl.COelim.mttmptpmu	1.211e+45	11.02	11.02	1.141e+37	4.54e-06
21585	TS.triHPacyl.COelim.mmtmptpmu	2.559e+45	11.47	11.47	1.131e+37	4.5e-06
21586	TS.triHPacyl.COelim.mtmmpptpmu	1.085e+45	10.96	10.96	1.130e+37	4.49e-06
21587	TS.triHPacyl.COelim.mpptmtppu	3.948e+44	10.36	10.36	1.129e+37	4.49e-06
21588	TS.triHPacyl.COelim.pmpmpmpu	6.755e+44	10.68	10.68	1.116e+37	4.44e-06
21589	TS.triHPacyl.COelim.tmtppptpu	6.733e+45	12.05	12.05	1.114e+37	4.43e-06
21590	TS.triHPacyl.COelim.tttppmmpu	1.276e+45	11.26	11.26	1.110e+37	4.41e-06
21591	TS.triHPacyl.COelim.ttptmnmmpu	2.237e+45	11.41	11.41	1.097e+37	4.36e-06
21592	TS.triHPacyl.COelim.pmpmtmmpu	2.881e+44	10.19	10.19	1.095e+37	4.35e-06
21593	TS.triHPacyl.COelim.pptmptppu	8.340e+44	10.82	10.82	1.095e+37	4.35e-06
21594	TS.triHPacyl.COelim.pmtppmpmpu	2.175e+44	10.03	10.03	1.069e+37	4.25e-06
21595	TS.triHPacyl.COelim.mptmtmpmu	5.969e+44	10.63	10.63	1.068e+37	4.25e-06
21596	TS.triHPacyl.COelim.pmmtmpmmu	4.368e+43	9.10	9.10	1.030e+37	4.1e-06
21597	TS.triHPacyl.COelim.pmpptpppu	1.059e+44	9.64	9.64	1.007e+37	4.01e-06
21598	TS.triHPacyl.COelim.pmmppmpmpu	1.673e+43	8.55	8.55	9.959e+36	3.96e-06
21599	TS.triHPacyl.COelim.mmmmmmtmpu	2.667e+45	11.59	11.59	9.686e+36	3.85e-06
21600	TS.triHPacyl.COelim.pmpptppu	4.513e+44	10.54	10.54	9.535e+36	3.79e-06
21601	TS.triHPacyl.COelim.mpptmtmmu	4.407e+44	10.52	10.52	9.501e+36	3.78e-06
21602	TS.triHPacyl.COelim.tpmptppu	3.142e+44	10.34	10.34	9.279e+36	3.69e-06
21603	TS.triHPacyl.COelim.pmmtmpmpu	2.912e+44	10.30	10.30	9.083e+36	3.61e-06
21604	TS.triHPacyl.COelim.mmpmtppmu	1.004e+46	12.42	12.42	8.998e+36	3.58e-06
21605	TS.triHPacyl.COelim.tmpmmtmmu	2.906e+44	10.31	10.31	8.950e+36	3.56e-06
21606	TS.triHPacyl.COelim.mmmmmmmmpu	3.509e+45	11.80	11.80	8.930e+36	3.55e-06
21607	TS.triHPacyl.COelim.mpmmtmmu	7.074e+43	9.47	9.47	8.880e+36	3.53e-06
21608	TS.triHPacyl.COelim.ppmmtmmu	3.804e+44	10.49	10.49	8.749e+36	3.48e-06
21609	TS.triHPacyl.COelim.ptmmpmpmmu	4.318e+44	10.57	10.57	8.652e+36	3.44e-06
21610	TS.triHPacyl.COelim.mptmmtmmu	3.600e+45	11.83	11.83	8.637e+36	3.43e-06
21611	TS.triHPacyl.COelim.mttppmtppu	1.778e+45	11.43	11.43	8.345e+36	3.32e-06
21612	TS.triHPacyl.COelim.pmtppptpmu	6.429e+44	10.84	10.84	8.108e+36	3.22e-06
21613	TS.triHPacyl.COelim.mttmmpmpu	9.020e+44	11.05	11.05	8.026e+36	3.19e-06
21614	TS.triHPacyl.COelim.mpptmnmmpu	4.725e+44	10.67	10.67	8.020e+36	3.19e-06
21615	TS.triHPacyl.COelim.pmmtmnmmpu	2.130e+44	10.19	10.19	7.984e+36	3.17e-06
21616	TS.triHPacyl.COelim.mmpmpmpmpu	9.503e+44	11.09	11.09	7.981e+36	3.17e-06
21617	TS.triHPacyl.COelim.ppmmtmmmpu	5.107e+44	10.72	10.72	7.974e+36	3.17e-06
21618	TS.triHPacyl.COelim.mpttpmnmmpu	5.864e+44	10.81	10.81	7.813e+36	3.11e-06
21619	TS.triHPacyl.COelim.mmtmptppu	5.027e+45	12.10	12.10	7.765e+36	3.09e-06
21620	TS.triHPacyl.COelim.mtmptmpmu	2.352e+45	11.65	11.65	7.697e+36	3.06e-06
21621	TS.triHPacyl.COelim.mpmptpppu	2.032e+44	10.20	10.20	7.605e+36	3.02e-06
21622	TS.triHPacyl.COelim.mtmppptmpu	4.940e+44	10.74	10.74	7.401e+36	2.94e-06
21623	TS.triHPacyl.COelim.mmtmmtppu	5.660e+45	12.21	12.21	7.246e+36	2.88e-06
21624	TS.triHPacyl.COelim.mptmptppu	4.835e+44	10.74	10.74	7.231e+36	2.88e-06
21625	TS.triHPacyl.COelim.ppmptpppu	3.192e+44	10.51	10.51	7.097e+36	2.82e-06
21626	TS.triHPacyl.COelim.mtmmtmpmu	2.894e+44	10.45	10.45	7.064e+36	2.81e-06
21627	TS.triHPacyl.COelim.pmmtppmpmu	6.852e+43	9.59	9.59	7.041e+36	2.8e-06
21628	TS.triHPacyl.COelim.ppmmtmmmpu	4.568e+44	10.73	10.73	6.979e+36	2.78e-06
21629	TS.triHPacyl.COelim.mptmmtmmu	7.765e+44	11.05	11.05	6.885e+36	2.74e-06
21630	TS.triHPacyl.COelim.pmtmpmtmmu	4.768e+44	10.77	10.77	6.814e+36	2.71e-06
21631	TS.triHPacyl.COelim.mmpmtppmu	7.621e+43	9.69	9.69	6.608e+36	2.63e-06
21632	TS.triHPacyl.COelim.mpptmtmmpu	3.599e+44	10.62	10.62	6.592e+36	2.62e-06
21633	TS.triHPacyl.COelim.mttmptppu	1.028e+45	11.25	11.25	6.567e+36	2.61e-06
21634	TS.triHPacyl.COelim.mmmmtmmmpu	1.110e+46	12.67	12.67	6.496e+36	2.58e-06
21635	TS.triHPacyl.COelim.mtmppmnmmpu	1.105e+44	9.93	9.93	6.465e+36	2.57e-06
21636	TS.triHPacyl.COelim.mmmmtmtpu	4.545e+45	12.15	12.15	6.438e+36	2.56e-06
21637	TS.triHPacyl.COelim.mpptmtmmu	4.700e+45	12.17	12.17	6.434e+36	2.56e-06
21638	TS.triHPacyl.COelim.mtptmnmmpu	1.596e+45	11.53	11.53	6.332e+36	2.52e-06
21639	TS.triHPacyl.COelim.tmmtppmpmu	3.703e+44	10.66	10.66	6.317e+36	2.51e-06
21640	TS.triHPacyl.COelim.mttmptpmu	2.204e+45	11.73	11.73	6.287e+36	2.5e-06
21641	TS.triHPacyl.COelim.mmtmptppu	1.334e+45	11.43	11.43	6.251e+36	2.49e-06
21642	TS.triHPacyl.COelim.mpttpptpmu	1.179e+45	11.36	11.36	6.209e+36	2.47e-06
21643	TS.triHPacyl.COelim.mmpmnmmpu	2.838e+45	11.89	11.89	6.202e+36	2.47e-06
21644	TS.triHPacyl.COelim.mptmmpnmmpu	2.817e+45	11.89	11.89	6.094e+36	2.42e-06
21645	TS.triHPacyl.COelim.ppmmpmpmpu	5.321e+43	9.53	9.53	6.071e+36	2.41e-06
21646	TS.triHPacyl.COelim.tpmmpptpmu	1.054e+45	11.32	11.32	5.963e+36	2.37e-06
21647	TS.triHPacyl.COelim.pmpmpmtmpu	1.141e+45	11.39	11.39	5.792e+36	2.3e-06

21648	TS.triHPacyl.COelim.mpttmmmpmu	6.109e+44	11.02	11.02	5.698e+36	2.27e-06
21649	TS.triHPacyl.COelim.mpmtmtppmu	1.843e+44	10.32	10.32	5.625e+36	2.24e-06
21650	TS.triHPacyl.COelim.pmtppmmpmu	1.332e+44	10.15	10.15	5.332e+36	2.12e-06
21651	TS.triHPacyl.COelim.mmmmtmmmpmu	8.620e+45	12.66	12.66	5.198e+36	2.07e-06
21652	TS.triHPacyl.COelim.mmmmpmmpmu	4.851e+44	10.98	10.98	4.879e+36	1.94e-06
21653	TS.triHPacyl.COelim.mttptmpmu	5.308e+44	11.03	11.03	4.863e+36	1.93e-06
21654	TS.triHPacyl.COelim.pmtppptmu	2.387e+44	10.56	10.56	4.807e+36	1.91e-06
21655	TS.triHPacyl.COelim.mppmtmmpmu	1.845e+44	10.42	10.42	4.750e+36	1.89e-06
21656	TS.triHPacyl.COelim.pmpptmmpmu	1.691e+44	10.37	10.37	4.710e+36	1.87e-06
21657	TS.triHPacyl.COelim.mtttppptmu	2.555e+45	12.01	12.01	4.523e+36	1.8e-06
21658	TS.triHPacyl.COelim.pmptmtmmpmu	1.379e+44	10.28	10.28	4.443e+36	1.77e-06
21659	TS.triHPacyl.COelim.tpmmpmmpmu	1.050e+44	10.13	10.13	4.360e+36	1.73e-06
21660	TS.triHPacyl.COelim.pmpptmmpmu	4.592e+44	11.02	11.02	4.305e+36	1.71e-06
21661	TS.triHPacyl.COelim.mpmtmmpmu	1.153e+45	11.59	11.59	4.191e+36	1.67e-06
21662	TS.triHPacyl.COelim.mpmmtmmpmu	1.574e+44	10.40	10.40	4.185e+36	1.66e-06
21663	TS.triHPacyl.COelim.mppmptmmpmu	1.546e+45	11.77	11.77	4.144e+36	1.65e-06
21664	TS.triHPacyl.COelim.mmmmtmtpmu	3.793e+45	12.30	12.30	4.143e+36	1.65e-06
21665	TS.triHPacyl.COelim.mmpmtmmpmu	5.153e+45	12.49	12.49	4.131e+36	1.64e-06
21666	TS.triHPacyl.COelim.ppmptmmpmu	3.584e+44	10.90	10.90	4.096e+36	1.63e-06
21667	TS.triHPacyl.COelim.mpmptmmpmu	2.232e+44	10.62	10.62	4.061e+36	1.61e-06
21668	TS.triHPacyl.COelim.mtppmptmu	1.550e+45	11.79	11.79	4.012e+36	1.6e-06
21669	TS.triHPacyl.COelim.mmmmpmmpmu	1.869e+44	10.53	10.53	3.988e+36	1.59e-06
21670	TS.triHPacyl.COelim.mmmmmtpmu	6.844e+44	11.30	11.30	3.984e+36	1.58e-06
21671	TS.triHPacyl.COelim.mppmptmmpmu	1.711e+45	11.85	11.85	3.960e+36	1.57e-06
21672	TS.triHPacyl.COelim.pmtmtmmpmu	2.634e+44	10.75	10.75	3.863e+36	1.54e-06
21673	TS.triHPacyl.COelim.pmmmpmmpmu	2.234e+44	10.66	10.66	3.836e+36	1.53e-06
21674	TS.triHPacyl.COelim.ppmptmmpmu	4.261e+44	11.06	11.06	3.766e+36	1.5e-06
21675	TS.triHPacyl.COelim.mtmtpptmu	2.103e+45	12.02	12.02	3.709e+36	1.47e-06
21676	TS.triHPacyl.COelim.mmtmtpmu	4.869e+45	12.59	12.59	3.297e+36	1.31e-06
21677	TS.triHPacyl.COelim.tpmtpmmpmu	2.062e+45	12.08	12.08	3.276e+36	1.3e-06
21678	TS.triHPacyl.COelim.mtppmtpmu	1.084e+45	11.70	11.70	3.272e+36	1.3e-06
21679	TS.triHPacyl.COelim.tpmppmmpmu	2.428e+44	10.82	10.82	3.169e+36	1.26e-06
21680	TS.triHPacyl.COelim.mmpmtmmpmu	6.599e+45	12.81	12.81	3.099e+36	1.23e-06
21681	TS.triHPacyl.COelim.mpmmtmmpmu	1.484e+44	10.55	10.55	3.073e+36	1.22e-06
21682	TS.triHPacyl.COelim.tmmmpmmpmu	3.496e+44	11.06	11.06	3.061e+36	1.22e-06
21683	TS.triHPacyl.COelim.mtmppmmpmu	8.016e+43	10.19	10.19	3.041e+36	1.21e-06
21684	TS.triHPacyl.COelim.mptmmpmmpmu	4.517e+44	11.23	11.23	2.956e+36	1.18e-06
21685	TS.triHPacyl.COelim.mttpttppmu	9.083e+44	11.67	11.67	2.852e+36	1.13e-06
21686	TS.triHPacyl.COelim.mppmmpmmpmu	3.373e+45	12.46	12.46	2.839e+36	1.13e-06
21687	TS.triHPacyl.COelim.tppmptmmpmu	2.791e+44	10.99	10.99	2.742e+36	1.09e-06
21688	TS.triHPacyl.COelim.mmmmtmmpmu	1.223e+45	11.88	11.88	2.729e+36	1.09e-06
21689	TS.triHPacyl.COelim.mtttppptmu	2.825e+45	12.39	12.39	2.652e+36	1.05e-06
21690	TS.triHPacyl.COelim.mmmmmtpmu	1.177e+45	11.88	11.88	2.630e+36	1.05e-06
21691	TS.triHPacyl.COelim.mpmptmmpmu	5.086e+44	11.44	11.44	2.350e+36	9.34e-07
21692	TS.triHPacyl.COelim.ppmptmmpmu	5.431e+44	11.51	11.51	2.221e+36	8.83e-07
21693	TS.triHPacyl.COelim.tmmtpmmpmu	5.705e+45	12.93	12.93	2.155e+36	8.57e-07
21694	TS.triHPacyl.COelim.mpttmtppmu	4.936e+45	12.85	12.85	2.154e+36	8.56e-07
21695	TS.triHPacyl.COelim.pmttmtppmu	4.248e+45	12.76	12.76	2.144e+36	8.53e-07
21696	TS.triHPacyl.COelim.ppmptmmpmu	1.520e+44	10.78	10.78	2.129e+36	8.46e-07
21697	TS.triHPacyl.COelim.pmpptmmpmu	1.084e+45	11.96	11.96	2.107e+36	8.38e-07
21698	TS.triHPacyl.COelim.mptmmpmmpmu	4.010e+45	12.74	12.74	2.085e+36	8.29e-07
21699	TS.triHPacyl.COelim.pmttmtppmu	1.008e+46	13.30	13.30	2.076e+36	8.26e-07
21700	TS.triHPacyl.COelim.mmtmtpmu	5.045e+45	12.89	12.89	2.061e+36	8.19e-07
21701	TS.triHPacyl.COelim.mtmppmtpmu	3.126e+44	11.24	11.24	2.043e+36	8.12e-07
21702	TS.triHPacyl.COelim.mmmmpmtpmu	2.981e+45	12.59	12.59	2.017e+36	8.02e-07
21703	TS.triHPacyl.COelim.tpmppmmpmu	1.002e+44	10.57	10.57	1.985e+36	7.89e-07
21704	TS.triHPacyl.COelim.mtmppmtpmu	1.909e+44	10.96	10.96	1.984e+36	7.89e-07
21705	TS.triHPacyl.COelim.mtmmpmtpmu	2.438e+44	11.10	11.10	1.984e+36	7.89e-07
21706	TS.triHPacyl.COelim.pmpmmpmmpmu	8.630e+44	11.86	11.86	1.983e+36	7.88e-07
21707	TS.triHPacyl.COelim.pmpptmmpmu	1.275e+45	12.12	12.12	1.884e+36	7.49e-07
21708	TS.triHPacyl.COelim.mmmmtmmpmu	9.886e+44	11.97	11.97	1.882e+36	7.48e-07
21709	TS.triHPacyl.COelim.pmpptmmpmu	2.591e+45	12.59	12.59	1.736e+36	6.9e-07
21710	TS.triHPacyl.COelim.mtmmpmmpmu	1.545e+44	10.91	10.91	1.730e+36	6.88e-07
21711	TS.triHPacyl.COelim.tpmppmmpmu	6.578e+43	10.48	10.48	1.517e+36	6.03e-07
21712	TS.triHPacyl.COelim.mtmppppmmpmu	7.754e+43	10.58	10.58	1.511e+36	6.01e-07
21713	TS.triHPacyl.COelim.mtmppptppmu	3.160e+44	11.42	11.42	1.509e+36	6e-07
21714	TS.triHPacyl.COelim.ppmptmmpmu	3.452e+44	11.48	11.48	1.500e+36	5.97e-07
21715	TS.triHPacyl.COelim.mppmtpmmpmu	3.411e+44	11.50	11.50	1.434e+36	5.7e-07
21716	TS.triHPacyl.COelim.mpmptmmpmu	4.627e+44	11.69	11.69	1.411e+36	5.61e-07
21717	TS.triHPacyl.COelim.mmpmtpmmpmu	2.699e+45	12.75	12.75	1.399e+36	5.56e-07
21718	TS.triHPacyl.COelim.tmmtpmmpmu	5.020e+45	13.13	13.13	1.363e+36	5.42e-07
21719	TS.triHPacyl.COelim.mmpmtmtpmu	4.515e+45	13.14	13.14	1.201e+36	4.77e-07

21720	TS.triHPacyl.COelim.pppmpmpmpu	2.255e+44	11.39	11.39	1.136e+36	4.52e-07
21721	TS.triHPacyl.COelim.mmmmtmpmmmu	3.544e+44	11.66	11.66	1.133e+36	4.51e-07
21722	TS.triHPacyl.COelim.pppmpptpmu	3.660e+44	11.68	11.68	1.130e+36	4.49e-07
21723	TS.triHPacyl.COelim.mptmtmmmu	4.491e+45	13.23	13.23	1.030e+36	4.1e-07
21724	TS.triHPacyl.COelim.tppmpptppu	1.338e+44	11.16	11.16	9.973e+35	3.97e-07
21725	TS.triHPacyl.COelim.mptmpmmmu	4.212e+45	13.21	13.21	9.972e+35	3.97e-07
21726	TS.triHPacyl.COelim.mtptmptpmu	3.286e+45	13.07	13.07	9.938e+35	3.95e-07
21727	TS.triHPacyl.COelim.mptmtppmu	6.621e+45	13.52	13.52	9.439e+35	3.75e-07
21728	TS.triHPacyl.COelim.mtmppmtmpu	1.737e+44	11.35	11.35	9.405e+35	3.74e-07
21729	TS.triHPacyl.COelim.mtppmmtpmu	7.325e+44	12.21	12.21	9.379e+35	3.73e-07
21730	TS.triHPacyl.COelim.mtptmptpmu	1.575e+45	12.68	12.68	9.050e+35	3.6e-07
21731	TS.triHPacyl.COelim.mppmmmtmpu	2.702e+44	11.64	11.64	9.000e+35	3.58e-07
21732	TS.triHPacyl.COelim.mtmpppppmu	1.314e+44	11.25	11.25	8.420e+35	3.35e-07
21733	TS.triHPacyl.COelim.pppmmmmmpu	1.087e+44	11.14	11.14	8.396e+35	3.34e-07
21734	TS.triHPacyl.COelim.mptmtppmu	4.291e+45	13.34	13.34	8.164e+35	3.25e-07
21735	TS.triHPacyl.COelim.mtmpppppmu	1.236e+44	11.26	11.26	7.698e+35	3.06e-07
21736	TS.triHPacyl.COelim.mppmmmmmpu	5.721e+43	10.81	10.81	7.581e+35	3.01e-07
21737	TS.triHPacyl.COelim.mtptmmtmpu	1.426e+45	12.76	12.76	7.261e+35	2.89e-07
21738	TS.triHPacyl.COelim.mtptmptpmu	2.574e+45	13.11	13.11	7.020e+35	2.79e-07
21739	TS.triHPacyl.COelim.pppmpmtmpu	1.368e+44	11.39	11.39	6.956e+35	2.77e-07
21740	TS.triHPacyl.COelim.pmmppmtpu	5.620e+43	10.87	10.87	6.796e+35	2.7e-07
21741	TS.triHPacyl.COelim.mmpmtmtpmu	3.892e+45	13.42	13.42	6.498e+35	2.58e-07
21742	TS.triHPacyl.COelim.mtmppptmpu	1.585e+44	11.58	11.58	5.945e+35	2.36e-07
21743	TS.triHPacyl.COelim.tmmppmtpu	7.566e+43	11.19	11.19	5.367e+35	2.13e-07
21744	TS.triHPacyl.COelim.mtppmpmpu	5.804e+45	13.79	13.79	5.194e+35	2.07e-07
21745	TS.triHPacyl.COelim.mtppmtmpu	9.795e+45	14.18	14.18	4.556e+35	1.81e-07
21746	TS.triHPacyl.COelim.mptmpmmu	5.379e+45	13.83	13.83	4.542e+35	1.81e-07
21747	TS.triHPacyl.COelim.pppmpptppu	9.457e+43	11.42	11.42	4.530e+35	1.8e-07
21748	TS.triHPacyl.COelim.mmpmtppmu	4.347e+44	12.38	12.38	4.199e+35	1.67e-07
21749	TS.triHPacyl.COelim.mptmtmmpu	5.053e+45	13.84	13.84	4.148e+35	1.65e-07
21750	TS.triHPacyl.COelim.mmmppmmmpu	2.206e+45	13.38	13.38	3.941e+35	1.57e-07
21751	TS.triHPacyl.COelim.mmpmtmtpmu	3.472e+45	13.66	13.66	3.908e+35	1.55e-07
21752	TS.triHPacyl.COelim.mmmppmpmpu	2.477e+44	12.17	12.17	3.376e+35	1.34e-07
21753	TS.triHPacyl.COelim.mmpmtmtpmu	1.065e+45	13.13	13.13	2.922e+35	1.16e-07
21754	TS.triHPacyl.COelim.pppmpmmmu	7.747e+43	11.57	11.57	2.875e+35	1.14e-07
21755	TS.triHPacyl.COelim.mppmmpppmu	8.548e+44	13.07	13.07	2.560e+35	1.02e-07
21756	TS.triHPacyl.COelim.pmtppptppu	6.648e+44	12.99	12.99	2.287e+35	9.1e-08
21757	TS.triHPacyl.COelim.mmmppmtpu	6.717e+43	11.75	11.75	1.838e+35	7.31e-08
21758	TS.triHPacyl.COelim.mtmppptpmu	2.217e+44	12.55	12.55	1.610e+35	6.4e-08
21759	TS.triHPacyl.COelim.mptmptppu	4.797e+44	13.10	13.10	1.384e+35	5.5e-08
21760	TS.triHPacyl.COelim.pmmppmpmpu	4.490e+43	11.69	11.69	1.376e+35	5.47e-08
21761	TS.triHPacyl.COelim.mppmmtpmu	2.002e+45	14.14	14.14	1.005e+35	3.99e-08
21762	TS.triHPacyl.COelim.pmmppmmppu	3.251e+43	11.94	11.94	6.537e+34	2.6e-08
21763	TS.triHPacyl.COelim.mmpmmtpmu	1.256e+45	14.26	14.26	5.179e+34	2.06e-08
21764	TS.triHPacyl.COelim.mtptmmmmmu	1.545e+45	14.79	14.79	2.597e+34	1.03e-08
21765	TS.triHPacyl.COelim.mppmpmtpmu	5.384e+44	14.22	14.22	2.356e+34	9.37e-09
21766	TS.triHPacyl.COelim.tmmppmtpu	1.405e+44	13.45	13.45	2.240e+34	8.91e-09
21767	TS.triHPacyl.COelim.mmpmmtpmu	2.046e+44	13.88	13.88	1.580e+34	6.28e-09
21768	TS.triHPacyl.COelim.mmpmmtpmu	7.409e+44	14.78	14.78	1.275e+34	5.07e-09
21769	TS.triHPacyl.COelim.mmpmmtpmu	8.055e+44	14.85	14.85	1.216e+34	4.84e-09
21770	TS.triHPacyl.COelim.mmpmmtpmu	4.592e+44	15.07	15.07	4.823e+33	1.92e-09
21771	Total				2.515e+44	100

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21774
21775 #####
21776 M06-2X/aug-cc-pVTZ data
21777 #####

21778
21779 Only the lowest energy conformers were re-optimized at this level of theory,
21780 but enough conformers were included to account for ~80% or more of the thermal
21781 population. We provide a population contribution analysis here for this
21782 truncated population. Note that the kinetic analysis accounts for all conformers
21783 by merging the M06-2X/aug-cc-pVTZ and /cc-pVDZ data (see main text).
21784 The raw quantum chemical data is provided below.
21785 (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
21786 =====

21787
21788 Population analysis at 300K. Vibrational scaling: 0.971.
21789 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
21790 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
21791 %: contribution to the population (with current data set assumed 100%)

21792	Compound	Qtot	Erel	Erel2	n*Q*MB	%
21793						
21794	diHPCARP_I.tmmmpmtmpd	2.936e+43	0.00	0.00	2.936e+43	14
21795	diHPCARP_I.mmmmpmtmd	2.948e+43	0.02	0.02	2.860e+43	13.7
21796	diHPCARP_I.tmmmpptpd	2.520e+43	0.20	0.20	1.792e+43	8.56
21797	diHPCARP_I.tmmmptttd	4.222e+43	0.67	0.67	1.375e+43	6.56
21798	diHPCARP_I.tmmmpttmd	3.504e+43	0.73	0.73	1.034e+43	4.93
21799	diHPCARP_I.mmmmpmtmpd	2.083e+43	0.45	0.45	9.755e+42	4.66
21800	diHPCARP_I.pmmmpmtmd	3.464e+43	0.86	0.86	8.225e+42	3.93
21801	diHPCARP_I.pmtmptmmd	2.136e+43	0.73	0.73	6.280e+42	3
21802	diHPCARP_I.pmmmpmtmpd	1.816e+43	0.76	0.76	5.078e+42	2.42
21803	diHPCARP_I.tttmptmmd	2.022e+43	0.87	0.87	4.686e+42	2.24
21804	diHPCARP_I.tttptmmd	1.917e+43	0.94	0.94	3.930e+42	1.88
21805	diHPCARP_I.pmtpptmmd	1.431e+44	2.24	2.24	3.346e+42	1.6
21806	diHPCARP_I.tmtmptmmd	4.270e+43	1.58	1.58	3.038e+42	1.45
21807	diHPCARP_I.pmmmpptpd	2.234e+43	1.19	1.19	3.037e+42	1.45
21808	diHPCARP_I.pmtmmtmmd	3.599e+43	1.48	1.48	2.994e+42	1.43
21809	diHPCARP_I.tmmmttmpd	1.350e+44	2.28	2.28	2.924e+42	1.4
21810	diHPCARP_I.pmtppttpd	7.551e+43	1.96	1.96	2.815e+42	1.34
21811	diHPCARP_I.pmmmpmtmpd	1.673e+43	1.12	1.12	2.546e+42	1.22
21812	diHPCARP_I.mttmptmmd	2.388e+43	1.34	1.34	2.505e+42	1.2
21813	diHPCARP_I.mmmmpptpd	5.258e+43	1.83	1.83	2.461e+42	1.17
21814	diHPCARP_I.pmmmptttd	4.336e+43	1.72	1.72	2.403e+42	1.15
21815	diHPCARP_I.mmmmptttd	7.161e+43	2.07	2.07	2.219e+42	1.06
21816	diHPCARP_I.tmmmtmtd	1.388e+44	2.47	2.47	2.214e+42	1.06
21817	diHPCARP_I.pmtmptmmd	4.558e+43	1.83	1.83	2.133e+42	1.02
21818	diHPCARP_I.tmtptmtd	1.311e+44	2.47	2.47	2.080e+42	0.993
21819	diHPCARP_I.ttpmpttpd	1.380e+43	1.17	1.17	1.926e+42	0.919
21820	diHPCARP_I.mttptmmd	2.370e+43	1.52	1.52	1.836e+42	0.877
21821	diHPCARP_I.pmtmtttd	9.834e+43	2.39	2.39	1.783e+42	0.851
21822	diHPCARP_I.mmmmpttmd	7.992e+43	2.31	2.31	1.650e+42	0.788
21823	diHPCARP_I.mmmmpptpd	6.198e+43	2.18	2.18	1.610e+42	0.768
21824	diHPCARP_I.tttmmtmmd	2.471e+43	1.65	1.65	1.547e+42	0.738
21825	diHPCARP_I.tpmmpmtmpd	1.948e+43	1.52	1.52	1.520e+42	0.725
21826	diHPCARP_I.tmtptmmd	9.444e+43	2.49	2.49	1.456e+42	0.695
21827	diHPCARP_I.pmmmttptd	5.315e+43	2.16	2.16	1.427e+42	0.681
21828	diHPCARP_I.pmmmpttmd	3.334e+43	1.93	1.93	1.299e+42	0.62
21829	diHPCARP_I.pptptpmd	3.042e+44	3.34	3.34	1.124e+42	0.536
21830	diHPCARP_I.ptmmmtmpd	3.365e+43	2.03	2.03	1.113e+42	0.531
21831	diHPCARP_I.mtmmmtmtd	3.989e+44	3.51	3.51	1.105e+42	0.527
21832	diHPCARP_I.tmpptttd	4.343e+43	2.20	2.20	1.087e+42	0.519
21833	diHPCARP_I.tmpmpttpd	4.333e+43	2.20	2.20	1.083e+42	0.517
21834	diHPCARP_I.pttptmtd	5.678e+43	2.39	2.39	1.025e+42	0.489
21835	diHPCARP_I.pmtmpttpd	3.918e+43	2.18	2.18	1.015e+42	0.484
21836	diHPCARP_I.pmmmpptmd	5.498e+43	2.40	2.40	9.740e+41	0.465
21837	diHPCARP_I.tmtmmtmmd	6.277e+43	2.54	2.54	8.890e+41	0.424
21838	diHPCARP_I.mmmmtmpd	6.465e+43	2.58	2.58	8.599e+41	0.411
21839	diHPCARP_I.ttmmmtmtd	1.011e+44	2.86	2.86	8.407e+41	0.401
21840	diHPCARP_I.ttpmptmmd	7.593e+42	1.32	1.32	8.254e+41	0.394
21841	diHPCARP_I.pttptmtd	4.486e+43	2.42	2.42	7.787e+41	0.372
21842	diHPCARP_I.pptmptpmd	8.819e+43	2.82	2.82	7.743e+41	0.37
21843	diHPCARP_I.mttmmtmmd	3.138e+43	2.21	2.21	7.729e+41	0.369
21844	diHPCARP_I.mtppmptpd	1.349e+43	1.76	1.76	7.035e+41	0.336
21845	diHPCARP_I.pppmptpmd	5.358e+43	2.74	2.74	5.377e+41	0.257
21846	diHPCARP_I.mtpmptmmd	9.527e+42	1.80	1.80	4.635e+41	0.221
21847	diHPCARP_I.pmmmtmpd	2.544e+43	2.41	2.41	4.451e+41	0.212
21848	diHPCARP_I.pptmptmpd	1.920e+43	2.37	2.37	3.616e+41	0.173
21849	diHPCARP_I.pppmpttpd	1.413e+44	3.57	3.57	3.520e+41	0.168
21850	diHPCARP_I.pttptmtd	1.650e+43	2.30	2.30	3.492e+41	0.167
21851	diHPCARP_I.ttpptmmd	6.257e+42	1.82	1.82	2.938e+41	0.14
21852	diHPCARP_I.pppmptmpd	1.003e+43	2.29	2.29	2.144e+41	0.102
21853	diHPCARP_I.tmpmptmmd	5.768e+43	3.37	3.37	2.040e+41	0.0974
21854	diHPCARP_I.mtppmptmmd	7.775e+42	2.25	2.25	1.781e+41	0.085
21855	diHPCARP_I.pptmptmmd	6.415e+43	3.53	3.53	1.722e+41	0.0822
21856	diHPCARP_I.ptppmptpd	1.041e+43	2.66	2.66	1.199e+41	0.0573
21857	diHPCARP_I.tppmptmpd	1.416e+43	2.86	2.86	1.177e+41	0.0562
21858	Total				2.095e+44	100
21859						
21860						
21861						
21862	(2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)					
21863						

21864
 21865 Population analysis at 300K. Vibrational scaling: 0.971.
 21866 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 21867 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 21868 %: contribution to the population (with current data set assumed 100%)
 21869 Compound Qtot Erel Erel2 n*Q*MB %
 21870 -----

21871	diHPCARP_Ib.tmmmppttpd	3.633e+43	0.33	0.33	2.106e+43	8.87
21872	diHPCARP_Ib.mmmmpmtmpd	2.095e+43	0.00	0.00	2.095e+43	8.82
21873	diHPCARP_Ib.tmmmpptppd	2.840e+43	0.30	0.30	1.716e+43	7.23
21874	diHPCARP_Ib.tmmmppttmd	5.199e+43	0.78	0.78	1.407e+43	5.92
21875	diHPCARP_Ib.mttptmtpd	1.467e+44	1.45	1.45	1.293e+43	5.45
21876	diHPCARP_Ib.mmmmpttmd	5.609e+43	1.01	1.01	1.027e+43	4.32
21877	diHPCARP_Ib.pmpmttmd	7.556e+43	1.26	1.26	9.163e+42	3.86
21878	diHPCARP_Ib.tmmmpptpmd	3.606e+43	0.87	0.87	8.354e+42	3.52
21879	diHPCARP_Ib.mmmmppttpd	4.570e+43	1.02	1.02	8.321e+42	3.5
21880	diHPCARP_Ib.pppmmmtmd	5.988e+43	1.18	1.18	8.296e+42	3.49
21881	diHPCARP_Ib.pptpmtppd	3.564e+43	0.88	0.88	8.177e+42	3.44
21882	diHPCARP_Ib.mmmmpptpmd	3.532e+43	0.91	0.91	7.643e+42	3.22
21883	diHPCARP_Ib.tmmmpmtmpd	3.230e+43	0.87	0.87	7.543e+42	3.18
21884	diHPCARP_Ib.mttptppd	8.611e+43	1.49	1.49	7.016e+42	2.95
21885	diHPCARP_Ib.pmpmtmpd	3.350e+43	1.03	1.03	5.974e+42	2.52
21886	diHPCARP_Ib.mmmmpptppd	3.447e+43	1.05	1.05	5.883e+42	2.48
21887	diHPCARP_Ib.pmpmttmd	2.514e+43	0.90	0.90	5.555e+42	2.34
21888	diHPCARP_Ib.pmmmpmtmd	1.084e+43	0.46	0.46	4.971e+42	2.09
21889	diHPCARP_Ib.pppmmmtmd	3.007e+43	1.08	1.08	4.950e+42	2.08
21890	diHPCARP_Ib.pmtppmtmd	5.429e+43	1.56	1.56	3.976e+42	1.67
21891	diHPCARP_Ib.pppmppppd	1.678e+43	0.88	0.88	3.828e+42	1.61
21892	diHPCARP_Ib.tmmmpmtmd	4.211e+43	1.44	1.44	3.732e+42	1.57
21893	diHPCARP_Ib.pppmppmpd	1.403e+43	0.87	0.87	3.261e+42	1.37
21894	diHPCARP_Ib.pmpmtmpd	6.315e+43	1.81	1.81	3.048e+42	1.28
21895	diHPCARP_Ib.pmmmpptppd	3.261e+43	1.46	1.46	2.807e+42	1.18
21896	diHPCARP_Ib.pmmmppttpd	3.900e+43	1.60	1.60	2.653e+42	1.12
21897	diHPCARP_Ib.pppmptppd	2.809e+43	1.42	1.42	2.594e+42	1.09
21898	diHPCARP_Ib.pppppptpd	7.480e+43	2.04	2.04	2.452e+42	1.03
21899	diHPCARP_Ib.pmtppmtmd	9.328e+43	2.18	2.18	2.413e+42	1.02
21900	diHPCARP_Ib.pppmptmmd	2.492e+43	1.46	1.46	2.143e+42	0.902
21901	diHPCARP_Ib.mmpmpttpd	3.269e+43	1.77	1.77	1.682e+42	0.708
21902	diHPCARP_Ib.pppppptmd	6.535e+43	2.21	2.21	1.606e+42	0.676
21903	diHPCARP_Ib.mtmmpptppd	2.547e+44	3.09	3.09	1.431e+42	0.603
21904	diHPCARP_Ib.pmmmpmtmpd	4.430e+43	2.05	2.05	1.411e+42	0.594
21905	diHPCARP_Ib.pmtppmtmd	8.219e+43	2.53	2.53	1.173e+42	0.494
21906	diHPCARP_Ib.mmpmptppd	3.329e+43	2.00	2.00	1.153e+42	0.485
21907	diHPCARP_Ib.ptppmttmd	2.896e+43	1.93	1.93	1.135e+42	0.478
21908	diHPCARP_Ib.mppmmtmd	5.698e+43	2.39	2.39	1.034e+42	0.435
21909	diHPCARP_Ib.mtpmptppd	1.627e+43	1.70	1.70	9.468e+41	0.399
21910	diHPCARP_Ib.ppppppppd	8.228e+43	2.69	2.69	9.000e+41	0.379
21911	diHPCARP_Ib.ptppmtmpd	1.414e+43	1.64	1.64	8.986e+41	0.378
21912	diHPCARP_Ib.mppppmtpd	8.911e+43	2.78	2.78	8.449e+41	0.356
21913	diHPCARP_Ib.mppmptppd	3.809e+43	2.37	2.37	7.190e+41	0.303
21914	diHPCARP_Ib.mppmptpmd	2.324e+43	2.42	2.42	4.002e+41	0.168
21915	diHPCARP_Ib.pppmpttmd	2.954e+43	2.57	2.57	3.997e+41	0.168
21916	diHPCARP_Ib.pppmptmpd	2.654e+43	2.51	2.51	3.911e+41	0.165
21917	diHPCARP_Ib.mppmptmpd	2.138e+43	2.77	2.77	2.053e+41	0.0864
21918	Total				2.375e+44	100

21919
 21920
 21921
 21922 (2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)
 21923 =====

21924
 21925 Population analysis at 300K. Vibrational scaling: 0.971.
 21926 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 21927 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 21928 %: contribution to the population (with current data set assumed 100%)
 21929 Compound Qtot Erel Erel2 n*Q*MB %
 21930 -----

21931	diHPCARP_Ic.pppppptpd	3.897e+43	0.00	0.00	3.897e+43	36.2
21932	diHPCARP_Ic.pptmptmmd	1.894e+43	0.53	0.53	7.835e+42	7.28
21933	diHPCARP_Ic.mtmptmmd	2.036e+43	0.61	0.61	7.360e+42	6.84
21934	diHPCARP_Ic.pptmptpmd	3.130e+43	1.07	1.07	5.200e+42	4.83
21935	diHPCARP_Ic.pptmptppd	7.689e+43	1.62	1.62	5.078e+42	4.72

21936	diHPCARP_Ic.ppmmtmpmd	3.759e+43	1.34	1.34	3.994e+42	3.71
21937	diHPCARP_Ic.mttmptmmd	2.091e+43	1.02	1.02	3.748e+42	3.48
21938	diHPCARP_Ic.pttmmtmmd	1.800e+43	1.05	1.05	3.094e+42	2.87
21939	diHPCARP_Ic.pmtmmmtmmd	1.407e+43	0.91	0.91	3.038e+42	2.82
21940	diHPCARP_Ic.pmpmttptd	1.595e+43	1.09	1.09	2.551e+42	2.37
21941	diHPCARP_Ic.tptmmmmmd	7.300e+43	2.00	2.00	2.530e+42	2.35
21942	diHPCARP_Ic.pptppptpd	7.703e+43	2.15	2.15	2.100e+42	1.95
21943	diHPCARP_Ic.pptpppppd	1.508e+44	2.57	2.57	2.021e+42	1.88
21944	diHPCARP_Ic.tppmmtpd	3.520e+43	1.71	1.71	1.998e+42	1.86
21945	diHPCARP_Ic.pmpmptpd	7.731e+43	2.20	2.20	1.928e+42	1.79
21946	diHPCARP_Ic.pppmptmmd	7.730e+43	2.20	2.20	1.928e+42	1.79
21947	diHPCARP_Ic.ppttppptpd	1.112e+44	2.52	2.52	1.614e+42	1.5
21948	diHPCARP_Ic.pptmppppd	1.460e+44	2.79	2.79	1.355e+42	1.26
21949	diHPCARP_Ic.mmppttptd	2.566e+43	1.78	1.78	1.305e+42	1.21
21950	diHPCARP_Ic.mttpttptd	3.749e+43	2.11	2.11	1.096e+42	1.02
21951	diHPCARP_Ic.ppttppppd	1.089e+44	2.75	2.75	1.073e+42	0.997
21952	diHPCARP_Ic.pmtmptmmd	3.489e+43	2.24	2.24	8.203e+41	0.762
21953	diHPCARP_Ic.pptppppmmd	3.834e+43	2.31	2.31	7.966e+41	0.74
21954	diHPCARP_Ic.pptpmtmmd	9.516e+43	2.86	2.86	7.894e+41	0.734
21955	diHPCARP_Ic.mttppptmmd	5.403e+43	2.60	2.60	6.943e+41	0.645
21956	diHPCARP_Ic.tmtmptmmd	6.463e+43	2.77	2.77	6.254e+41	0.581
21957	diHPCARP_Ic.pmtppppmd	3.082e+43	2.44	2.44	5.158e+41	0.479
21958	diHPCARP_Ic.pmmmpmmpd	2.895e+43	2.42	2.42	4.957e+41	0.461
21959	diHPCARP_Ic.tmtppmmmpd	1.077e+44	3.25	3.25	4.608e+41	0.428
21960	diHPCARP_Ic.tmmmmmmmpd	3.733e+43	2.62	2.62	4.599e+41	0.427
21961	diHPCARP_Ic.tmtmmmpmmd	2.487e+43	2.52	2.52	3.604e+41	0.335
21962	diHPCARP_Ic.pppppptpd	5.980e+43	3.11	3.11	3.265e+41	0.303
21963	diHPCARP_Ic.mmtppptmmd	5.732e+43	3.15	3.15	2.922e+41	0.272
21964	diHPCARP_Ic.ppmmtmpd	1.251e+43	2.24	2.24	2.912e+41	0.271
21965	diHPCARP_Ic.pttpmtmpd	3.494e+43	2.86	2.86	2.859e+41	0.266
21966	diHPCARP_Ic.pmtpmtmmd	3.764e+43	3.13	3.13	1.984e+41	0.184
21967	diHPCARP_Ic.pptpmtmpd	2.117e+43	2.88	2.88	1.690e+41	0.157
21968	diHPCARP_Ic.ppppppmmd	2.135e+43	3.05	3.05	1.274e+41	0.118
21969	diHPCARP_Ic.ptmmmtmpd	3.933e+43	3.62	3.62	8.999e+40	0.0836
21970	Total				1.076e+44	100

21971
21972
21973
21974 1,4-aldehyde-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
21975 =====

21976
21977 Population analysis at 300K. Vibrational scaling: 0.971.
21978 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
21979 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
21980 %: contribution to the population (with current data set assumed 100%)

21981 Compound	Qtot	Erel	Erel2	n*Q*MB	%
21982 -----					
21983 TS.diHPCARP_I.14aldHshift.mmtmmpd	1.414e+43	0.00	0.00	1.414e+43	16
21984 TS.diHPCARP_I.14aldHshift.mmmmmmpd	1.675e+43	0.20	0.20	1.195e+43	13.5
21985 TS.diHPCARP_I.14aldHshift.mmmmtppd	1.111e+44	1.58	1.58	7.863e+42	8.91
21986 TS.diHPCARP_I.14aldHshift.mtppmmpd	3.162e+43	1.02	1.02	5.699e+42	6.46
21987 TS.diHPCARP_I.14aldHshift.tmtptpd	5.499e+43	1.37	1.37	5.516e+42	6.25
21988 TS.diHPCARP_I.14aldHshift.mtttppd	5.836e+43	1.53	1.53	4.472e+42	5.07
21989 TS.diHPCARP_I.14aldHshift.mmmmtmmd	2.760e+43	1.13	1.13	4.138e+42	4.69
21990 TS.diHPCARP_I.14aldHshift.tmpmmpd	2.103e+43	1.00	1.00	3.944e+42	4.47
21991 TS.diHPCARP_I.14aldHshift.mppmmpd	1.633e+43	0.89	0.89	3.683e+42	4.17
21992 TS.diHPCARP_I.14aldHshift.mtmmpd	2.644e+43	1.20	1.20	3.548e+42	4.02
21993 TS.diHPCARP_I.14aldHshift.tppmmmpd	4.999e+43	1.59	1.59	3.480e+42	3.94
21994 TS.diHPCARP_I.14aldHshift.mtttmmd	7.691e+43	1.92	1.92	3.060e+42	3.47
21995 TS.diHPCARP_I.14aldHshift.tmtpppd	3.919e+43	1.52	1.52	3.043e+42	3.45
21996 TS.diHPCARP_I.14aldHshift.tppppmd	5.813e+42	0.41	0.41	2.899e+42	3.29
21997 TS.diHPCARP_I.14aldHshift.mtptmpd	2.359e+43	1.59	1.59	1.647e+42	1.87
21998 TS.diHPCARP_I.14aldHshift.tmtppmd	2.173e+43	1.58	1.58	1.528e+42	1.73
21999 TS.diHPCARP_I.14aldHshift.mtppppmd	1.478e+43	1.45	1.45	1.293e+42	1.47
22000 TS.diHPCARP_I.14aldHshift.ppmmpd	1.333e+43	1.39	1.39	1.287e+42	1.46
22001 TS.diHPCARP_I.14aldHshift.mppppmd	8.295e+42	1.21	1.21	1.094e+42	1.24
22002 TS.diHPCARP_I.14aldHshift.mtmmpd	5.672e+43	2.36	2.36	1.085e+42	1.23
22003 TS.diHPCARP_I.14aldHshift.mmmmtmmd	1.923e+43	1.73	1.73	1.064e+42	1.21
22004 TS.diHPCARP_I.14aldHshift.pmpmmpd	8.057e+42	1.51	1.51	6.413e+41	0.727
22005 TS.diHPCARP_I.14aldHshift.tppppmd	1.174e+43	1.76	1.76	6.180e+41	0.701
22006 TS.diHPCARP_I.14aldHshift.mmpmmpd	1.506e+43	2.00	2.00	5.295e+41	0.6
22007 Total				8.822e+43	100

22008
 22009
 22010
 22011 1,5-aldehyde-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)
 22012 =====

22013
 22014 Note: both enantiomers (R,R and S,S) were calculated at the M06-2X/cc-pVDZ level based
 22015 on
 22016 a different template, to check the robustness of the conformer space search. As can be
 22017 seen,
 22018 most conformers are found in both enantiomers, though some higher-energy conformers
 22019 are
 22020 missing in either the R,R or S,S set. The impact on the rate predictions was
 22021 found to be negligible. At the M06-02X/aug-cc-pVTZ level of theory, only a single set
 22022 of
 22023 enantiomers was calculated.

22024 Population analysis at 300K. Vibrational scaling: 0.971.
 22025 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
 22026 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22027 %: contribution to the population (with current data set assumed 100%)

22028 Compound	Qtot	Erel	Erel2	n*Q*MB	%
22029 -----					
22030 TS.diHPCARP_Ib.15aldHshift.dtdppdud	8.564e+42	0.00	0.00	8.564e+42	52.6
22031 TS.diHPCARP_Ib.15aldHshift.ututpddu	3.974e+43	1.91	1.91	1.612e+42	9.9
22032 TS.diHPCARP_Ib.15aldHshift.umdmmudu	7.388e+42	1.00	1.00	1.390e+42	8.54
22033 TS.diHPCARP_Ib.15aldHshift.ututmudu	2.338e+43	1.68	1.68	1.388e+42	8.53
22034 TS.diHPCARP_Ib.15aldHshift.utuppddu	1.499e+43	1.70	1.70	8.694e+41	5.34
22035 TS.diHPCARP_Ib.15aldHshift.umdtpddu	3.724e+43	2.47	2.47	5.952e+41	3.65
22036 TS.diHPCARP_Ib.15aldHshift.umdmmudu	2.081e+43	2.31	2.31	4.292e+41	2.64
22037 TS.diHPCARP_Ib.15aldHshift.utdmmddu	1.325e+43	2.09	2.09	3.985e+41	2.45
22038 TS.diHPCARP_Ib.15aldHshift.umdmpddu	8.056e+42	2.08	2.08	2.455e+41	1.51
22039 TS.diHPCARP_Ib.15aldHshift.umdppddu	1.668e+43	2.66	2.66	1.930e+41	1.19
22040 TS.diHPCARP_Ib.15aldHshift.upummuud	1.361e+43	2.64	2.64	1.616e+41	0.993
22041 TS.diHPCARP_Ib.15aldHshift.utuppuud	2.790e+43	3.47	3.47	8.280e+40	0.508
22042 TS.diHPCARP_Ib.15aldHshift.utuppudu	2.372e+43	3.37	3.37	8.275e+40	0.508
22043 TS.diHPCARP_Ib.15aldHshift.utummuud	5.260e+42	2.57	2.57	7.095e+40	0.436
22044 TS.diHPCARP_Ib.15aldHshift.upupmudu	2.110e+43	3.42	3.42	6.772e+40	0.416
22045 TS.diHPCARP_Ib.15aldHshift.umdmmudu	2.012e+43	3.43	3.43	6.375e+40	0.391
22046 TS.diHPCARP_Ib.15aldHshift.utdmpddu	6.855e+42	3.12	3.12	3.633e+40	0.223
22047 TS.diHPCARP_Ib.15aldHshift.updmmuud	1.166e+43	3.49	3.49	3.357e+40	0.206
22048 Total				1.628e+43	100

22049
 22050
 22051
 22052 1,6-aldehyde-H-shift in (2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)
 22053 =====

22054
 22055 Population analysis at 300K. Vibrational scaling: 0.971.
 22056 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
 22057 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22058 %: contribution to the population (with current data set assumed 100%)

22059 Compound	Qtot	Erel	Erel2	n*Q*MB	%
22060 -----					
22061 TS.diHPCARP_Ic.16aldHshift.a.mptpuu	6.760e+42	0.27	0.27	4.293e+42	17.8
22062 TS.diHPCARP_Ic.16aldHshift.a.mppmuu	3.249e+42	0.00	0.00	3.249e+42	13.4
22063 TS.diHPCARP_Ic.16aldHshift.a.pmpuud	5.297e+42	0.39	0.39	2.757e+42	11.4
22064 TS.diHPCARP_Ic.16aldHshift.b.pmpuud	5.037e+42	0.37	0.37	2.709e+42	11.2
22065 TS.diHPCARP_Ic.16aldHshift.b.mptpuu	7.611e+42	0.70	0.70	2.362e+42	9.77
22066 TS.diHPCARP_Ic.16aldHshift.a.mppmuu	8.350e+42	0.89	0.89	1.874e+42	7.75
22067 TS.diHPCARP_Ic.16aldHshift.a.mpppuu	1.254e+43	1.21	1.21	1.634e+42	6.76
22068 TS.diHPCARP_Ic.16aldHshift.a.mppmuu	6.291e+42	1.27	1.27	7.448e+41	3.08
22069 TS.diHPCARP_Ic.16aldHshift.b.pmmuud	7.879e+42	1.62	1.62	5.193e+41	2.15
22070 TS.diHPCARP_Ic.16aldHshift.a.pmmuud	2.901e+42	1.07	1.07	4.821e+41	1.99
22071 TS.diHPCARP_Ic.16aldHshift.a.tmpuud	8.935e+42	1.80	1.80	4.376e+41	1.81
22072 TS.diHPCARP_Ic.16aldHshift.a.pmpddu	1.735e+43	2.22	2.22	4.199e+41	1.74
22073 TS.diHPCARP_Ic.16aldHshift.a.pmpmuu	2.793e+42	1.19	1.19	3.810e+41	1.58
22074 TS.diHPCARP_Ic.16aldHshift.b.mpppuu	1.139e+43	2.05	2.05	3.642e+41	1.51
22075 TS.diHPCARP_Ic.16aldHshift.a.tmpuud	6.894e+42	1.81	1.81	3.283e+41	1.36
22076 TS.diHPCARP_Ic.16aldHshift.a.pppmuu	2.938e+42	1.43	1.43	2.656e+41	1.1
22077 TS.diHPCARP_Ic.16aldHshift.b.pppmuu	1.430e+43	2.46	2.46	2.315e+41	0.958
22078 TS.diHPCARP_Ic.16aldHshift.b.pmpuud	3.879e+42	1.75	1.75	2.060e+41	0.852
22079 TS.diHPCARP_Ic.16aldHshift.e.tmpuud	1.033e+43	2.40	2.40	1.846e+41	0.764

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22080 TS.diHPCARP_Ic.16aldHshift.b.mppmuu 4.317e+42 1.97 1.97 1.596e+41 0.66
22081 TS.diHPCARP_Ic.16aldHshift.a.pmpmdd 3.698e+43 3.25 3.25 1.592e+41 0.658
22082 TS.diHPCARP_Ic.16aldHshift.c.mppmuu 9.446e+42 2.51 2.51 1.404e+41 0.581
22083 TS.diHPCARP_Ic.16aldHshift.a.pmpmdd 2.992e+43 3.35 3.35 1.079e+41 0.446
22084 TS.diHPCARP_Ic.16aldHshift.a.pppmuu 3.368e+42 2.53 2.53 4.872e+40 0.202
22085 TS.diHPCARP_Ic.16aldHshift.b.pppmuu 3.221e+42 2.60 2.60 4.083e+40 0.169
22086 TS.diHPCARP_Ic.16aldHshift.b.pppmuu 7.926e+42 3.23 3.23 3.534e+40 0.146
22087 TS.diHPCARP_Ic.16aldHshift.b.pmpmuu 3.368e+42 2.72 2.72 3.522e+40 0.146
22088 Total 2.417e+43 100
22089
22090
22091
22092 1,6-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
22093 HPCARP-Ia), forming B (di-HPCARP-Ib)
22094 =====
22095 =====
22096
22097 Population analysis at 300K. Vibrational scaling: 0.971.
22098 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22099 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22100 %: contribution to the population (with current data set assumed 100%)
22101 Compound Qtot Erel Erel2 n*Q*MB %
22102 -----
22103 TS.diHPCARP_I.16OOHHshift.a.tppmdd 3.382e+42 0.00 0.00 3.382e+42 32.4
22104 TS.diHPCARP_I.16OOHHshift.a.tmmuuu 6.884e+43 2.18 2.18 1.781e+42 17.1
22105 TS.diHPCARP_I.16OOHHshift.a.htppuu 3.766e+43 1.94 1.94 1.447e+42 13.9
22106 TS.diHPCARP_I.16OOHHshift.a.ttptuu 3.353e+43 1.89 1.89 1.418e+42 13.6
22107 TS.diHPCARP_I.16OOHHshift.b.ttptuu 4.175e+43 2.05 2.05 1.340e+42 12.8
22108 TS.diHPCARP_I.16OOHHshift.b.htppuu 4.018e+43 2.16 2.16 1.067e+42 10.2
22109 Total 1.044e+43 100
22110
22111
22112
22113 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
22114 HPCARP-Ia), forming C (di-HPCARP-Ic)
22115 =====
22116 =====
22117
22118 Population analysis at 300K. Vibrational scaling: 0.971.
22119 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22120 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22121 %: contribution to the population (with current data set assumed 100%)
22122 Compound Qtot Erel Erel2 n*Q*MB %
22123 -----
22124 TS.diHPCARP_I.17OOHHshift.BB.hpddd 5.702e+42 0.00 0.00 5.702e+42 91.3
22125 TS.diHPCARP_I.17OOHHshift.BB.ltddd 3.148e+43 2.81 2.81 2.834e+41 4.54
22126 TS.diHPCARP_I.17OOHHshift.BB.tmuud 3.756e+42 1.96 1.96 1.395e+41 2.23
22127 TS.diHPCARP_I.17OOHHshift.BB.lpudd 1.278e+43 3.41 3.41 4.162e+40 0.667
22128 TS.diHPCARP_I.17OOHHshift.BB.ltduu 7.557e+42 3.13 3.13 3.974e+40 0.636
22129 TS.diHPCARP_I.17OOHHshift.CR.hmddd 4.619e+42 3.86 3.86 7.080e+39 0.113
22130 TS.diHPCARP_I.17OOHHshift.BB.lmduu 1.023e+43 4.37 4.37 6.659e+39 0.107
22131 TS.diHPCARP_I.17OOHHshift.BB.lmuuu 1.319e+43 4.57 4.57 6.173e+39 0.0989
22132 TS.diHPCARP_I.17OOHHshift.BB.hmddd 9.002e+42 4.42 4.42 5.387e+39 0.0863
22133 TS.diHPCARP_I.17OOHHshift.BB.hpudd 5.223e+42 4.14 4.14 4.998e+39 0.08
22134 TS.diHPCARP_I.17OOHHshift.BC.tmuuu 1.757e+43 4.88 4.88 4.925e+39 0.0789
22135 TS.diHPCARP_I.17OOHHshift.BB.ctddd 2.016e+43 5.38 5.38 2.439e+39 0.0391
22136 TS.diHPCARP_I.17OOHHshift.BB.tpduu 5.112e+42 5.55 5.55 4.629e+38 0.00741
22137 TS.diHPCARP_I.17OOHHshift.BB.lpuuu 3.566e+42 5.68 5.68 2.608e+38 0.00418
22138 Total 6.244e+42 100
22139
22140
22141
22142 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-
22143 HPCARP-Ib), forming C (di-HPCARP-Ic)
22144 =====
22145 =====
22146
22147 Population analysis at 300K. Vibrational scaling: 0.971.
22148 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22149 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22150 %: contribution to the population (with current data set assumed 100%)
22151 Compound Qtot Erel Erel2 n*Q*MB %

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22152	-----						
22153	TS.diHPCARP_Ib.1600HHshift.b.hpmmuu	1.256e+43	0.11	0.11	1.043e+43	23.4	
22154	TS.diHPCARP_Ib.1600HHshift.b.ctmpuu	6.980e+42	0.00	0.00	6.980e+42	15.7	
22155	TS.diHPCARP_Ib.1600HHshift.a.hpmmuu	8.743e+42	0.15	0.15	6.814e+42	15.3	
22156	TS.diHPCARP_Ib.1600HHshift.b.htpmuu	7.373e+42	0.41	0.41	3.701e+42	8.3	
22157	TS.diHPCARP_Ib.1600HHshift.b.lmppdd	7.609e+42	0.57	0.57	2.902e+42	6.51	
22158	TS.diHPCARP_Ib.1600HHshift.b.ctpmuu	5.975e+43	1.81	1.81	2.876e+42	6.45	
22159	TS.diHPCARP_Ib.1600HHshift.a.ctpmdd	4.354e+42	0.29	0.29	2.664e+42	5.98	
22160	TS.diHPCARP_Ib.1600HHshift.b.cptpuu	1.117e+43	1.26	1.26	1.350e+42	3.03	
22161	TS.diHPCARP_Ib.1600HHshift.a.hptpuu	1.634e+43	1.74	1.74	8.811e+41	1.98	
22162	TS.diHPCARP_Ib.1600HHshift.a.ctmmuu	1.630e+43	1.85	1.85	7.374e+41	1.65	
22163	TS.diHPCARP_Ib.1600HHshift.a.ctmpuu	1.871e+43	2.01	2.01	6.384e+41	1.43	
22164	TS.diHPCARP_Ib.1600HHshift.b.hptpuu	1.778e+43	2.06	2.06	5.646e+41	1.27	
22165	TS.diHPCARP_Ib.1600HHshift.a.lmppdd	5.543e+42	1.39	1.39	5.351e+41	1.2	
22166	TS.diHPCARP_Ib.1600HHshift.b.ctpmuu	3.292e+43	2.56	2.56	4.500e+41	1.01	
22167	TS.diHPCARP_Ib.1600HHshift.a.mttmuu	2.694e+43	2.54	2.54	3.802e+41	0.853	
22168	TS.diHPCARP_Ib.1600HHshift.a.mmpmuu	2.816e+43	2.62	2.62	3.468e+41	0.778	
22169	TS.diHPCARP_Ib.1600HHshift.a.httpuu	1.064e+43	2.10	2.10	3.133e+41	0.703	
22170	TS.diHPCARP_Ib.1600HHshift.a.ctpmuu	1.542e+43	2.32	2.32	3.128e+41	0.702	
22171	TS.diHPCARP_Ib.1600HHshift.a.cpmuu	2.304e+43	2.64	2.64	2.773e+41	0.622	
22172	TS.diHPCARP_Ib.1600HHshift.b.mmpmuu	2.098e+43	2.66	2.66	2.434e+41	0.546	
22173	TS.diHPCARP_Ib.1600HHshift.a.cmpmuu	1.785e+43	2.61	2.61	2.231e+41	0.501	
22174	TS.diHPCARP_Ib.1600HHshift.b.cttmuu	3.826e+43	3.15	3.15	1.946e+41	0.437	
22175	TS.diHPCARP_Ib.1600HHshift.b.pttpdd	3.940e+43	3.18	3.18	1.908e+41	0.428	
22176	TS.diHPCARP_Ib.1600HHshift.b.pptpdd	8.291e+42	2.26	2.26	1.868e+41	0.419	
22177	TS.diHPCARP_Ib.1600HHshift.a.ctppuu	2.182e+43	2.98	2.98	1.483e+41	0.333	
22178	TS.diHPCARP_Ib.1600HHshift.b.ctmmuu	2.079e+43	3.16	3.16	1.032e+41	0.232	
22179	TS.diHPCARP_Ib.1600HHshift.a.ctpmdd	5.018e+42	2.51	2.51	7.417e+40	0.166	
22180	TS.diHPCARP_Ib.1600HHshift.a.lmtmdd	7.583e+42	3.01	3.01	4.906e+40	0.11	
22181	Total				4.457e+43	100	

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22185 1,4-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-
22186 di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde
22187 =====
22188 =====

22189
22190 Population analysis at 300K. Vibrational scaling: 0.971.
22191 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
22192 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22193 %: contribution to the population (with current data set assumed 100%)
22194 Compound Qtot Erel Erel2 n*Q*MB %
22195 -----

22196	TS.diHPCARP_I.14HPHshift.mmmmmmtu	5.651e+42	0.10	0.10	4.757e+42	39.6	
22197	TS.diHPCARP_I.14HPHshift.mtmmttu	4.097e+42	0.00	0.00	4.097e+42	34.1	
22198	TS.diHPCARP_I.14HPHshift.mmtmttu	7.336e+42	0.83	0.83	1.821e+42	15.2	
22199	TS.diHPCARP_I.14HPHshift.mtmmttu	8.460e+42	1.46	1.46	7.364e+41	6.14	
22200	TS.diHPCARP_I.14HPHshift.mmmmttu	5.754e+42	1.61	1.61	3.876e+41	3.23	
22201	TS.diHPCARP_I.14HPHshift.mmtmttu	8.135e+42	2.20	2.20	2.024e+41	1.69	
22202	Total				1.200e+43	100	

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22206 1,5-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-
22207 di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde
22208 =====
22209 =====

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22211 Population analysis at 300K. Vibrational scaling: 0.971.
22212 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
22213 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22214 %: contribution to the population (with current data set assumed 100%)
22215 Compound Qtot Erel Erel2 n*Q*MB %
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22217	TS.diHPCARP_I.15HPHshift.dmtdpdud	2.461e+43	0.14	0.14	1.935e+43	29.2	
22218	TS.diHPCARP_I.15HPHshift.dmtdmuud	1.117e+43	0.00	0.00	1.117e+43	16.8	
22219	TS.diHPCARP_I.15HPHshift.dcpdpddd	4.251e+43	1.01	1.01	7.839e+42	11.8	
22220	TS.diHPCARP_I.15HPHshift.dlpdtddd	6.503e+43	1.31	1.31	7.190e+42	10.8	
22221	TS.diHPCARP_I.15HPHshift.dmpupuud	4.145e+43	1.28	1.28	4.825e+42	7.27	
22222	TS.diHPCARP_I.15HPHshift.dcmupddd	4.121e+43	1.65	1.65	2.572e+42	3.88	
22223	TS.diHPCARP_I.15HPHshift.dcmupudd	3.533e+43	1.72	1.72	1.983e+42	2.99	

22224	TS.diHPCARP_I.15HPHshift.dmtmdud	2.294e+43	1.48	1.48	1.916e+42	2.89
22225	TS.diHPCARP_I.15HPHshift.dcpdpudd	3.912e+43	1.97	1.97	1.447e+42	2.18
22226	TS.diHPCARP_I.15HPHshift.dcpdmudd	2.638e+43	1.78	1.78	1.333e+42	2.01
22227	TS.diHPCARP_I.15HPHshift.dcpumdud	4.195e+43	2.08	2.08	1.287e+42	1.94
22228	TS.diHPCARP_I.15HPHshift.dmpumuud	1.340e+43	1.44	1.44	1.201e+42	1.81
22229	TS.diHPCARP_I.15HPHshift.dppdmudd	2.360e+43	1.90	1.90	9.753e+41	1.47
22230	TS.diHPCARP_I.15HPHshift.dcmdpddd	2.451e+43	1.98	1.98	8.884e+41	1.34
22231	TS.diHPCARP_I.15HPHshift.dtpdmdud	2.440e+43	1.98	1.98	8.801e+41	1.33
22232	TS.diHPCARP_I.15HPHshift.dcmutudd	1.102e+43	1.92	1.92	4.434e+41	0.668
22233	TS.diHPCARP_I.15HPHshift.umpupuud	4.078e+43	2.86	2.86	3.340e+41	0.503
22234	TS.diHPCARP_I.15HPHshift.umpupddd	2.994e+43	2.73	2.73	3.066e+41	0.462
22235	TS.diHPCARP_I.15HPHshift.dcmumudd	1.535e+43	2.73	2.73	1.562e+41	0.235
22236	TS.diHPCARP_I.15HPHshift.dcmumddd	8.170e+42	2.48	2.48	1.269e+41	0.191
22237	TS.diHPCARP_I.15HPHshift.uppupuud	3.474e+43	3.81	3.81	5.818e+40	0.0877
22238	TS.diHPCARP_I.15HPHshift.umtumddd	1.159e+43	3.16	3.16	5.809e+40	0.0876
22239	Total				6.634e+43	100

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(2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia)

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Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
22251					
22252	diHPCARP_I.tmmmppttmu	8.428e+42	0.00	0.00	8.428e+42 34.3
22253	diHPCARP_I.mmmmppttmu	1.046e+43	0.72	0.72	3.134e+42 12.7
22254	diHPCARP_I.tmmmpptpmu	1.836e+43	1.63	1.63	1.198e+42 4.87
22255	diHPCARP_I.tpmmppttmu	2.766e+43	1.92	1.92	1.113e+42 4.53
22256	diHPCARP_I.mmmmpptpmu	2.002e+43	1.78	1.78	1.015e+42 4.13
22257	diHPCARP_I.pmmmppttmu	8.064e+42	1.25	1.25	9.953e+41 4.05
22258	diHPCARP_I.tmmmpptmpu	1.635e+43	1.70	1.70	9.437e+41 3.84
22259	diHPCARP_I.tptmppttmu	4.955e+43	2.38	2.38	9.149e+41 3.72
22260	diHPCARP_I.ppmmpptmpu	1.556e+43	1.76	1.76	8.093e+41 3.29
22261	diHPCARP_I.ptppmtpmu	1.425e+43	1.73	1.73	7.880e+41 3.2
22262	diHPCARP_I.tpmmpptmtu	3.231e+43	2.37	2.37	6.051e+41 2.46
22263	diHPCARP_I.mmmmpptmpu	1.446e+43	1.94	1.94	5.590e+41 2.27
22264	diHPCARP_I.tpmmpptmmu	2.318e+43	2.24	2.24	5.391e+41 2.19
22265	diHPCARP_I.tptpmtppu	2.973e+43	2.46	2.46	4.787e+41 1.95
22266	diHPCARP_I.tmtppmpppu	3.231e+43	2.59	2.59	4.211e+41 1.71
22267	diHPCARP_I.tmmmpptmtu	2.138e+43	2.38	2.38	3.974e+41 1.62
22268	diHPCARP_I.mmtppmpppu	2.807e+43	2.55	2.55	3.908e+41 1.59
22269	diHPCARP_I.tmmmppttpu	2.587e+43	2.53	2.53	3.725e+41 1.51
22270	diHPCARP_I.pttpmtppu	7.607e+43	3.25	3.25	3.278e+41 1.33
22271	diHPCARP_I.tmpmpptpmu	2.267e+43	2.60	2.60	2.909e+41 1.18
22272	diHPCARP_I.mmpmpptpmu	3.522e+43	3.06	3.06	2.065e+41 0.84
22273	diHPCARP_I.ptmmppttmu	7.082e+43	3.58	3.58	1.758e+41 0.715
22274	diHPCARP_I.mmmtpmpppu	1.897e+43	2.85	2.85	1.598e+41 0.65
22275	diHPCARP_I.tmmtpmpppu	1.690e+43	2.80	2.80	1.535e+41 0.624
22276	diHPCARP_I.ptmmpmtpu	1.328e+44	4.27	4.27	1.024e+41 0.416
22277	diHPCARP_I.pmmmpptpmu	1.268e+43	3.10	3.10	7.038e+40 0.286
22278	Total				2.459e+43 100

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(2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-Ib)

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Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
22289					
22290					
22291	diHPCARP_Ib.ptppmpmmu	1.158e+43	0.00	0.00	1.158e+43 25.2
22292	diHPCARP_Ib.ptmmtmmu	7.497e+43	1.27	1.27	8.962e+42 19.5
22293	diHPCARP_Ib.ptmptmmu	1.005e+44	1.65	1.65	6.330e+42 13.8
22294	diHPCARP_Ib.ptttptmmu	7.512e+43	2.11	2.11	2.165e+42 4.72
22295	diHPCARP_Ib.ptppmtpmu	1.165e+43	1.06	1.06	1.980e+42 4.32

22296	diHPCARP_Ib.ptttmtmmu	7.804e+43	2.26	2.26	1.752e+42	3.82
22297	diHPCARP_Ib.pttpptmmu	1.256e+44	2.57	2.57	1.680e+42	3.66
22298	diHPCARP_Ib.pttpmtmmu	5.840e+43	2.23	2.23	1.394e+42	3.04
22299	diHPCARP_Ib.ptppmtmmu	3.302e+43	1.96	1.96	1.224e+42	2.67
22300	diHPCARP_Ib.pptmppmpu	9.656e+43	2.75	2.75	9.609e+41	2.09
22301	diHPCARP_Ib.pptmmppmu	8.083e+43	2.65	2.65	9.474e+41	2.06
22302	diHPCARP_Ib.pppmptmmu	2.653e+43	2.11	2.11	7.668e+41	1.67
22303	diHPCARP_Ib.pttmptmmu	1.184e+44	3.11	3.11	6.461e+41	1.41
22304	diHPCARP_Ib.pptmpmtpu	2.264e+43	2.19	2.19	5.728e+41	1.25
22305	diHPCARP_Ib.pppppptpu	6.517e+43	2.84	2.84	5.524e+41	1.2
22306	diHPCARP_Ib.tmmppmtmmu	2.732e+43	2.51	2.51	4.061e+41	0.885
22307	diHPCARP_Ib.ptmmmtmmu	3.954e+43	2.81	2.81	3.521e+41	0.767
22308	diHPCARP_Ib.ptmtptmmu	1.104e+44	3.46	3.46	3.325e+41	0.725
22309	diHPCARP_Ib.pmmmmmtmu	3.550e+43	2.80	2.80	3.235e+41	0.705
22310	diHPCARP_Ib.ptmmpmtmmu	2.675e+43	2.66	2.66	3.074e+41	0.67
22311	diHPCARP_Ib.ptmtmtmmu	1.983e+44	3.88	3.88	2.954e+41	0.644
22312	diHPCARP_Ib.tmtmpmtmu	5.191e+43	3.11	3.11	2.811e+41	0.613
22313	diHPCARP_Ib.pppppmpu	6.266e+43	3.24	3.24	2.751e+41	0.6
22314	diHPCARP_Ib.tmmppmmmmu	2.713e+43	2.83	2.83	2.353e+41	0.513
22315	diHPCARP_Ib.pptmptmmu	3.179e+43	2.96	2.96	2.236e+41	0.487
22316	diHPCARP_Ib.tmmmmmtmu	7.286e+43	3.50	3.50	2.065e+41	0.45
22317	diHPCARP_Ib.mmmmpmtmu	2.944e+43	3.05	3.05	1.773e+41	0.386
22318	diHPCARP_Ib.mmmmpmtmu	2.804e+43	3.16	3.16	1.388e+41	0.302
22319	diHPCARP_Ib.pmmmmmpmu	3.940e+43	3.40	3.40	1.308e+41	0.285
22320	diHPCARP_Ib.pppmptmmu	2.255e+43	3.07	3.07	1.306e+41	0.285
22321	diHPCARP_Ib.pmpmpmpu	2.834e+43	3.50	3.50	8.030e+40	0.175
22322	diHPCARP_Ib.ptmmpmmmu	4.866e+43	3.84	3.84	7.750e+40	0.169
22323	diHPCARP_Ib.ptmpmmpmu	1.998e+43	3.36	3.36	7.132e+40	0.155
22324	diHPCARP_Ib.tmpmpmpmu	1.794e+43	3.43	3.43	5.668e+40	0.124
22325	diHPCARP_Ib.ptmpmtmmu	1.718e+43	3.44	3.44	5.404e+40	0.118
22326	diHPCARP_Ib.tpmmpmmmu	1.221e+43	3.27	3.27	5.058e+40	0.11
22327	diHPCARP_Ib.ptmpptmmu	4.616e+43	4.07	4.07	5.012e+40	0.109
22328	diHPCARP_Ib.pppmpmpmu	1.026e+43	3.17	3.17	5.004e+40	0.109
22329	diHPCARP_Ib.pmpmptmmu	1.586e+43	3.55	3.55	4.114e+40	0.0897
22330	diHPCARP_Ib.pppmptpmu	1.143e+43	3.83	3.83	1.860e+40	0.0405
22331	Total				4.588e+43	100

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(2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-Ic)

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Population analysis at 300K. Vibrational scaling: 0.971.

22339 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

22340 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

22341 %: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
22344	diHPCARP_Ic.tmtmpmpu	3.952e+43	0.00	0.00	3.952e+43	44.5
22345	diHPCARP_Ic.pmmmpmtmu	2.063e+43	0.85	0.85	4.926e+42	5.54
22346	diHPCARP_Ic.pmtppppu	2.091e+43	0.91	0.91	4.562e+42	5.13
22347	diHPCARP_Ic.pttpmtppu	1.867e+43	0.91	0.91	4.080e+42	4.59
22348	diHPCARP_Ic.tmmmmmtmu	2.883e+43	1.19	1.19	3.937e+42	4.43
22349	diHPCARP_Ic.pttmmtmmu	7.946e+43	1.90	1.90	3.293e+42	3.7
22350	diHPCARP_Ic.ptmmmtmmu	2.295e+43	1.21	1.21	3.009e+42	3.39
22351	diHPCARP_Ic.ptttmtmmu	8.369e+43	2.19	2.19	2.132e+42	2.4
22352	diHPCARP_Ic.pttpmtmmu	8.339e+43	2.36	2.36	1.591e+42	1.79
22353	diHPCARP_Ic.ptppmtmmu	8.868e+43	2.40	2.40	1.583e+42	1.78
22354	diHPCARP_Ic.pttmmtmpu	5.802e+43	2.16	2.16	1.560e+42	1.75
22355	diHPCARP_Ic.ptttmtmpu	7.473e+43	2.33	2.33	1.491e+42	1.68
22356	diHPCARP_Ic.tptmmpmpu	5.217e+43	2.14	2.14	1.442e+42	1.62
22357	diHPCARP_Ic.pptppmpu	1.157e+43	1.25	1.25	1.417e+42	1.59
22358	diHPCARP_Ic.tmttmppu	1.933e+44	2.94	2.94	1.397e+42	1.57
22359	diHPCARP_Ic.tmtmmppu	5.658e+43	2.25	2.25	1.298e+42	1.46
22360	diHPCARP_Ic.pptmpmtmu	5.702e+43	2.35	2.35	1.111e+42	1.25
22361	diHPCARP_Ic.pptpmtppu	1.364e+43	1.58	1.58	9.708e+41	1.09
22362	diHPCARP_Ic.pttpmtmpu	8.561e+43	2.75	2.75	8.538e+41	0.961
22363	diHPCARP_Ic.pptppmtmu	5.323e+43	2.47	2.47	8.431e+41	0.949
22364	diHPCARP_Ic.pppppmpu	2.514e+43	2.03	2.03	8.280e+41	0.932
22365	diHPCARP_Ic.pppmptpu	7.106e+43	2.67	2.67	8.038e+41	0.904
22366	diHPCARP_Ic.tppmmpmu	5.801e+43	2.68	2.68	6.452e+41	0.726
22367	diHPCARP_Ic.tppppmpu	6.716e+43	2.79	2.79	6.195e+41	0.697

22368	diHPCARP_Ic.pptmpmpmu	1.286e+44	3.26	3.26	5.447e+41	0.613
22369	diHPCARP_Ic.ppmmttmu	3.922e+43	2.65	2.65	4.575e+41	0.515
22370	diHPCARP_Ic.pttmmtppu	9.890e+43	3.23	3.23	4.404e+41	0.495
22371	diHPCARP_Ic.pppmpmpmu	5.830e+43	2.94	2.94	4.226e+41	0.475
22372	diHPCARP_Ic.pttmmtpmu	4.006e+43	2.79	2.79	3.730e+41	0.42
22373	diHPCARP_Ic.ppptmpmpmu	4.589e+43	3.02	3.02	2.898e+41	0.326
22374	diHPCARP_Ic.pppppmpmu	1.533e+43	2.38	2.38	2.844e+41	0.32
22375	diHPCARP_Ic.ptmtmtmpu	7.717e+43	3.39	3.39	2.617e+41	0.294
22376	diHPCARP_Ic.pmtmppppu	4.094e+43	3.02	3.02	2.583e+41	0.291
22377	diHPCARP_Ic.mmtppmpmu	4.230e+43	3.06	3.06	2.488e+41	0.28
22378	diHPCARP_Ic.mttppppu	1.772e+43	2.66	2.66	2.046e+41	0.23
22379	diHPCARP_Ic.pmmmpmpmu	2.430e+43	2.94	2.94	1.753e+41	0.197
22380	diHPCARP_Ic.ptmmmtmpu	6.894e+43	3.60	3.60	1.635e+41	0.184
22381	diHPCARP_Ic.tmmmmmpmu	2.666e+43	3.10	3.10	1.464e+41	0.165
22382	diHPCARP_Ic.mptppppu	1.608e+43	2.82	2.82	1.408e+41	0.158
22383	diHPCARP_Ic.mtmmtppu	2.083e+43	3.04	3.04	1.273e+41	0.143
22384	diHPCARP_Ic.pmpmmtmpu	3.607e+43	3.54	3.54	9.490e+40	0.107
22385	diHPCARP_Ic.pmpmtpmu	1.949e+43	3.20	3.20	9.139e+40	0.103
22386	diHPCARP_Ic.mmtmptmpu	4.199e+43	3.67	3.67	8.951e+40	0.101
22387	diHPCARP_Ic.mmpppppu	4.407e+43	3.74	3.74	8.364e+40	0.0941
22388	diHPCARP_Ic.ptmmmtppu	2.550e+43	3.78	3.78	4.503e+40	0.0507
22389	diHPCARP_Ic.tmmmtmpu	7.957e+43	4.66	4.66	3.184e+40	0.0358
22390	Total				8.889e+43	100

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22394 1,4-aldehyde-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia)
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22399 Population analysis at 300K. Vibrational scaling: 0.971.
22400 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
22401 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22402 %: contribution to the population (with current data set assumed 100%)

22403	Compound	Qtot	Erel	Erel2	n*Q*MB	%
22404	-----					
22405	TS.diHPCARP_I.14aldHshift.tmmmpu	6.607e+42	0.00	0.00	6.607e+42	39.1
22406	TS.diHPCARP_I.14aldHshift.tppppmu	9.907e+42	1.16	1.16	1.405e+42	8.31
22407	TS.diHPCARP_I.14aldHshift.mmpmpmu	1.095e+43	1.23	1.23	1.392e+42	8.23
22408	TS.diHPCARP_I.14aldHshift.mppppu	4.089e+43	2.29	2.29	8.746e+41	5.17
22409	TS.diHPCARP_I.14aldHshift.tmmppmu	1.286e+43	1.64	1.64	8.215e+41	4.86
22410	TS.diHPCARP_I.14aldHshift.tpptmpu	1.675e+43	1.94	1.94	6.431e+41	3.8
22411	TS.diHPCARP_I.14aldHshift.ttmtpu	1.937e+44	3.43	3.43	6.173e+41	3.65
22412	TS.diHPCARP_I.14aldHshift.mtppppu	2.316e+44	3.61	3.61	5.438e+41	3.22
22413	TS.diHPCARP_I.14aldHshift.mtmmpu	1.364e+43	1.95	1.95	5.151e+41	3.05
22414	TS.diHPCARP_I.14aldHshift.mppppu	3.410e+43	2.69	2.69	3.714e+41	2.2
22415	TS.diHPCARP_I.14aldHshift.ttpmpu	1.788e+43	2.39	2.39	3.257e+41	1.93
22416	TS.diHPCARP_I.14aldHshift.mtmtmpu	2.739e+43	2.69	2.69	2.996e+41	1.77
22417	TS.diHPCARP_I.14aldHshift.ttmppmu	2.528e+43	2.72	2.72	2.641e+41	1.56
22418	TS.diHPCARP_I.14aldHshift.tpptmmpu	8.332e+43	3.47	3.47	2.465e+41	1.46
22419	TS.diHPCARP_I.14aldHshift.tmmmpmu	1.395e+43	2.43	2.43	2.385e+41	1.41
22420	TS.diHPCARP_I.14aldHshift.tmmmpmu	2.583e+43	2.80	2.80	2.353e+41	1.39
22421	TS.diHPCARP_I.14aldHshift.tpptppu	2.369e+43	2.78	2.78	2.238e+41	1.32
22422	TS.diHPCARP_I.14aldHshift.mmmmpmu	1.147e+43	2.36	2.36	2.202e+41	1.3
22423	TS.diHPCARP_I.14aldHshift.mmpmpmu	1.060e+43	2.31	2.31	2.199e+41	1.3
22424	TS.diHPCARP_I.14aldHshift.tppppmu	1.968e+43	2.77	2.77	1.904e+41	1.13
22425	TS.diHPCARP_I.14aldHshift.tptmpu	6.164e+42	2.08	2.08	1.892e+41	1.12
22426	TS.diHPCARP_I.14aldHshift.tppppmu	1.077e+43	2.67	2.67	1.220e+41	0.722
22427	TS.diHPCARP_I.14aldHshift.tppmpmu	1.060e+43	2.68	2.68	1.188e+41	0.703
22428	TS.diHPCARP_I.14aldHshift.ttmtpu	4.072e+43	3.48	3.48	1.184e+41	0.7
22429	TS.diHPCARP_I.14aldHshift.tpmmpmu	1.545e+43	3.00	3.00	1.016e+41	0.601
22430	Total				1.690e+43	100

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22434 1,5-aldehyde-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-Ib)
22435
22436 =====
22437 =

22438

22439 Note: both enantiomers (R,R and S,S) were calculated at the M06-2X/cc-pVDZ level based
 22440 on
 22441 a different template, to check the robustness of the conformer space search. As can be
 22442 seen,
 22443 most conformers are found in both enantiomers, though some higher-energy conformers
 22444 are
 22445 missing in either the R,R or S,S set. The impact on the rate predictions was
 22446 found to be negligible. At the M06-02X/aug-cc-pVTZ level of theory, only a single set
 22447 of
 22448 enantiomers was calculated.

22449 Population analysis at 300K. Vibrational scaling: 0.971.
 22450 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 22451 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22452 %: contribution to the population (with current data set assumed 100%)

22453 Compound	Qtot	Erel	Erel2	n*Q*MB	%
22454 -----					
22455 TS.diHPCARP_Ib.15aldHshift.upuppudd	1.380e+43	0.18	0.18	1.027e+43	24.5
22456 TS.diHPCARP_Ib.15aldHshift.umdmuudd	7.662e+42	0.00	0.00	7.662e+42	18.3
22457 TS.diHPCARP_Ib.15aldHshift.utuppudd	8.593e+42	0.42	0.42	4.278e+42	10.2
22458 TS.diHPCARP_Ib.15aldHshift.utdtpduu	5.653e+43	1.57	1.57	4.082e+42	9.75
22459 TS.diHPCARP_Ib.15aldHshift.utdttuud	2.630e+43	1.41	1.41	2.479e+42	5.92
22460 TS.diHPCARP_Ib.15aldHshift.utupmuuu	9.121e+42	0.86	0.86	2.154e+42	5.15
22461 TS.diHPCARP_Ib.15aldHshift.utdmuudd	2.821e+43	1.76	1.76	1.481e+42	3.54
22462 TS.diHPCARP_Ib.15aldHshift.utummuud	5.666e+43	2.21	2.21	1.385e+42	3.31
22463 TS.diHPCARP_Ib.15aldHshift.upuptddd	1.943e+43	1.58	1.58	1.381e+42	3.3
22464 TS.diHPCARP_Ib.15aldHshift.umdtmddd	4.487e+43	2.17	2.17	1.176e+42	2.81
22465 TS.diHPCARP_Ib.15aldHshift.utummudd	5.481e+42	1.13	1.13	8.195e+41	1.96
22466 TS.diHPCARP_Ib.15aldHshift.umdtpddd	1.845e+43	1.87	1.87	7.992e+41	1.91
22467 TS.diHPCARP_Ib.15aldHshift.utdppudd	1.500e+43	1.81	1.81	7.172e+41	1.71
22468 TS.diHPCARP_Ib.15aldHshift.uputmudd	4.961e+43	2.64	2.64	5.936e+41	1.42
22469 TS.diHPCARP_Ib.15aldHshift.umdmuudd	3.349e+43	2.48	2.48	5.244e+41	1.25
22470 TS.diHPCARP_Ib.15aldHshift.umdmtddd	5.362e+42	1.44	1.44	4.780e+41	1.14
22471 TS.diHPCARP_Ib.15aldHshift.updmuudd	1.093e+43	1.90	1.90	4.534e+41	1.08
22472 TS.diHPCARP_Ib.15aldHshift.utdmuudd	4.911e+42	1.80	1.80	2.398e+41	0.573
22473 TS.diHPCARP_Ib.15aldHshift.utupmuudd	8.325e+42	2.14	2.14	2.312e+41	0.552
22474 TS.diHPCARP_Ib.15aldHshift.utuppuuu	8.486e+42	2.21	2.21	2.096e+41	0.501
22475 TS.diHPCARP_Ib.15aldHshift.updmtddd	8.898e+42	2.34	2.34	1.754e+41	0.419
22476 TS.diHPCARP_Ib.15aldHshift.utdppddd	7.469e+42	2.39	2.39	1.353e+41	0.323
22477 TS.diHPCARP_Ib.15aldHshift.umdppduu	8.288e+42	2.86	2.86	6.840e+40	0.163
22478 TS.diHPCARP_Ib.15aldHshift.upumpddd	6.823e+42	2.82	2.82	6.025e+40	0.144
22479 Total				4.186e+43	100

22480
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 22483 1,6-aldehyde-H-shift in (2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-
 22484 Ic)
 22485 =====

22486 =
 22487

22488 Population analysis at 300K. Vibrational scaling: 0.971.
 22489 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)
 22490 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22491 %: contribution to the population (with current data set assumed 100%)

22492 Compound	Qtot	Erel	Erel2	n*Q*MB	%
22493 -----					
22494 TS.diHPCARP_Ic.16aldHshift.a.pmtmud	6.737e+42	0.00	0.00	6.737e+42	46.5
22495 TS.diHPCARP_Ic.16aldHshift.b.pmtmud	6.862e+42	0.66	0.66	2.265e+42	15.6
22496 TS.diHPCARP_Ic.16aldHshift.a.pmmuud	1.902e+43	1.44	1.44	1.706e+42	11.8
22497 TS.diHPCARP_Ic.16aldHshift.a.mptmud	7.452e+42	1.06	1.06	1.253e+42	8.66
22498 TS.diHPCARP_Ic.16aldHshift.a.pmpmdu	1.205e+43	1.92	1.92	4.798e+41	3.31
22499 TS.diHPCARP_Ic.16aldHshift.b.mptmud	7.069e+42	1.92	1.92	2.820e+41	1.95
22500 TS.diHPCARP_Ic.16aldHshift.e.pptmud	5.857e+42	1.82	1.82	2.779e+41	1.92
22501 TS.diHPCARP_Ic.16aldHshift.b.pmpmdu	6.102e+42	1.98	1.98	2.214e+41	1.53
22502 TS.diHPCARP_Ic.16aldHshift.a.pmpmdu	4.268e+43	3.20	3.20	2.002e+41	1.38
22503 TS.diHPCARP_Ic.16aldHshift.a.mppmuud	1.965e+43	2.85	2.85	1.662e+41	1.15
22504 TS.diHPCARP_Ic.16aldHshift.a.pptmud	5.882e+42	2.23	2.23	1.401e+41	0.968
22505 TS.diHPCARP_Ic.16aldHshift.a.pppmdu	9.226e+42	2.50	2.50	1.396e+41	0.964
22506 TS.diHPCARP_Ic.16aldHshift.e.pptpud	7.688e+42	2.49	2.49	1.178e+41	0.813
22507 TS.diHPCARP_Ic.16aldHshift.a.pmpmdu	1.896e+43	3.15	3.15	9.658e+40	0.667
22508 TS.diHPCARP_Ic.16aldHshift.a.pmpmdu	1.160e+43	2.86	2.86	9.612e+40	0.664
22509 TS.diHPCARP_Ic.16aldHshift.a.tmpmdu	9.360e+42	2.96	2.96	6.561e+40	0.453
22510 TS.diHPCARP_Ic.16aldHshift.a.pppmdu	3.377e+43	3.95	3.95	4.493e+40	0.31

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22511 TS.diHPCARP_Ic.16aldHshift.b.pppud 4.893e+42 2.80 2.80 4.489e+40 0.31
22512 TS.diHPCARP_Ic.16aldHshift.a.pptud 7.907e+42 3.13 3.13 4.176e+40 0.288
22513 TS.diHPCARP_Ic.16aldHshift.a.pmpdu 3.632e+43 4.11 4.11 3.654e+40 0.252
22514 TS.diHPCARP_Ic.16aldHshift.a.pmmdu 3.166e+43 4.45 4.45 1.816e+40 0.125
22515 TS.diHPCARP_Ic.16aldHshift.a.mppdu 7.236e+42 3.61 3.61 1.706e+40 0.118
22516 TS.diHPCARP_Ic.16aldHshift.b.mppud 6.912e+42 3.60 3.60 1.646e+40 0.114
22517 TS.diHPCARP_Ic.16aldHshift.e.pmpdu 1.694e+43 4.44 4.44 9.791e+39 0.0676
22518 TS.diHPCARP_Ic.16aldHshift.e.mppdu 5.903e+42 4.28 4.28 4.514e+39 0.0312
22519 Total 1.448e+43 100
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22521
22522
22523 1,6-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-
22524 HPCARP-Ia), forming B' (di-HPCARP-Ib)
22525 =====
22526 =====
22527
22528 Population analysis at 300K. Vibrational scaling: 0.971.
22529 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22530 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22531 %: contribution to the population (with current data set assumed 100%)
22532 Compound Qtot Erel Erel2 n*Q*MB %
22533 -----
22534 TS.diHPCARP_I.1600HHshift.b.lmmpdu 3.725e+42 0.00 0.00 3.725e+42 92.5
22535 TS.diHPCARP_I.1600HHshift.b.hppmud 3.044e+42 2.14 2.14 8.438e+40 2.1
22536 TS.diHPCARP_I.1600HHshift.a.tppud 1.594e+43 3.31 3.31 6.225e+40 1.55
22537 TS.diHPCARP_I.1600HHshift.b.ttpdu 1.888e+43 3.44 3.44 5.899e+40 1.47
22538 TS.diHPCARP_I.1600HHshift.b.tmpdu 6.185e+42 2.96 2.96 4.307e+40 1.07
22539 TS.diHPCARP_I.1600HHshift.b.lppmdu 1.128e+43 3.69 3.69 2.331e+40 0.579
22540 TS.diHPCARP_I.1600HHshift.a.ttpud 1.275e+43 3.94 3.94 1.706e+40 0.424
22541 TS.diHPCARP_I.1600HHshift.b.lppud 1.622e+43 4.66 4.66 6.570e+39 0.163
22542 TS.diHPCARP_I.1600HHshift.a.lmmpdu 6.360e+42 4.29 4.29 4.762e+39 0.118
22543 Total 4.025e+42 100
22544
22545
22546
22547 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-
22548 HPCARP-Ia), forming C' (di-HPCARP-Ic)
22549 =====
22550 =====
22551
22552 Population analysis at 300K. Vibrational scaling: 0.971.
22553 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22554 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22555 %: contribution to the population (with current data set assumed 100%)
22556 Compound Qtot Erel Erel2 n*Q*MB %
22557 -----
22558 TS.diHPCARP_I.1700HHshift.BB.tmuud 7.055e+42 0.00 0.00 7.055e+42 46.9
22559 TS.diHPCARP_I.1700HHshift.BB.ttdud 1.269e+43 0.65 0.65 4.267e+42 28.4
22560 TS.diHPCARP_I.1700HHshift.BB.ttudu 1.097e+43 0.99 0.99 2.070e+42 13.8
22561 TS.diHPCARP_I.1700HHshift.BB.htdud 2.185e+43 2.59 2.59 2.849e+41 1.89
22562 TS.diHPCARP_I.1700HHshift.BB.ttuud 3.101e+43 2.82 2.82 2.739e+41 1.82
22563 TS.diHPCARP_I.1700HHshift.CR.hpddu 4.723e+42 1.70 1.70 2.728e+41 1.81
22564 TS.diHPCARP_I.1700HHshift.BB.mmdud 6.497e+42 2.19 2.19 1.653e+41 1.1
22565 TS.diHPCARP_I.1700HHshift.BB.tmuud 2.330e+42 1.68 1.68 1.394e+41 0.926
22566 TS.diHPCARP_I.1700HHshift.BB.ltuud 1.559e+43 2.84 2.84 1.331e+41 0.885
22567 TS.diHPCARP_I.1700HHshift.BB.lmddu 1.043e+43 2.69 2.69 1.136e+41 0.755
22568 TS.diHPCARP_I.1700HHshift.BB.tpdud 5.503e+42 2.39 2.39 9.941e+40 0.661
22569 TS.diHPCARP_I.1700HHshift.BB.ltdud 1.714e+43 3.19 3.19 8.189e+40 0.544
22570 TS.diHPCARP_I.1700HHshift.BB.lpuud 1.231e+43 3.00 3.00 8.059e+40 0.535
22571 TS.diHPCARP_I.1700HHshift.BB.cmudu 2.420e+42 3.13 3.13 1.270e+40 0.0844
22572 Total 1.505e+43 100
22573
22574
22575
22576 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-
22577 HPCARP-Ib), forming C' (di-HPCARP-Ic)
22578 =====
22579 =====
22580
22581 Population analysis at 300K. Vibrational scaling: 0.971.
22582 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)

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22583 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22584 %: contribution to the population (with current data set assumed 100%)
 22585 Compound Qtot Erel Erel2 n*Q*MB %
 22586 -----

22587	TS.diHPCARP_Ib.1600HHshift.b.cppmud	3.170e+43	0.63	0.63	1.109e+43	20.2
22588	TS.diHPCARP_Ib.1600HHshift.a.cppmud	1.544e+43	0.42	0.42	7.608e+42	13.9
22589	TS.diHPCARP_Ib.1600HHshift.a.lttmud	1.453e+43	0.50	0.50	6.288e+42	11.5
22590	TS.diHPCARP_Ib.1600HHshift.b.pmpmud	6.225e+42	0.00	0.00	6.225e+42	11.4
22591	TS.diHPCARP_Ib.1600HHshift.b.lttmud	1.359e+43	0.67	0.67	4.439e+42	8.09
22592	TS.diHPCARP_Ib.1600HHshift.b.ltpud	1.070e+43	0.53	0.53	4.379e+42	7.99
22593	TS.diHPCARP_Ib.1600HHshift.a.lmppud	6.043e+42	0.46	0.46	2.792e+42	5.09
22594	TS.diHPCARP_Ib.1600HHshift.a.httpdu	4.274e+42	0.33	0.33	2.448e+42	4.47
22595	TS.diHPCARP_Ib.1600HHshift.b.cmpmud	1.410e+43	1.06	1.06	2.378e+42	4.34
22596	TS.diHPCARP_Ib.1600HHshift.a.ltpud	9.452e+42	0.97	0.97	1.871e+42	3.41
22597	TS.diHPCARP_Ib.1600HHshift.a.cmpmud	5.683e+42	0.81	0.81	1.452e+42	2.65
22598	TS.diHPCARP_Ib.1600HHshift.b.lmppud	8.776e+42	1.13	1.13	1.321e+42	2.41
22599	TS.diHPCARP_Ib.1600HHshift.a.cmpmud	1.005e+43	1.38	1.38	9.995e+41	1.82
22600	TS.diHPCARP_Ib.1600HHshift.a.lmtmud	9.776e+42	1.63	1.63	6.313e+41	1.15
22601	TS.diHPCARP_Ib.1600HHshift.b.pmpmud	1.113e+43	1.93	1.93	4.400e+41	0.802
22602	TS.diHPCARP_Ib.1600HHshift.b.lmtmud	1.470e+43	2.10	2.10	4.321e+41	0.788
22603	TS.diHPCARP_Ib.1600HHshift.a.ltpud	1.490e+43	3.45	3.45	4.568e+40	0.0833
22604	Total				5.484e+43	100

22605
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 22607
 22608 1,4-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-
 22609 di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde
 22610 =====
 22611 =====

22612
 22613 Population analysis at 300K. Vibrational scaling: 0.971.
 22614 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
 22615 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22616 %: contribution to the population (with current data set assumed 100%)
 22617 Compound Qtot Erel Erel2 n*Q*MB %
 22618 -----

22619	TS.diHPCARP_I.14HPHshift.mtppptd	4.550e+42	0.00	0.00	4.550e+42	94.8
22620	TS.diHPCARP_I.14HPHshift.mttmtd	3.146e+43	3.00	3.00	2.043e+41	4.25
22621	TS.diHPCARP_I.14HPHshift.mptmtd	1.785e+43	3.93	3.93	2.446e+40	0.509
22622	TS.diHPCARP_I.14HPHshift.mppmtd	1.291e+43	3.78	3.78	2.267e+40	0.472
22623	Total				4.801e+42	100

22624
 22625
 22626
 22627 1,5-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,R-
 22628 di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde
 22629 =====
 22630 =====

22631
 22632 Population analysis at 300K. Vibrational scaling: 0.971.
 22633 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
 22634 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
 22635 %: contribution to the population (with current data set assumed 100%)
 22636 Compound Qtot Erel Erel2 n*Q*MB %
 22637 -----

22638	TS.diHPCARP_I.15HPHshift.dmmmdmudu	4.206e+43	0.27	0.27	2.653e+43	30.7
22639	TS.diHPCARP_I.15HPHshift.dmpumudu	9.276e+43	1.19	1.19	1.261e+43	14.6
22640	TS.diHPCARP_I.15HPHshift.dmpdmudu	1.153e+44	1.34	1.34	1.216e+43	14.1
22641	TS.diHPCARP_I.15HPHshift.dcmumudu	8.863e+43	1.54	1.54	6.731e+42	7.78
22642	TS.diHPCARP_I.15HPHshift.dmpupudu	2.831e+43	1.12	1.12	4.314e+42	4.99
22643	TS.diHPCARP_I.15HPHshift.dmtdpuuu	3.618e+42	0.00	0.00	3.618e+42	4.18
22644	TS.diHPCARP_I.15HPHshift.dmmtdtddu	6.638e+42	0.37	0.37	3.569e+42	4.12
22645	TS.diHPCARP_I.15HPHshift.dctdmudu	1.067e+44	2.14	2.14	2.932e+42	3.39
22646	TS.diHPCARP_I.15HPHshift.dmpdpudu	2.633e+43	1.37	1.37	2.645e+42	3.06
22647	TS.diHPCARP_I.15HPHshift.dmmdpudu	1.164e+43	1.14	1.14	1.714e+42	1.98
22648	TS.diHPCARP_I.15HPHshift.dmtdpddu	6.539e+43	2.34	2.34	1.286e+42	1.49
22649	TS.diHPCARP_I.15HPHshift.dctmudu	1.609e+44	2.96	2.96	1.116e+42	1.29
22650	TS.diHPCARP_I.15HPHshift.dmmdpddu	1.834e+43	1.69	1.69	1.082e+42	1.25
22651	TS.diHPCARP_I.15HPHshift.dmmupddu	3.080e+43	2.05	2.05	9.897e+41	1.14
22652	TS.diHPCARP_I.15HPHshift.dcmupddu	3.053e+43	2.05	2.05	9.745e+41	1.13
22653	TS.diHPCARP_I.15HPHshift.dmpdtddu	1.681e+43	1.90	1.90	6.910e+41	0.799
22654	TS.diHPCARP_I.15HPHshift.dmpdtddu	1.700e+43	1.92	1.92	6.815e+41	0.788

22655	TS.diHPCARP_I.15HPHshift.dmmupudu	1.649e+43	1.91	1.91	6.721e+41	0.777
22656	TS.diHPCARP_I.15HPHshift.dmmutddu	1.544e+43	1.93	1.93	6.107e+41	0.706
22657	TS.diHPCARP_I.15HPHshift.dmtdddu	1.199e+43	2.01	2.01	4.096e+41	0.473
22658	TS.diHPCARP_I.15HPHshift.dmmtdudu	4.230e+43	2.81	2.81	3.824e+41	0.442
22659	TS.diHPCARP_I.15HPHshift.dmmupuuu	8.892e+42	1.93	1.93	3.481e+41	0.402
22660	TS.diHPCARP_I.15HPHshift.dcpdpudu	2.138e+43	3.02	3.02	1.342e+41	0.155
22661	TS.diHPCARP_I.15HPHshift.dcpdpddu	2.012e+43	3.08	3.08	1.156e+41	0.134
22662	TS.diHPCARP_I.15HPHshift.dmpupuuu	3.003e+42	2.12	2.12	8.531e+40	0.0986
22663	TS.diHPCARP_I.15HPHshift.dmpuutdu	6.164e+42	2.58	2.58	8.115e+40	0.0938
22664	TS.diHPCARP_I.15HPHshift.dcmuutdu	3.521e+42	2.52	2.52	5.129e+40	0.0593
22665	Total				8.654e+43	100

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22669 #####
22670 M06-2X/aug-cc-pVTZ data for tri-HPACYL-I
22671 #####

(2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)

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22674 =====
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22676 Population analysis at 300K. Vibrational scaling: 0.971.
22677 Qtot: Total partition function (m^-3). Erel, Erel2: Relative energy (kcal/mol)
22678 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.
22679 %: contribution to the population (with current data set assumed 100%)

22680	Compound	Qtot	Erel	Erel2	n*Q*MB	%
22681	-----					
22682	triHPacyl.tmmmtmppd	2.982e+43	0.00	0.00	2.982e+43	10.5
22683	triHPacyl.ppmmpmmd	1.084e+44	1.29	1.29	1.236e+43	4.34
22684	triHPacyl.ppmmpmmd	1.083e+44	1.29	1.29	1.233e+43	4.33
22685	triHPacyl.ppmptmppd	1.393e+43	0.11	0.11	1.155e+43	4.05
22686	triHPacyl.pptmptmmd	2.426e+44	1.85	1.85	1.092e+43	3.83
22687	triHPacyl.pptpmtmmd	1.620e+44	1.66	1.66	1.007e+43	3.53
22688	triHPacyl.pptmptmmd	1.676e+44	1.70	1.70	9.691e+42	3.4
22689	triHPacyl.ppmppmmd	2.270e+43	0.52	0.52	9.427e+42	3.31
22690	triHPacyl.ppppmtmmd	1.806e+44	1.91	1.91	7.306e+42	2.56
22691	triHPacyl.tmmmmmpmd	3.510e+43	0.98	0.98	6.770e+42	2.37
22692	triHPacyl.ppmmpmmd	3.165e+43	0.93	0.93	6.635e+42	2.33
22693	triHPacyl.pptmppmmd	1.008e+44	1.65	1.65	6.306e+42	2.21
22694	triHPacyl.pmmmpmmd	2.214e+43	0.75	0.75	6.305e+42	2.21
22695	triHPacyl.tmmmmmpmd	2.422e+44	2.21	2.21	5.969e+42	2.09
22696	triHPacyl.tmtmmtmmd	3.173e+44	2.42	2.42	5.515e+42	1.93
22697	triHPacyl.ppppmtmmd	4.949e+43	1.31	1.31	5.454e+42	1.91
22698	triHPacyl.ppppmtmmd	1.476e+44	1.97	1.97	5.406e+42	1.9
22699	triHPacyl.pptmptmmd	4.861e+43	1.39	1.39	4.745e+42	1.66
22700	triHPacyl.ppmppmmd	1.804e+43	0.80	0.80	4.733e+42	1.66
22701	triHPacyl.ppppmtmmd	3.462e+43	1.19	1.19	4.677e+42	1.64
22702	triHPacyl.tmtmmtmmd	5.831e+43	1.51	1.51	4.665e+42	1.64
22703	triHPacyl.tmmmtmmd	6.068e+43	1.53	1.53	4.643e+42	1.63
22704	triHPacyl.tmmmmmpmd	7.074e+43	1.65	1.65	4.431e+42	1.55
22705	triHPacyl.ppppmtmmd	6.418e+43	1.64	1.64	4.130e+42	1.45
22706	triHPacyl.pptpmtmmd	5.524e+43	1.56	1.56	4.056e+42	1.42
22707	triHPacyl.ppppmtmmd	8.832e+43	1.84	1.84	4.042e+42	1.42
22708	triHPacyl.tpmmmmpmd	2.751e+43	1.17	1.17	3.893e+42	1.37
22709	triHPacyl.pptmptmmd	9.848e+43	1.95	1.95	3.733e+42	1.31
22710	triHPacyl.tmtmmtmmd	7.804e+43	1.83	1.83	3.627e+42	1.27
22711	triHPacyl.ppmmpmmd	6.873e+43	1.80	1.80	3.369e+42	1.18
22712	triHPacyl.pptmppmmd	3.098e+43	1.34	1.34	3.249e+42	1.14
22713	triHPacyl.pmtmptmmd	2.013e+44	2.48	2.48	3.168e+42	1.11
22714	triHPacyl.pptpmtmmd	3.519e+43	1.46	1.46	3.064e+42	1.07
22715	triHPacyl.pptpmtmmd	4.111e+43	1.61	1.61	2.782e+42	0.976
22716	triHPacyl.tpmmmmpmd	1.948e+43	1.19	1.19	2.646e+42	0.928
22717	triHPacyl.tmmmtmmd	5.325e+43	1.80	1.80	2.594e+42	0.91
22718	triHPacyl.pppppmmd	6.569e+43	1.95	1.95	2.503e+42	0.878
22719	triHPacyl.pmmmpmmd	2.080e+43	1.28	1.28	2.435e+42	0.854
22720	triHPacyl.tmtmmtmmd	3.693e+43	1.68	1.68	2.192e+42	0.769
22721	triHPacyl.ptmmpmmd	1.015e+44	2.30	2.30	2.135e+42	0.749
22722	triHPacyl.pmpmmtmmd	2.261e+43	1.41	1.41	2.124e+42	0.745
22723	triHPacyl.mtptmmd	4.771e+43	1.87	1.87	2.073e+42	0.727
22724	triHPacyl.pmtmptmmd	3.025e+43	1.63	1.63	1.976e+42	0.693
22725	triHPacyl.ptmmpmmd	3.383e+43	1.73	1.73	1.872e+42	0.657
22726	triHPacyl.pmmmpmmd	4.693e+43	1.96	1.96	1.750e+42	0.614

22727	triHPacyl.pppmptmpmd	3.621e+43	1.82	1.82	1.711e+42	0.6
22728	triHPacyl.tpmmtmpmd	3.436e+43	1.80	1.80	1.685e+42	0.591
22729	triHPacyl.ptmmmtmpmd	4.355e+43	1.94	1.94	1.685e+42	0.591
22730	triHPacyl.pptmptmpmd	2.699e+43	1.72	1.72	1.508e+42	0.529
22731	triHPacyl.pptppmmpmd	2.489e+43	1.68	1.68	1.486e+42	0.521
22732	triHPacyl.ttpmmtmpmd	1.609e+43	1.42	1.42	1.482e+42	0.52
22733	triHPacyl.ttmmmtmpmd	4.945e+43	2.13	2.13	1.399e+42	0.491
22734	triHPacyl.pptmptmpmd	5.053e+43	2.19	2.19	1.275e+42	0.447
22735	triHPacyl.mmtmptmpmd	3.750e+43	2.02	2.02	1.274e+42	0.447
22736	triHPacyl.tmpmmtmpmd	3.756e+43	2.03	2.03	1.245e+42	0.437
22737	triHPacyl.ttpmmtmpmd	3.260e+43	1.97	1.97	1.201e+42	0.421
22738	triHPacyl.pmmmtmpmd	6.815e+43	2.46	2.46	1.106e+42	0.388
22739	triHPacyl.mtmmtmpmd	3.616e+43	2.09	2.09	1.086e+42	0.381
22740	triHPacyl.ptmmtmpmd	3.301e+43	2.04	2.04	1.071e+42	0.376
22741	triHPacyl.tmtmptmpmd	6.989e+43	2.49	2.49	1.070e+42	0.375
22742	triHPacyl.ppppmpmd	1.613e+43	1.66	1.66	1.004e+42	0.352
22743	triHPacyl.tpmmmmpmd	1.915e+43	1.81	1.81	9.155e+41	0.321
22744	triHPacyl.pmpmmtmpmd	1.834e+43	1.82	1.82	8.673e+41	0.304
22745	triHPacyl.pmtmmtmpmd	2.010e+43	1.89	1.89	8.476e+41	0.297
22746	triHPacyl.tmpmmtmpmd	2.996e+43	2.14	2.14	8.225e+41	0.289
22747	triHPacyl.ttpmmtmpmd	1.322e+43	1.72	1.72	7.424e+41	0.26
22748	triHPacyl.mmtmptmpmd	4.079e+43	2.44	2.44	6.832e+41	0.24
22749	triHPacyl.mmpmptmpmd	2.922e+43	2.29	2.29	6.321e+41	0.222
22750	triHPacyl.mmtppmmpmd	3.321e+43	2.39	2.39	6.073e+41	0.213
22751	triHPacyl.pmpmptmpmd	8.540e+42	1.59	1.59	5.886e+41	0.206
22752	triHPacyl.ptmmmtmpmd	6.157e+43	2.81	2.81	5.508e+41	0.193
22753	triHPacyl.mmpmptmpmd	4.534e+43	2.69	2.69	4.935e+41	0.173
22754	triHPacyl.pmtmmtmpmd	2.291e+43	2.38	2.38	4.246e+41	0.149
22755	triHPacyl.pmpmptmpmd	7.744e+42	1.75	1.75	4.080e+41	0.143
22756	triHPacyl.mmpmptmpmd	4.576e+43	2.84	2.84	3.929e+41	0.138
22757	triHPacyl.pppmmtmpmd	1.977e+43	2.35	2.35	3.826e+41	0.134
22758	triHPacyl.pppppmpmd	1.844e+43	2.43	2.43	3.152e+41	0.111
22759	triHPacyl.mtpmptmpmd	8.382e+43	3.36	3.36	3.010e+41	0.106
22760	triHPacyl.pmpmptmpmd	1.721e+43	2.45	2.45	2.825e+41	0.0991
22761	triHPacyl.ptpmtmpmd	1.216e+43	2.37	2.37	2.288e+41	0.0803
22762	triHPacyl.mmpmptmpmd	1.848e+43	3.15	3.15	9.298e+40	0.0326
22763	triHPacyl.mppmptmpmd	7.423e+42	3.07	3.07	4.301e+40	0.0151
22764	Total				2.851e+44	100

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CO elimination from (2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)

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Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m^{-3}). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
22776					
22777	TS.triHPacyl.COelim.tmtmmtmpmd	1.619e+44	0.00	0.00	1.619e+44 6.02
22778	TS.triHPacyl.COelim.tmtmmmtmpmd	1.633e+44	0.07	0.07	1.446e+44 5.38
22779	TS.triHPacyl.COelim.tmtmptmpmd	2.617e+44	0.58	0.58	9.915e+43 3.69
22780	TS.triHPacyl.COelim.ppppmpmd	1.378e+44	0.22	0.22	9.576e+43 3.56
22781	TS.triHPacyl.COelim.ppmmtmpmd	4.720e+44	1.06	1.06	7.952e+43 2.96
22782	TS.triHPacyl.COelim.tmtmmtmpmd	3.495e+44	0.90	0.90	7.727e+43 2.87
22783	TS.triHPacyl.COelim.ppmmtmpmd	7.869e+44	1.41	1.41	7.429e+43 2.76
22784	TS.triHPacyl.COelim.tmtmptmpmd	4.725e+44	1.11	1.11	7.378e+43 2.74
22785	TS.triHPacyl.COelim.tmtmptmpmd	4.625e+44	1.14	1.14	6.779e+43 2.52
22786	TS.triHPacyl.COelim.ppmmpmpmd	1.309e+44	0.48	0.48	5.871e+43 2.18
22787	TS.triHPacyl.COelim.tmtmmtmpmd	1.760e+44	0.66	0.66	5.802e+43 2.16
22788	TS.triHPacyl.COelim.ppmmtmpmd	1.638e+44	0.66	0.66	5.419e+43 2.02
22789	TS.triHPacyl.COelim.pptmptmpmd	4.777e+44	1.30	1.30	5.415e+43 2.01
22790	TS.triHPacyl.COelim.tmtmmtmpmd	3.103e+44	1.06	1.06	5.237e+43 1.95
22791	TS.triHPacyl.COelim.ppmmtmpmd	6.304e+43	0.12	0.12	5.141e+43 1.91
22792	TS.triHPacyl.COelim.tmtmmtmpmd	2.584e+44	0.98	0.98	4.995e+43 1.86
22793	TS.triHPacyl.COelim.ppppmpmd	2.069e+44	0.85	0.85	4.990e+43 1.86
22794	TS.triHPacyl.COelim.ppppmpmd	2.011e+44	0.84	0.84	4.889e+43 1.82
22795	TS.triHPacyl.COelim.tmtmmtmpmd	6.758e+44	1.57	1.57	4.872e+43 1.81
22796	TS.triHPacyl.COelim.pptmptmpmd	3.417e+44	1.17	1.17	4.834e+43 1.8
22797	TS.triHPacyl.COelim.pptmptmpmd	3.663e+44	1.21	1.21	4.821e+43 1.79
22798	TS.triHPacyl.COelim.tmtmmtmpmd	6.245e+44	1.54	1.54	4.755e+43 1.77

22799	TS.triHPacyl.COelim.ppppptomnd	4.321e+44	1.39	1.39	4.228e+43	1.57
22800	TS.triHPacyl.COelim.tmtmtmnmnd	2.541e+44	1.09	1.09	4.049e+43	1.51
22801	TS.triHPacyl.COelim.pptpptomnd	1.664e+44	0.89	0.89	3.720e+43	1.38
22802	TS.triHPacyl.COelim.tmtmmmmnmnd	2.744e+44	1.21	1.21	3.596e+43	1.34
22803	TS.triHPacyl.COelim.pptmptomnd	8.868e+43	0.55	0.55	3.543e+43	1.32
22804	TS.triHPacyl.COelim.tmtppmnmnd	3.836e+44	1.44	1.44	3.442e+43	1.28
22805	TS.triHPacyl.COelim.tmmmtmnmnd	1.661e+44	1.00	1.00	3.111e+43	1.16
22806	TS.triHPacyl.COelim.pppppptomnd	5.180e+44	1.71	1.71	2.949e+43	1.1
22807	TS.triHPacyl.COelim.ppmptomnd	1.055e+44	0.81	0.81	2.732e+43	1.02
22808	TS.triHPacyl.COelim.pmmptomnd	6.716e+43	0.54	0.54	2.716e+43	1.01
22809	TS.triHPacyl.COelim.tmmmmnmnd	1.880e+44	1.20	1.20	2.527e+43	0.94
22810	TS.triHPacyl.COelim.tppptomnd	5.139e+44	1.80	1.80	2.523e+43	0.938
22811	TS.triHPacyl.COelim.pptptomnd	4.539e+44	1.72	1.72	2.515e+43	0.936
22812	TS.triHPacyl.COelim.tmtmmmmnmnd	5.192e+44	1.81	1.81	2.507e+43	0.932
22813	TS.triHPacyl.COelim.tmtmptomnd	1.413e+44	1.04	1.04	2.480e+43	0.923
22814	TS.triHPacyl.COelim.tptmtmnmnd	8.987e+44	2.15	2.15	2.428e+43	0.903
22815	TS.triHPacyl.COelim.tpmmmnmnd	8.905e+43	0.78	0.78	2.407e+43	0.895
22816	TS.triHPacyl.COelim.pppppptomnd	3.427e+44	1.59	1.59	2.390e+43	0.889
22817	TS.triHPacyl.COelim.pptmptomnd	1.328e+44	1.05	1.05	2.277e+43	0.847
22818	TS.triHPacyl.COelim.pptptomnd	1.248e+44	1.02	1.02	2.263e+43	0.842
22819	TS.triHPacyl.COelim.pptptomnd	4.700e+44	1.82	1.82	2.202e+43	0.819
22820	TS.triHPacyl.COelim.tmtptomnd	7.045e+44	2.08	2.08	2.139e+43	0.796
22821	TS.triHPacyl.COelim.pptptomnd	5.731e+44	1.96	1.96	2.131e+43	0.793
22822	TS.triHPacyl.COelim.pmmptomnd	4.411e+44	1.81	1.81	2.129e+43	0.792
22823	TS.triHPacyl.COelim.tmtppnmnmnd	7.883e+44	2.16	2.16	2.118e+43	0.788
22824	TS.triHPacyl.COelim.pmtmptomnd	2.088e+44	1.39	1.39	2.015e+43	0.749
22825	TS.triHPacyl.COelim.tmtmtmnmnd	4.445e+44	1.85	1.85	2.003e+43	0.745
22826	TS.triHPacyl.COelim.pptptomnd	2.343e+44	1.48	1.48	1.972e+43	0.734
22827	TS.triHPacyl.COelim.tmmmmnmnmnd	2.039e+44	1.43	1.43	1.866e+43	0.694
22828	TS.triHPacyl.COelim.tmmmtmnmnd	4.040e+44	1.86	1.86	1.780e+43	0.662
22829	TS.triHPacyl.COelim.pptptomnd	2.000e+44	1.48	1.48	1.670e+43	0.621
22830	TS.triHPacyl.COelim.tptmtmnmnd	7.269e+44	2.27	2.27	1.613e+43	0.6
22831	TS.triHPacyl.COelim.pptptomnd	2.317e+44	1.59	1.59	1.600e+43	0.595
22832	TS.triHPacyl.COelim.pptptomnd	1.264e+44	1.23	1.23	1.595e+43	0.593
22833	TS.triHPacyl.COelim.tmmmtmnmnd	1.600e+44	1.38	1.38	1.591e+43	0.592
22834	TS.triHPacyl.COelim.tppnmnmnd	3.612e+44	1.90	1.90	1.501e+43	0.558
22835	TS.triHPacyl.COelim.tmtmptomnd	5.049e+44	2.10	2.10	1.494e+43	0.556
22836	TS.triHPacyl.COelim.pptptomnd	6.020e+44	2.22	2.22	1.443e+43	0.537
22837	TS.triHPacyl.COelim.tppptomnd	1.047e+45	2.55	2.55	1.443e+43	0.537
22838	TS.triHPacyl.COelim.pptppnmnmnd	1.573e+44	1.44	1.44	1.399e+43	0.52
22839	TS.triHPacyl.COelim.ppmptomnd	8.550e+44	2.47	2.47	1.357e+43	0.505
22840	TS.triHPacyl.COelim.tpmmmnmnmnd	6.095e+43	0.94	0.94	1.254e+43	0.467
22841	TS.triHPacyl.COelim.tpmmtmnmnd	7.813e+43	1.24	1.24	9.806e+42	0.365
22842	TS.triHPacyl.COelim.tppnmnmnd	4.182e+44	2.25	2.25	9.594e+42	0.357
22843	TS.triHPacyl.COelim.ppmptomnd	3.621e+44	2.21	2.21	8.897e+42	0.331
22844	TS.triHPacyl.COelim.pppptomnd	1.143e+44	1.53	1.53	8.840e+42	0.329
22845	TS.triHPacyl.COelim.pmtptomnd	1.158e+44	1.55	1.55	8.667e+42	0.322
22846	TS.triHPacyl.COelim.tppnmnmnd	4.414e+43	0.98	0.98	8.514e+42	0.317
22847	TS.triHPacyl.COelim.mmtmptomnd	1.547e+44	1.74	1.74	8.288e+42	0.308
22848	TS.triHPacyl.COelim.mmtppnmnmnd	1.461e+44	1.74	1.74	7.850e+42	0.292
22849	TS.triHPacyl.COelim.tpmmtmnmnd	1.357e+44	1.73	1.73	7.473e+42	0.278
22850	TS.triHPacyl.COelim.pmtmmnmnmnd	1.279e+44	1.70	1.70	7.349e+42	0.273
22851	TS.triHPacyl.COelim.pmmmtppnd	8.928e+43	1.50	1.50	7.155e+42	0.266
22852	TS.triHPacyl.COelim.pppptomnd	1.585e+44	1.85	1.85	7.059e+42	0.263
22853	TS.triHPacyl.COelim.ppmptomnd	1.678e+44	1.89	1.89	7.017e+42	0.261
22854	TS.triHPacyl.COelim.mmtptomnd	1.230e+44	1.82	1.82	5.789e+42	0.215
22855	TS.triHPacyl.COelim.pptppnmnmnd	1.619e+44	1.99	1.99	5.704e+42	0.212
22856	TS.triHPacyl.COelim.ptppptomnd	3.213e+43	1.18	1.18	4.434e+42	0.165
22857	TS.triHPacyl.COelim.pmtmmnmnmnd	1.642e+44	2.24	2.24	3.826e+42	0.142
22858	TS.triHPacyl.COelim.mmtptomnd	1.654e+44	2.25	2.25	3.769e+42	0.14
22859	TS.triHPacyl.COelim.ptppptomnd	3.923e+43	1.41	1.41	3.713e+42	0.138
22860	TS.triHPacyl.COelim.tptmmnmnmnd	2.533e+44	2.58	2.58	3.330e+42	0.124
22861	TS.triHPacyl.COelim.pmpptomnd	2.954e+43	1.37	1.37	2.983e+42	0.111
22862	TS.triHPacyl.COelim.tppptomnd	3.049e+43	1.40	1.40	2.929e+42	0.109
22863	TS.triHPacyl.COelim.tpmmtmnmnd	1.449e+44	2.35	2.35	2.827e+42	0.105
22864	TS.triHPacyl.COelim.pmtmtmnmnd	1.543e+44	2.42	2.42	2.675e+42	0.0995
22865	TS.triHPacyl.COelim.pmmmtmnmnd	1.076e+44	2.21	2.21	2.622e+42	0.0975
22866	TS.triHPacyl.COelim.pmpnmnmnd	1.029e+44	2.23	2.23	2.458e+42	0.0914
22867	TS.triHPacyl.COelim.ppmptomnd	7.009e+43	2.00	2.00	2.437e+42	0.0907
22868	TS.triHPacyl.COelim.pmpptomnd	6.470e+43	2.00	2.00	2.245e+42	0.0835
22869	TS.triHPacyl.COelim.pmpptomnd	5.882e+43	1.96	1.96	2.188e+42	0.0814
22870	TS.triHPacyl.COelim.ppmptomnd	3.510e+44	3.09	3.09	1.969e+42	0.0732

22871	TS.triHPacyl.COelim.pmpmpmpmd	3.043e+43	1.66	1.66	1.872e+42	0.0696
22872	TS.triHPacyl.COelim.pmmmmmpmd	9.561e+43	2.36	2.36	1.829e+42	0.068
22873	TS.triHPacyl.COelim.ptmmmtmpmd	2.688e+44	3.01	3.01	1.736e+42	0.0646
22874	TS.triHPacyl.COelim.pppptmpmd	5.430e+43	2.11	2.11	1.571e+42	0.0584
22875	TS.triHPacyl.COelim.tmpmtmmmd	1.637e+44	2.80	2.80	1.487e+42	0.0553
22876	TS.triHPacyl.COelim.mmpmpmpmd	5.812e+43	2.23	2.23	1.380e+42	0.0513
22877	TS.triHPacyl.COelim.pppppmpmd	3.524e+43	1.96	1.96	1.315e+42	0.0489
22878	TS.triHPacyl.COelim.ptppmtmpmd	3.878e+43	2.06	2.06	1.233e+42	0.0459
22879	TS.triHPacyl.COelim.mmpmpmpmd	1.044e+44	2.79	2.79	9.705e+41	0.0361
22880	TS.triHPacyl.COelim.pmpmtmpmd	9.802e+43	2.78	2.78	9.179e+41	0.0341
22881	Total				2.688e+45	100

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(2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)

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Population analysis at 300K. Vibrational scaling: 0.971.

22889 Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

22890 n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

22891 %: contribution to the population (with current data set assumed 100%)

22892	Compound	Qtot	Erel	Erel2	n*Q*MB	%
22893	-----					
22894	triHPacyl.tmmmtmpu	1.549e+43	0.00	0.00	1.549e+43	19.8
22895	triHPacyl.tmmmtmpu	1.999e+43	0.45	0.45	9.382e+42	12
22896	triHPacyl.pmmptmpu	1.424e+43	0.57	0.57	5.437e+42	6.95
22897	triHPacyl.tmtppmpu	4.877e+43	1.71	1.71	2.792e+42	3.57
22898	triHPacyl.pmmptmpu	1.533e+43	1.04	1.04	2.688e+42	3.44
22899	triHPacyl.ptppmpmpu	4.977e+43	1.81	1.81	2.383e+42	3.05
22900	triHPacyl.tmtppmpu	2.041e+44	2.75	2.75	2.019e+42	2.58
22901	triHPacyl.pttpmpmpu	5.757e+43	2.00	2.00	1.997e+42	2.55
22902	triHPacyl.tmtppmpu	7.286e+43	2.23	2.23	1.733e+42	2.22
22903	triHPacyl.ptppmpmpu	3.118e+43	1.74	1.74	1.689e+42	2.16
22904	triHPacyl.pmtppppmpu	2.949e+43	1.78	1.78	1.486e+42	1.9
22905	triHPacyl.tppmpmpmpu	8.411e+43	2.42	2.42	1.456e+42	1.86
22906	triHPacyl.tppmpmpmpu	8.394e+43	2.42	2.42	1.453e+42	1.86
22907	triHPacyl.ptppmpmpmpu	1.080e+43	1.21	1.21	1.413e+42	1.81
22908	triHPacyl.tmtppmpmpu	8.681e+43	2.53	2.53	1.243e+42	1.59
22909	triHPacyl.pppptmpmpu	5.640e+43	2.30	2.30	1.188e+42	1.52
22910	triHPacyl.pmtppptmpmpu	5.384e+43	2.34	2.34	1.070e+42	1.37
22911	triHPacyl.tppmpmpmpmpu	2.603e+43	1.92	1.92	1.044e+42	1.34
22912	triHPacyl.pppmpmpmpmpu	1.173e+43	1.46	1.46	1.019e+42	1.3
22913	triHPacyl.pptppmpmpmpu	2.872e+43	1.99	1.99	1.013e+42	1.3
22914	triHPacyl.tppmpmpmpmpmpu	4.008e+43	2.19	2.19	1.011e+42	1.29
22915	triHPacyl.pppppmpmpmpmpu	5.293e+43	2.39	2.39	9.686e+41	1.24
22916	triHPacyl.ptppmpmpmpmpmpu	4.159e+43	2.29	2.29	8.996e+41	1.15
22917	triHPacyl.pppmpmpmpmpmpmpu	3.392e+43	2.18	2.18	8.705e+41	1.11
22918	triHPacyl.tppmpmpmpmpmpmpu	9.284e+43	2.79	2.79	8.674e+41	1.11
22919	triHPacyl.mmmmtmpmpmpmpmpu	1.876e+43	1.88	1.88	8.077e+41	1.03
22920	triHPacyl.tmtmmmtmpmpmpmpu	6.231e+43	2.59	2.59	8.032e+41	1.03
22921	triHPacyl.ptmpmpmpmpmpmpmpu	4.593e+43	2.43	2.43	7.790e+41	0.996
22922	triHPacyl.pttpmpmpmpmpmpmpu	2.337e+43	2.06	2.06	7.426e+41	0.95
22923	triHPacyl.ptppmpmpmpmpmpmpu	2.868e+43	2.19	2.19	7.257e+41	0.928
22924	triHPacyl.tppmpmpmpmpmpmpmpu	3.251e+43	2.30	2.30	6.916e+41	0.884
22925	triHPacyl.tmtmpmpmpmpmpmpmpu	6.478e+43	2.75	2.75	6.474e+41	0.828
22926	triHPacyl.tppmpmpmpmpmpmpmpmpu	2.574e+43	2.21	2.21	6.323e+41	0.809
22927	triHPacyl.pmtmpmpmpmpmpmpmpmpu	3.690e+43	2.46	2.46	5.943e+41	0.76
22928	triHPacyl.tppmpmpmpmpmpmpmpmpmpu	1.774e+43	2.05	2.05	5.686e+41	0.727
22929	triHPacyl.pmtmpmpmpmpmpmpmpmpmpu	1.630e+44	3.39	3.39	5.533e+41	0.708
22930	triHPacyl.pppmpmpmpmpmpmpmpmpmpu	1.687e+43	2.05	2.05	5.422e+41	0.693
22931	triHPacyl.tmmmtmpmpmpmpmpmpmpmpu	5.607e+43	2.77	2.77	5.375e+41	0.687
22932	triHPacyl.tmmptmpmpmpmpmpmpmpmpu	1.657e+43	2.06	2.06	5.237e+41	0.67
22933	triHPacyl.pppmpmpmpmpmpmpmpmpmpmpu	8.692e+42	1.69	1.69	5.106e+41	0.653
22934	triHPacyl.tmmmtmpmpmpmpmpmpmpmpmpu	3.098e+43	2.45	2.45	5.086e+41	0.65
22935	triHPacyl.pttpmpmpmpmpmpmpmpmpmpmpu	3.865e+43	2.61	2.61	4.882e+41	0.624
22936	triHPacyl.pppmpmpmpmpmpmpmpmpmpmpmpu	9.963e+42	1.80	1.80	4.861e+41	0.622
22937	triHPacyl.pppmpmpmpmpmpmpmpmpmpmpmpmpu	8.714e+42	1.79	1.79	4.333e+41	0.554
22938	triHPacyl.ptppmpmpmpmpmpmpmpmpmpmpmpu	1.827e+43	2.24	2.24	4.232e+41	0.541
22939	triHPacyl.tmmmtmpmpmpmpmpmpmpmpmpmpu	6.079e+43	3.02	3.02	3.820e+41	0.488
22940	triHPacyl.ptmmmtmpmpmpmpmpmpmpmpmpu	3.555e+43	2.71	2.71	3.790e+41	0.485
22941	triHPacyl.pmtppppmpmpmpmpmpmpmpmpu	3.841e+43	2.77	2.77	3.664e+41	0.469
22942	triHPacyl.tppmpmpmpmpmpmpmpmpmpmpmpmpu	3.115e+43	2.72	2.72	3.255e+41	0.416

22943	triHPacyl.mmmmmmtmpu	4.238e+43	2.91	2.91	3.238e+41	0.414
22944	triHPacyl.ptppptpmu	1.553e+43	2.32	2.32	3.182e+41	0.407
22945	triHPacyl.tmpptppmu	4.845e+43	3.31	3.31	1.877e+41	0.24
22946	triHPacyl.tmpptppmu	3.155e+43	3.11	3.11	1.713e+41	0.219
22947	triHPacyl.pppmmtpmu	1.084e+43	2.54	2.54	1.528e+41	0.195
22948	triHPacyl.pppmmtpmu	1.872e+43	2.90	2.90	1.452e+41	0.186
22949	triHPacyl.tmmmmmpmu	3.031e+43	3.20	3.20	1.405e+41	0.18
22950	triHPacyl.pppmmtpmu	8.997e+42	2.56	2.56	1.233e+41	0.158
22951	triHPacyl.tmmmmmpmu	4.269e+43	3.56	3.56	1.082e+41	0.138
22952	triHPacyl.pppmmtpmu	1.222e+43	2.88	2.88	9.792e+40	0.125
22953	triHPacyl.ptmmmtmpu	1.357e+43	2.96	2.96	9.442e+40	0.121
22954	triHPacyl.mppmmtpmu	3.130e+43	3.62	3.62	7.251e+40	0.0927
22955	triHPacyl.tmmmmmpmu	2.078e+43	3.44	3.44	6.495e+40	0.0831
22956	triHPacyl.pppmmtpmu	1.149e+43	3.10	3.10	6.333e+40	0.081
22957	triHPacyl.tmmmtppmu	1.415e+43	3.37	3.37	4.998e+40	0.0639
22958	triHPacyl.pppmmtpmu	1.206e+43	3.80	3.80	2.066e+40	0.0264
22959	Total				7.819e+43	100

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CO elimination from (2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)

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Population analysis at 300K. Vibrational scaling: 0.971.

Qtot: Total partition function (m⁻³). Erel, Erel2: Relative energy (kcal/mol)

n*Q*MB: Multiplicity-corrected and Boltzmann-weighted partition function.

#: contribution to the population (with current data set assumed 100%)

22966

Compound	Qtot	Erel	Erel2	n*Q*MB	%	
22970						
22971						
22972	TS.triHPacyl.COelim.pttpmmpmu	1.013e+44	0.16	0.16	7.703e+43	7.44
22973	TS.triHPacyl.COelim.tmmmmmtmpu	5.748e+43	0.02	0.02	5.555e+43	5.37
22974	TS.triHPacyl.COelim.pttpmmtmpu	4.047e+44	1.25	1.25	4.974e+43	4.8
22975	TS.triHPacyl.COelim.tmmmmmtmpu	4.366e+43	0.00	0.00	4.366e+43	4.22
22976	TS.triHPacyl.COelim.pttpmtppmu	1.220e+44	0.67	0.67	3.960e+43	3.82
22977	TS.triHPacyl.COelim.tmtptppmu	1.822e+44	0.98	0.98	3.545e+43	3.42
22978	TS.triHPacyl.COelim.pttpmmpmu	1.692e+44	0.94	0.94	3.521e+43	3.4
22979	TS.triHPacyl.COelim.tppmmmtmpu	1.732e+44	0.95	0.95	3.500e+43	3.38
22980	TS.triHPacyl.COelim.ptmmmmmtmpu	1.176e+44	0.74	0.74	3.410e+43	3.29
22981	TS.triHPacyl.COelim.ptppmmmpmu	5.271e+43	0.26	0.26	3.410e+43	3.29
22982	TS.triHPacyl.COelim.ptppppppmu	1.670e+44	0.96	0.96	3.324e+43	3.21
22983	TS.triHPacyl.COelim.ptppmmmpmu	4.838e+43	0.26	0.26	3.103e+43	3
22984	TS.triHPacyl.COelim.ptppmmmmmu	7.294e+43	0.57	0.57	2.788e+43	2.69
22985	TS.triHPacyl.COelim.tpppmtppmu	3.454e+44	1.55	1.55	2.545e+43	2.46
22986	TS.triHPacyl.COelim.pttpmmmpmu	2.091e+44	1.26	1.26	2.533e+43	2.45
22987	TS.triHPacyl.COelim.pttmmmtmpu	2.006e+44	1.26	1.26	2.414e+43	2.33
22988	TS.triHPacyl.COelim.ptppmmpmu	6.969e+43	0.65	0.65	2.351e+43	2.27
22989	TS.triHPacyl.COelim.pttmmmpmu	2.902e+44	1.57	1.57	2.074e+43	2
22990	TS.triHPacyl.COelim.tppmmmtmpu	1.369e+44	1.14	1.14	2.017e+43	1.95
22991	TS.triHPacyl.COelim.ptppmpmmu	7.466e+43	0.79	0.79	1.976e+43	1.91
22992	TS.triHPacyl.COelim.tmtmmmtmpu	3.326e+44	1.69	1.69	1.948e+43	1.88
22993	TS.triHPacyl.COelim.ptmmmtmpu	1.558e+44	1.28	1.28	1.809e+43	1.75
22994	TS.triHPacyl.COelim.tppmmmpmu	3.929e+44	1.85	1.85	1.751e+43	1.69
22995	TS.triHPacyl.COelim.ptmmmtmpu	1.492e+44	1.34	1.34	1.578e+43	1.52
22996	TS.triHPacyl.COelim.pptmptmpu	8.482e+43	1.00	1.00	1.576e+43	1.52
22997	TS.triHPacyl.COelim.pppmptmpu	2.935e+43	0.40	0.40	1.501e+43	1.45
22998	TS.triHPacyl.COelim.ppppptmpu	2.085e+44	1.59	1.59	1.446e+43	1.4
22999	TS.triHPacyl.COelim.tppmmmtppu	8.294e+43	1.05	1.05	1.427e+43	1.38
23000	TS.triHPacyl.COelim.ptppmtmpu	5.286e+43	0.89	0.89	1.188e+43	1.15
23001	TS.triHPacyl.COelim.ptmmmmppmu	1.348e+44	1.47	1.47	1.150e+43	1.11
23002	TS.triHPacyl.COelim.pmtppmtmpu	2.254e+44	1.83	1.83	1.048e+43	1.01
23003	TS.triHPacyl.COelim.pptpmtmpu	2.242e+44	1.83	1.83	1.039e+43	1
23004	TS.triHPacyl.COelim.pptmptmpu	9.018e+43	1.29	1.29	1.031e+43	0.996
23005	TS.triHPacyl.COelim.tmtptmpu	6.038e+44	2.44	2.44	1.000e+43	0.966
23006	TS.triHPacyl.COelim.pppmptmpu	3.322e+43	0.78	0.78	8.933e+42	0.863
23007	TS.triHPacyl.COelim.tppmmmpmu	9.432e+43	1.44	1.44	8.490e+42	0.82
23008	TS.triHPacyl.COelim.tmtmmmtmpu	2.994e+44	2.15	2.15	8.112e+42	0.784
23009	TS.triHPacyl.COelim.tmtppmmpmu	1.746e+44	1.83	1.83	8.103e+42	0.783
23010	TS.triHPacyl.COelim.pttpptppmu	1.059e+44	1.54	1.54	8.024e+42	0.775
23011	TS.triHPacyl.COelim.tmtmmtppmu	1.630e+44	1.85	1.85	7.357e+42	0.711
23012	TS.triHPacyl.COelim.pppmmmpmu	3.729e+43	0.97	0.97	7.282e+42	0.703
23013	TS.triHPacyl.COelim.ptppppppmu	8.779e+43	1.58	1.58	6.168e+42	0.596
23014	TS.triHPacyl.COelim.tmtppmmpmu	1.236e+44	1.80	1.80	6.056e+42	0.585

23015	TS.triHPacyl.COelim.ptppptpmu	1.038e+44	1.72	1.72	5.823e+42	0.562
23016	TS.triHPacyl.COelim.ptppmpmpmu	7.276e+43	1.52	1.52	5.658e+42	0.547
23017	TS.triHPacyl.COelim.pmtpppppmu	1.200e+44	1.83	1.83	5.600e+42	0.541
23018	TS.triHPacyl.COelim.ptmmmmmpmu	1.473e+44	1.99	1.99	5.275e+42	0.51
23019	TS.triHPacyl.COelim.ptmmpmpmu	7.653e+43	1.60	1.60	5.259e+42	0.508
23020	TS.triHPacyl.COelim.ptmmpmpmu	7.347e+43	1.58	1.58	5.171e+42	0.5
23021	TS.triHPacyl.COelim.ppmmmtmpmu	5.347e+43	1.41	1.41	5.054e+42	0.488
23022	TS.triHPacyl.COelim.ptmmmpmpmu	8.334e+43	1.67	1.67	5.030e+42	0.486
23023	TS.triHPacyl.COelim.tmtptppmu	1.680e+44	2.11	2.11	4.903e+42	0.474
23024	TS.triHPacyl.COelim.pmtptppmu	8.221e+43	1.73	1.73	4.518e+42	0.436
23025	TS.triHPacyl.COelim.ptmmmtppmu	1.398e+44	2.07	2.07	4.377e+42	0.423
23026	TS.triHPacyl.COelim.ppmpmtmpmu	3.348e+43	1.41	1.41	3.119e+42	0.301
23027	TS.triHPacyl.COelim.pmmptmpmu	3.843e+43	1.51	1.51	3.043e+42	0.294
23028	TS.triHPacyl.COelim.ppmpmtmpmu	5.866e+43	1.83	1.83	2.743e+42	0.265
23029	TS.triHPacyl.COelim.pmtptppmu	7.792e+43	2.05	2.05	2.520e+42	0.243
23030	TS.triHPacyl.COelim.pmmmpmpmu	5.046e+43	1.84	1.84	2.314e+42	0.224
23031	TS.triHPacyl.COelim.ptmmmtppmu	6.471e+43	2.00	2.00	2.242e+42	0.217
23032	TS.triHPacyl.COelim.mpmmpppmu	1.688e+44	2.64	2.64	2.000e+42	0.193
23033	TS.triHPacyl.COelim.ppmmmtppmu	3.925e+43	1.86	1.86	1.729e+42	0.167
23034	TS.triHPacyl.COelim.ppmmmtppmu	3.109e+43	2.06	2.06	9.890e+41	0.0955
23035	TS.triHPacyl.COelim.pptptppmu	5.637e+43	2.49	2.49	8.590e+41	0.083
23036	TS.triHPacyl.COelim.ppmpmpmpmu	2.078e+43	1.91	1.91	8.440e+41	0.0815
23037	TS.triHPacyl.COelim.mpmmptmpmu	8.096e+43	2.74	2.74	8.178e+41	0.079
23038	TS.triHPacyl.COelim.pmmmpmpmu	4.260e+43	2.46	2.46	6.893e+41	0.0666
23039	TS.triHPacyl.COelim.ppmmpppmu	2.573e+43	2.24	2.24	5.989e+41	0.0579
23040	Total				1.035e+45	100

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23045 Raw quantum chemical M06-2X/aug-cc-pVTZ data for di-HPCARP-I
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(2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
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23050
23051 diHPCARP_I.mmmmtmpd
23052 -----
23053 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17891931
23054 Electronic state : 2-A
23055 Cartesian coordinates (Angs):

23056	O	-2.009594	0.295671	1.462689
23057	O	-0.799186	0.744390	1.377708
23058	C	-0.308140	0.869266	0.008102
23059	C	-0.053898	-0.503607	-0.657824
23060	C	0.550221	-1.517810	0.306330
23061	O	1.733625	-1.000238	0.879650
23062	O	2.711886	-0.925173	-0.153484
23063	H	3.360448	-1.570392	0.153849
23064	C	-1.247540	1.736633	-0.807617
23065	H	-1.389037	2.699469	-0.319320
23066	H	-2.208262	1.246237	-0.935899
23067	H	-0.797588	1.896444	-1.785384
23068	C	1.029017	1.585266	0.191726
23069	O	1.683474	1.928907	-0.747764
23070	H	1.328417	1.782245	1.233707
23071	H	0.666370	-0.293243	-1.452777
23072	O	-1.160736	-1.022859	-1.356073
23073	O	-2.025164	-1.722351	-0.470867
23074	H	-2.489975	-1.006108	-0.010249
23075	H	-0.105153	-1.705020	1.153647
23076	H	0.742383	-2.454897	-0.216753

23077 Rotational constants (GHz): 1.1476900 0.8701900 0.6872200
23078 Vibrational harmonic frequencies (cm-1):

23079	42.3175	77.7163	102.4505
23080	113.3531	151.1430	175.0978
23081	186.8253	205.9268	221.9515
23082	230.7787	248.2345	287.3666
23083	306.0541	316.1901	369.4638
23084	417.3465	465.9919	474.1830
23085	490.6741	559.9319	633.2879
23086	694.6019	755.4110	887.6106

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23087      929.3038      952.4542      978.6215
23088      988.8009      1033.3617     1107.0126
23089     1120.2076     1137.8863     1178.8963
23090     1204.7326     1243.1016     1280.0219
23091     1314.8568     1331.1144     1379.0791
23092     1399.5902     1403.7551     1410.9063
23093     1422.5744     1458.5186     1484.9544
23094     1487.1539     1496.3811     1871.2665
23095     3009.5519     3084.3284     3091.4540
23096     3093.5247     3164.2335     3165.0410
23097     3180.6587     3734.6715     3826.7401
23098 Zero-point correction (Hartree): 0.155778
23099
23100 diHPCARP_I.mmmmpmpd
23101 -----
23102 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18308300
23103 Electronic state : 2-A
23104 Cartesian coordinates (Angs):
23105 O      -2.219949      0.524380      1.230398
23106 O      -0.959594      0.814277      1.265066
23107 C      -0.323724      0.855962     -0.048437
23108 C      -0.056328     -0.556139     -0.614215
23109 C       0.594693     -1.475945      0.413287
23110 O       1.786300     -0.893022      0.902116
23111 O       2.769656     -0.992827     -0.116686
23112 H       2.862667     -0.070464     -0.407095
23113 C      -1.129110      1.717620     -1.003731
23114 H      -1.311706      2.699060     -0.568692
23115 H      -2.076386      1.238843     -1.233229
23116 H      -0.556693      1.834801     -1.921933
23117 C       1.010414      1.524478      0.249113
23118 O       1.845757      1.676494     -0.601985
23119 H       1.144743      1.890826      1.279033
23120 H       0.646137     -0.395057     -1.436326
23121 O      -1.165739     -1.141021     -1.251077
23122 O      -1.990694     -1.795975     -0.296393
23123 H      -2.572617     -1.081449      0.002334
23124 H      -0.033246     -1.602035      1.291887
23125 H       0.795534     -2.448822     -0.033597
23126 Rotational constants (GHz): 1.2197000      0.8573900      0.6715300
23127 Vibrational harmonic frequencies (cm-1):
23128      46.1783      82.0465      124.8523
23129     168.4767     182.5890     192.7337
23130     208.3176     214.0176     232.9920
23131     257.3364     280.3283     297.5277
23132     321.3911     360.9842     407.5387
23133     433.1299     471.6113     473.3141
23134     487.7456     568.1335     629.0241
23135     690.8730     757.4181     894.7183
23136     937.1556     954.7068     980.0294
23137     985.0589     1033.9800    1113.0462
23138    1123.5828     1141.2389    1178.5591
23139    1207.6576     1245.8008    1279.5324
23140    1312.9819     1332.0252    1377.9970
23141    1401.4720     1411.8533    1417.6841
23142    1439.5785     1459.5129    1485.4721
23143    1488.3870     1494.5348    1841.2437
23144    3021.2195     3083.0946    3090.2757
23145    3105.0888     3161.7706    3169.9378
23146    3184.1520     3717.4871    3761.5496
23147 Zero-point correction (Hartree): 0.156558
23148
23149 diHPCARP_I.mmmmpmtd
23150 -----
23151 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18331957
23152 Electronic state : 2-A
23153 Cartesian coordinates (Angs):
23154 O      -1.534451      1.761587      1.466925
23155 O      -1.100819      0.587764      1.121921
23156 C      -0.534854      0.597546     -0.217266
23157 C       0.021387     -0.804542     -0.504901
23158 C       0.847480     -1.346914      0.657126

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23159	O	1.889153	-0.447538	0.978234	
23160	O	2.875119	-0.551535	-0.038779	
23161	H	2.759418	0.280352	-0.527199	
23162	C	-1.583896	1.019599	-1.231623	
23163	H	-1.932361	2.026195	-1.014829	
23164	H	-2.418466	0.323294	-1.195378	
23165	H	-1.138591	0.997849	-2.224775	
23166	C	0.620882	1.592616	-0.206110	
23167	O	1.401992	1.668371	-1.117143	
23168	H	0.675822	2.248765	0.675436	
23169	H	0.667196	-0.695299	-1.379224	
23170	O	-0.950466	-1.717133	-0.952042	
23171	O	-1.883869	-1.915049	0.112712	
23172	H	-1.920442	-2.878373	0.147530	
23173	H	0.250361	-1.421301	1.563370	
23174	H	1.257794	-2.323033	0.397090	
23175	Rotational constants (GHz):		1.0947600	0.8940300	0.6847500
23176	Vibrational harmonic frequencies (cm-1):				
23177		64.6070		104.4281	112.3995
23178		125.1330		164.7733	177.5949
23179		186.9204		197.2365	204.9009
23180		240.3105		256.6317	274.8210
23181		308.1601		334.7182	374.2314
23182		408.5785		434.6902	473.8558
23183		515.5802		579.9763	627.8802
23184		703.7009		758.0068	903.8173
23185		947.8814		967.0154	977.7632
23186		980.7970		1041.4616	1111.6276
23187		1121.6436		1136.9320	1182.4063
23188		1209.0992		1244.1668	1273.1131
23189		1292.8137		1338.9757	1373.6533
23190		1396.9699		1398.3833	1410.8460
23191		1433.6576		1460.5478	1484.5088
23192		1490.5260		1502.0557	1836.4200
23193		3033.9702		3085.4378	3090.6688
23194		3099.9015		3163.0646	3168.2975
23195		3177.6981		3718.8410	3837.1085
23196	Zero-point correction (Hartree): 0.156103				
23197					
23198	diHPCARP_I.mmmmpptpd				
23199	-----				
23200	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18035271				
23201	Electronic state : 2-A				
23202	Cartesian coordinates (Angs):				
23203	O	1.867652	-0.944226	1.656018	
23204	O	0.674378	-1.221931	1.225452	
23205	C	0.423769	-0.755536	-0.128644	
23206	C	0.120763	0.753733	-0.116250	
23207	C	-0.855267	1.122730	0.998942	
23208	O	-2.021996	0.331801	0.929177	
23209	O	-2.809733	0.825811	-0.143496	
23210	H	-2.678991	0.148169	-0.827813	
23211	C	1.568449	-1.133033	-1.052111	
23212	H	1.735838	-2.209111	-1.017276	
23213	H	2.471755	-0.615406	-0.744549	
23214	H	1.310468	-0.838687	-2.067116	
23215	C	-0.824905	-1.519895	-0.530668	
23216	O	-1.444283	-1.258471	-1.528405	
23217	H	-1.101927	-2.357721	0.129556	
23218	H	-0.311402	1.003497	-1.087220	
23219	O	1.267891	1.538999	0.109125	
23220	O	1.921241	1.759486	-1.137335	
23221	H	1.867953	2.720849	-1.206270	
23222	H	-0.420408	0.909615	1.974775	
23223	H	-1.111338	2.179068	0.934009	
23224	Rotational constants (GHz):		1.1377600	0.8032300	0.7141800
23225	Vibrational harmonic frequencies (cm-1):				
23226		38.7420		82.6064	89.9765
23227		140.9355		166.2848	181.4542
23228		194.0073		198.0101	228.7183
23229		245.4862		271.4708	290.2566
23230		320.0335		345.5311	364.3045

23231	399.3889	435.5679	473.5512			
23232	507.6435	537.4915	617.8650			
23233	687.6906	757.4662	901.8988			
23234	951.9327	957.2108	978.9938			
23235	1022.9142	1033.3358	1111.2255			
23236	1121.7964	1150.7355	1176.7256			
23237	1216.8743	1246.4600	1280.9859			
23238	1291.1318	1334.4241	1379.2787			
23239	1402.0887	1409.7555	1411.8299			
23240	1415.6270	1465.5975	1481.8063			
23241	1487.2930	1509.7296	1840.3205			
23242	3012.0558	3081.2376	3095.5609			
23243	3098.5231	3155.4512	3160.6612			
23244	3190.2151	3710.8687	3823.9385			
23245	Zero-point correction (Hartree): 0.156016					
23246						
23247	diHPCARP_I.mmmmpptd					
23248	-----					
23249	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17971395					
23250	Electronic state : 2-A					
23251	Cartesian coordinates (Angs):					
23252	O	1.917216	-0.842451	1.647088		
23253	O	0.708081	-1.137589	1.277612		
23254	C	0.412716	-0.755605	-0.094043		
23255	C	0.121646	0.756044	-0.159787		
23256	C	-0.859635	1.186911	0.929326		
23257	O	-2.026060	0.393106	0.907765		
23258	O	-2.820335	0.828302	-0.184825		
23259	H	-2.696988	0.113097	-0.831263		
23260	C	1.515005	-1.218156	-1.030541		
23261	H	1.630019	-2.299871	-0.964225		
23262	H	2.453170	-0.747201	-0.756469		
23263	H	1.249890	-0.944033	-2.048849		
23264	C	-0.857723	-1.527386	-0.407797		
23265	O	-1.474843	-1.351421	-1.425339		
23266	H	-1.148765	-2.288914	0.333394		
23267	H	-0.302774	0.962796	-1.144813		
23268	O	1.259195	1.555644	0.039884		
23269	O	1.880529	1.755228	-1.229860		
23270	H	2.811111	1.677359	-0.986438		
23271	H	-0.424995	1.031812	1.916395		
23272	H	-1.112982	2.237557	0.800718		
23273	Rotational constants (GHz):			1.150200	0.8013700	0.7078800
23274	Vibrational harmonic frequencies (cm-1):					
23275		36.6210	72.4273	96.5199		
23276		144.2394	163.6111	181.7425		
23277		182.9277	197.1600	225.9842		
23278		244.6107	265.3313	290.1044		
23279		323.1033	346.5106	359.3028		
23280		396.6407	434.0948	473.1460		
23281		507.4716	536.9963	614.1669		
23282		684.0379	752.9995	899.1818		
23283		952.2992	953.5276	980.6430		
23284		1027.3409	1032.8992	1114.4014		
23285		1123.6708	1151.5538	1172.8188		
23286		1215.8067	1242.3346	1281.0873		
23287		1292.2826	1331.4565	1379.4509		
23288		1397.9584	1406.1580	1413.3250		
23289		1422.2441	1467.9181	1479.5559		
23290		1485.8313	1505.5387	1839.3951		
23291		3018.5533	3082.7132	3093.3167		
23292		3100.1019	3157.0601	3161.4968		
23293		3194.1474	3710.8304	3831.8080		
23294	Zero-point correction (Hartree): 0.155937					
23295						
23296	diHPCARP_I.mmmmpptmd					
23297	-----					
23298	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17927717					
23299	Electronic state : 2-A					
23300	Cartesian coordinates (Angs):					
23301	O	2.140971	-0.738502	1.442752		
23302	O	0.952411	-1.185962	1.174406		

23303	C	0.504466	-0.844534	-0.165513	
23304	C	0.141924	0.640530	-0.266691	
23305	C	-0.706532	1.099118	0.913501	
23306	O	-1.852907	0.282410	1.055377	
23307	O	-2.776166	0.657547	0.043783	
23308	H	-2.715540	-0.085300	-0.579021	
23309	C	1.526585	-1.285647	-1.199749	
23310	H	1.706470	-2.356781	-1.117075	
23311	H	2.457323	-0.748595	-1.045557	
23312	H	1.133659	-1.067538	-2.191183	
23313	C	-0.762372	-1.674088	-0.324247	
23314	O	-1.495753	-1.551133	-1.268444	
23315	H	-0.931922	-2.428974	0.460020	
23316	H	-0.417320	0.756641	-1.199577	
23317	O	1.340555	1.386642	-0.341121	
23318	O	0.975157	2.702652	-0.744625	
23319	H	1.416734	2.767608	-1.600199	
23320	H	-0.151649	0.980834	1.843721	
23321	H	-0.996319	2.140600	0.788038	
23322	Rotational constants (GHz):		1.0339700	0.8913200	0.6772500
23323	Vibrational harmonic frequencies (cm-1):				
23324		36.1536	84.9452		95.2118
23325		115.1148	168.8394		173.3731
23326		180.3136	187.7826		223.6854
23327		237.8501	253.0631		267.6497
23328		310.6981	329.0858		348.4527
23329		416.2058	443.6033		473.4913
23330		474.6904	538.1982		602.9672
23331		683.4428	780.9741		901.8610
23332		952.3650	954.7714		979.7158
23333		1018.2693	1050.0393		1105.5140
23334		1128.1165	1142.3889		1168.8576
23335		1222.1483	1254.4788		1278.7829
23336		1288.0917	1347.6911		1376.3467
23337		1397.2880	1403.6854		1414.0374
23338		1424.6994	1460.5583		1486.8406
23339		1488.7898	1502.1729		1844.6598
23340		3017.7042	3075.6673		3081.7763
23341		3102.4948	3157.3994		3160.1947
23342		3187.9718	3723.7643		3827.2629
23343	Zero-point correction (Hartree):		0.155718		
23344	diHPCARP_I.mmmmppttd				
23345	-----				
23347	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17962573		
23348	Electronic state : 2-A				
23349	Cartesian coordinates (Angs):				
23350	O	2.019937	-0.731648	1.519180	
23351	O	0.886334	-1.259447	1.173040	
23352	C	0.475351	-0.876028	-0.168317	
23353	C	0.177586	0.622422	-0.259558	
23354	C	-0.648925	1.112159	0.922875	
23355	O	-1.832061	0.350941	1.063987	
23356	O	-2.737293	0.771849	0.054593	
23357	H	-2.693414	0.040873	-0.583832	
23358	C	1.504552	-1.345082	-1.183478	
23359	H	1.616760	-2.427440	-1.133940	
23360	H	2.457377	-0.867204	-0.975605	
23361	H	1.167627	-1.064952	-2.179769	
23362	C	-0.816127	-1.657565	-0.361328	
23363	O	-1.552285	-1.468196	-1.291818	
23364	H	-1.003278	-2.445511	0.386103	
23365	H	-0.378757	0.761748	-1.190173	
23366	O	1.400183	1.325086	-0.353651	
23367	O	1.091976	2.578888	-0.960431	
23368	H	1.460857	3.194399	-0.315602	
23369	H	-0.101530	0.966774	1.854138	
23370	H	-0.894586	2.166097	0.798324	
23371	Rotational constants (GHz):		1.0286700	0.8892100	0.6887700
23372	Vibrational harmonic frequencies (cm-1):				
23373		44.4891	83.2399		98.3492
23374		113.9242	154.9143		176.0904

23375	180.4031	186.0442	221.2260			
23376	230.4824	251.1206	266.2548			
23377	302.3976	328.0474	354.5051			
23378	426.0878	443.6635	470.1840			
23379	475.0082	534.7251	602.8823			
23380	686.3058	781.3969	901.6747			
23381	954.0043	956.8469	979.1365			
23382	1019.8539	1052.0888	1106.8676			
23383	1126.9688	1138.4529	1169.6308			
23384	1220.9511	1257.1508	1281.0621			
23385	1290.9341	1350.1197	1374.9220			
23386	1397.7846	1409.9658	1415.2654			
23387	1420.5585	1461.6982	1485.8903			
23388	1488.0070	1498.0493	1846.7309			
23389	3012.7372	3080.6686	3084.0205			
23390	3093.1748	3149.5336	3159.4929			
23391	3185.8682	3719.4465	3834.5808			
23392	Zero-point correction (Hartree): 0.155681					
23393						
23394	diHPCARP_I.mtmmmtmd					
23395	-----					
23396	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17657443					
23397	Electronic state : 2-A					
23398	Cartesian coordinates (Angs):					
23399	O	-1.309421	2.038959	-1.286410		
23400	O	-1.786659	1.076624	-0.562892		
23401	C	-0.779587	0.471289	0.300597		
23402	C	0.315558	-0.131286	-0.597867		
23403	C	1.420071	-0.856224	0.172034		
23404	O	2.363506	0.036961	0.722677		
23405	O	3.009890	0.698161	-0.360971		
23406	H	3.917416	0.388157	-0.256498		
23407	C	-0.220609	1.509507	1.255281		
23408	H	-1.042923	2.033683	1.739936		
23409	H	0.399076	2.222521	0.716639		
23410	H	0.378156	1.013593	2.014585		
23411	C	-1.570975	-0.589644	1.059440		
23412	O	-1.167094	-1.081194	2.074602		
23413	H	-2.544300	-0.858177	0.618734		
23414	H	0.753797	0.693691	-1.161886		
23415	O	-0.227725	-0.950732	-1.608585		
23416	O	-0.798649	-2.088140	-0.956695		
23417	H	-0.459374	-2.807723	-1.501607		
23418	H	1.031366	-1.400001	1.032643		
23419	H	1.909262	-1.552708	-0.513258		
23420	Rotational constants (GHz):			1.0511400	0.7734100	0.7199300
23421	Vibrational harmonic frequencies (cm-1):					
23422		36.4446	53.8144	61.4112		
23423		101.3740	118.0838	135.4561		
23424		167.6778	189.8212	211.6408		
23425		218.2193	230.6300	258.4949		
23426		295.2955	303.9854	337.3901		
23427		352.7393	439.0580	471.5533		
23428		484.9981	525.9445	654.4390		
23429		685.6056	804.0683	886.8680		
23430		919.1548	957.1850	978.3437		
23431		1005.2749	1055.5570	1098.1149		
23432		1111.9642	1124.2290	1174.7324		
23433		1197.2631	1247.0145	1291.8202		
23434		1307.2463	1333.5601	1364.2902		
23435		1390.6906	1402.5317	1406.8035		
23436		1420.8958	1434.6277	1479.5810		
23437		1481.4482	1498.7130	1863.4473		
23438		3012.5480	3065.1402	3084.0022		
23439		3114.3308	3141.0315	3164.0900		
23440		3181.9111	3831.4813	3839.6263		
23441	Zero-point correction (Hartree): 0.154924					
23442						
23443	diHPCARP_I.mtppmtmmd					
23444	-----					
23445	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18145041					
23446	Electronic state : 2-A					

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23447 Cartesian coordinates (Angs):
23448 O 2.938644 0.118719 -0.708431
23449 O 2.214788 -0.115305 0.337106
23450 C 0.826970 -0.450499 0.005021
23451 C 0.221098 0.782649 -0.685193
23452 C -1.141933 0.630479 -1.352063
23453 O -2.213850 0.400726 -0.455942
23454 O -2.539123 -0.980765 -0.456913
23455 H -2.051346 -1.304829 0.324677
23456 C 0.803140 -1.677280 -0.888514
23457 H 1.407804 -2.466312 -0.444916
23458 H 1.206907 -1.431833 -1.868781
23459 H -0.218887 -2.033917 -0.991779
23460 C 0.255981 -0.770374 1.384760
23461 O -0.744796 -1.417433 1.550064
23462 H 0.872596 -0.434260 2.229307
23463 H 0.929390 1.038498 -1.479241
23464 O 0.253772 1.923168 0.152257
23465 O -0.420490 1.634360 1.367313
23466 H -1.354934 1.588841 1.105457
23467 H -1.359083 1.590313 -1.824628
23468 H -1.135546 -0.144111 -2.117792
23469 Rotational constants (GHz): 1.2814400 0.8092300 0.7361600
23470 Vibrational harmonic frequencies (cm-1):
23471 76.9259 97.4747 120.6449
23472 139.1322 173.6478 197.6812
23473 217.5111 224.6226 250.7408
23474 272.3199 298.4390 325.3947
23475 339.5374 365.1782 422.8480
23476 453.6254 480.8479 508.8620
23477 552.8744 625.2689 662.7669
23478 712.2404 840.9212 880.0117
23479 912.8593 921.8924 991.8437
23480 1001.4657 1015.4342 1074.1722
23481 1118.1514 1134.0171 1164.0116
23482 1200.7676 1256.0607 1296.5799
23483 1316.8704 1347.7437 1375.7388
23484 1405.2330 1407.0022 1427.7319
23485 1451.0571 1466.7942 1495.4615
23486 1501.4332 1510.3506 1839.9271
23487 3051.6590 3073.5575 3081.9811
23488 3084.0185 3137.4859 3161.9046
23489 3177.2965 3584.8616 3724.0720
23490 Zero-point correction (Hartree): 0.157077
23491
23492 diHPCARP_I.mtppmttptd
23493 -----
23494 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18147760
23495 Electronic state : 2-A
23496 Cartesian coordinates (Angs):
23497 O -2.831506 1.084118 0.438169
23498 O -2.253020 0.408018 -0.500544
23499 C -1.061620 -0.305282 -0.031776
23500 C -0.012748 0.730460 0.389994
23501 C 1.011552 0.253085 1.410637
23502 O 1.715366 -0.916402 1.071324
23503 O 2.569147 -0.609188 -0.024477
23504 H 2.054581 -1.002216 -0.751581
23505 C -1.471760 -1.268721 1.072093
23506 H -2.292599 -1.895028 0.724342
23507 H -1.807780 -0.707566 1.941931
23508 H -0.624655 -1.898730 1.334835
23509 C -0.684955 -1.123990 -1.262557
23510 O 0.381108 -1.640508 -1.436607
23511 H -1.514615 -1.261331 -1.976954
23512 H -0.555499 1.557452 0.861746
23513 O 0.545496 1.169774 -0.840098
23514 O 1.562636 2.114938 -0.584639
23515 H 2.342535 1.536876 -0.548615
23516 H 1.707241 1.065884 1.620976
23517 H 0.494152 0.005363 2.337947
23518 Rotational constants (GHz): 1.2978300 0.7844800 0.6955300

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23519 Vibrational harmonic frequencies (cm-1):
23520      63.0006      104.0733      119.3104
23521     134.8990     155.3282     184.0328
23522     209.3173     232.6127     247.7383
23523     271.8181     283.7266     310.1849
23524     343.0730     357.8084     442.5301
23525     474.6862     481.5425     511.5193
23526     539.0252     605.3101     650.4790
23527     717.3181     820.2024     882.1970
23528     894.3508     959.3406     974.9805
23529     990.3503    1053.4290    1070.7638
23530    1125.4617    1133.3694    1171.5596
23531    1202.3519    1282.9044    1298.2774
23532    1308.9956    1358.3494    1380.5545
23533    1396.5119    1410.6025    1432.8307
23534    1448.7930    1460.9239    1481.6627
23535    1500.0854    1505.4538    1872.7594
23536    2996.8928    3047.3739    3074.8097
23537    3091.5749    3135.3891    3153.7555
23538    3171.6065    3678.5893    3725.2141
23539 Zero-point correction (Hartree): 0.157038
23540
23541 diHPCARP_I.mtpptmmd
23542 -----
23543 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18062379
23544 Electronic state : 2-A
23545 Cartesian coordinates (Angs):
23546 O      2.959501      0.417874      -0.492471
23547 O      2.185820      0.080554      0.486954
23548 C      0.875716     -0.401256      0.038751
23549 C      0.187290      0.767903     -0.683810
23550 C     -1.042540      0.410618     -1.531210
23551 O     -1.904511     -0.603700     -1.078817
23552 O     -2.627569     -0.134034      0.051945
23553 H     -2.337114     -0.785995      0.712928
23554 C      1.058884     -1.605662     -0.866925
23555 H      1.720448     -2.325273     -0.387771
23556 H      1.500114     -1.299724     -1.813443
23557 H      0.091610     -2.072658     -1.034770
23558 C      0.236254     -0.814240      1.364916
23559 O     -0.703755     -1.558480      1.441967
23560 H      0.752777     -0.432308      2.257688
23561 H      0.932526      1.143775     -1.391283
23562 O     -0.002307      1.889305      0.152911
23563 O     -0.734422      1.521178      1.307812
23564 H     -1.632761      1.370229      0.965081
23565 H     -1.601024      1.333617     -1.709218
23566 H     -0.702251      0.022591     -2.491944
23567 Rotational constants (GHz): 1.3178300 0.8008200 0.7594200
23568 Vibrational harmonic frequencies (cm-1):
23569      79.0758      119.1178      132.1496
23570     155.7369     171.4964     196.3178
23571     222.5421     231.3197     242.4918
23572     245.1279     272.7970     321.6204
23573     340.9596     349.4047     426.5017
23574     432.6414     468.2613     482.5658
23575     595.1780     635.1594     652.4271
23576     689.7962     792.1075     870.4609
23577     898.1093     956.6065     993.4693
23578    1009.9842    1035.7251    1064.3488
23579    1117.8250    1134.4326    1176.1108
23580    1202.4329    1260.3132    1298.2878
23581    1309.3879    1354.3667    1390.5850
23582    1400.4304    1407.4062    1427.5501
23583    1443.3329    1463.7315    1486.3582
23584    1495.3738    1501.4930    1846.3233
23585    3032.1714    3061.6589    3074.6498
23586    3082.3170    3125.2822    3159.9097
23587    3179.2735    3680.4866    3705.0347
23588 Zero-point correction (Hartree): 0.156966
23589
23590 diHPCARP_I.mttmmtmmd

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23591 -----
23592 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18003973
23593 Electronic state : 2-A
23594 Cartesian coordinates (Angs):
23595 O 2.342456 -1.832547 0.107535
23596 O 2.095890 -0.744560 -0.550440
23597 C 1.191470 0.144976 0.163097
23598 C -0.160590 -0.574993 0.315591
23599 C -1.192636 0.290765 1.036006
23600 O -2.439250 -0.369844 1.139555
23601 O -3.143049 -0.188905 -0.085277
23602 H -3.888728 0.351528 0.203460
23603 C 1.791156 0.525502 1.505082
23604 H 2.832241 0.813825 1.369747
23605 H 1.744125 -0.314250 2.195362
23606 H 1.251757 1.378087 1.911617
23607 C 1.099306 1.364832 -0.751062
23608 O 0.710226 2.425020 -0.349388
23609 H 1.437226 1.208187 -1.786577
23610 H 0.021258 -1.482634 0.895596
23611 O -0.628320 -1.082709 -0.910328
23612 O -0.902940 0.005972 -1.777884
23613 H -1.852324 0.130075 -1.619108
23614 H -0.879431 0.446314 2.068182
23615 H -1.318456 1.262964 0.559254
23616 Rotational constants (GHz): 1.3342500 0.6983500 0.6483100
23617 Vibrational harmonic frequencies (cm-1):
23618 56.8251 73.3657 113.1993
23619 136.2671 156.9709 187.9667
23620 193.8087 223.4359 230.3517
23621 264.6978 276.0786 300.4016
23622 324.0408 332.5676 350.7699
23623 413.0475 469.6417 488.4844
23624 492.2664 574.8064 658.1892
23625 675.7699 824.4759 888.4842
23626 909.4985 955.7853 995.4453
23627 1002.5364 1012.7332 1093.3239
23628 1121.9250 1140.8944 1172.0932
23629 1201.0117 1240.2914 1292.7777
23630 1313.8935 1327.3357 1388.6983
23631 1398.0946 1398.4764 1417.2100
23632 1429.3103 1439.6292 1474.8371
23633 1490.9965 1503.5472 1858.3470
23634 3027.1118 3080.7919 3092.0797
23635 3098.0019 3146.6412 3159.7290
23636 3171.4722 3729.7287 3823.4254
23637 Zero-point correction (Hartree): 0.156313
23638
23639 diHPCARP_I.mttmptmmd
23640 -----
23641 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18179617
23642 Electronic state : 2-A
23643 Cartesian coordinates (Angs):
23644 O 2.202283 -1.932917 0.142131
23645 O 2.033461 -0.840469 -0.532973
23646 C 1.189858 0.119527 0.163264
23647 C -0.200719 -0.512080 0.341227
23648 C -1.198326 0.426525 1.013585
23649 O -2.455628 -0.194953 1.186585
23650 O -3.148453 -0.155623 -0.058023
23651 H -3.090382 -1.079998 -0.336682
23652 C 1.818477 0.491272 1.494795
23653 H 2.873477 0.716427 1.348079
23654 H 1.727773 -0.330860 2.201718
23655 H 1.331045 1.380938 1.887050
23656 C 1.171858 1.325141 -0.774086
23657 O 0.815312 2.406072 -0.399883
23658 H 1.533603 1.137497 -1.796496
23659 H -0.072872 -1.406837 0.954880
23660 O -0.697715 -1.040168 -0.872718
23661 O -0.877746 0.025764 -1.791377
23662 H -1.779814 0.320082 -1.580560

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23663	H	-0.867188	0.652751	2.026513	
23664	H	-1.314640	1.366029	0.472851	
23665	Rotational constants (GHz):			1.3180500	0.6544600
23666	Vibrational harmonic frequencies (cm-1):			0.7077400	
23667		56.9562	80.0522		112.5985
23668		136.5298	161.6949		178.0388
23669		205.8745	225.2391		232.1509
23670		261.8352	290.7056		325.4449
23671		330.0754	350.2419		396.1628
23672		419.4674	468.4117		477.4597
23673		572.1118	583.0027		658.4413
23674		674.6378	832.0966		888.7621
23675		912.3133	953.0334		995.4281
23676		1005.8812	1010.4513		1098.3999
23677		1121.0700	1137.0396		1166.0532
23678		1198.7784	1243.5929		1291.8754
23679		1310.2884	1324.3324		1387.9688
23680		1398.0629	1408.7721		1417.5878
23681		1421.8581	1438.1600		1481.5194
23682		1491.0001	1503.3914		1860.2372
23683		3026.4315	3081.6449		3093.9494
23684		3099.3023	3149.0705		3160.6805
23685		3172.7775	3705.8500		3795.6853
23686	Zero-point correction (Hartree): 0.156693				
23687					
23688	diHPCARP_I.mttpmtmmd				
23689	-----				
23690	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18159726				
23691	Electronic state : 2-A				
23692	Cartesian coordinates (Angs):				
23693	O	1.922483	-2.141526	-0.265891	
23694	O	1.962791	-0.903855	-0.645557	
23695	C	1.164522	-0.031324	0.205033	
23696	C	-0.300864	-0.470387	0.102678	
23697	C	-1.225873	0.379688	0.985565	
23698	O	-2.538802	0.384032	0.468069	
23699	O	-3.026995	-0.948659	0.507244	
23700	H	-2.813299	-1.262362	-0.383897	
23701	C	1.660181	-0.096949	1.637452	
23702	H	2.737838	0.054453	1.659390	
23703	H	1.427108	-1.065293	2.074904	
23704	H	1.193116	0.697585	2.215723	
23705	C	1.401674	1.353793	-0.394767	
23706	O	1.232395	2.354757	0.240997	
23707	H	1.757917	1.363370	-1.436227	
23708	H	-0.338741	-1.519611	0.400949	
23709	O	-0.766608	-0.511040	-1.231488	
23710	O	-0.822505	0.815472	-1.733339	
23711	H	-1.710945	1.093608	-1.459460	
23712	H	-1.222186	0.006257	2.010181	
23713	H	-0.930720	1.429633	0.982385	
23714	Rotational constants (GHz):			1.2630000	0.6490400
23715	Vibrational harmonic frequencies (cm-1):			0.7314800	
23716		60.5337	84.4298		109.9107
23717		128.1345	154.1846		176.5181
23718		199.2512	223.9823		233.3368
23719		268.1047	299.0596		310.1988
23720		349.2318	363.2705		405.4643
23721		437.3028	470.3620		476.8206
23722		497.0004	584.6950		663.7539
23723		737.7576	803.4173		884.9988
23724		915.2714	958.3673		993.1648
23725		1000.4856	1014.9616		1084.4057
23726		1125.2704	1136.3172		1177.5288
23727		1203.8576	1252.6538		1292.9668
23728		1306.9014	1328.8949		1394.4344
23729		1398.7563	1407.0030		1418.5768
23730		1424.1068	1432.1512		1486.2609
23731		1493.2757	1502.3272		1862.2730
23732		3024.1434	3082.1639		3084.0359
23733		3105.9400	3140.5847		3162.6564
23734		3171.2994	3743.0470		3773.7575

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23735 Zero-point correction (Hartree): 0.156782
23736
23737 diHPCARP_I.pmmptmpd
23738 -----
23739 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18230607
23740 Electronic state : 2-A
23741 Cartesian coordinates (Angs):
23742 O -0.680550 0.411094 2.114874
23743 O -1.248753 0.908815 1.054981
23744 C -0.388486 0.887114 -0.113115
23745 C -0.239332 -0.542592 -0.678437
23746 C 0.430454 -1.540338 0.261394
23747 O 1.689226 -1.066442 0.686834
23748 O 2.577282 -1.147017 -0.419119
23749 H 2.727305 -0.209852 -0.625373
23750 C -1.064284 1.806490 -1.117165
23751 H -1.193150 2.801073 -0.694055
23752 H -2.035276 1.404052 -1.397328
23753 H -0.440278 1.877331 -2.005161
23754 C 0.977626 1.448893 0.256258
23755 O 1.832422 1.594137 -0.576850
23756 H 1.113761 1.750892 1.305103
23757 H 0.388296 -0.431882 -1.566772
23758 O -1.453226 -1.039047 -1.195613
23759 O -2.270255 -1.492894 -0.122531
23760 H -2.819597 -0.721209 0.070284
23761 H -0.141370 -1.681675 1.173704
23762 H 0.535264 -2.495295 -0.254617
23763 Rotational constants (GHz): 1.1394500 0.8871400 0.7343500
23764 Vibrational harmonic frequencies (cm-1):
23765 54.7424 101.1708 128.7051
23766 164.5172 176.1270 181.8947
23767 206.7427 212.5676 236.7001
23768 258.6166 268.0380 290.6280
23769 314.2018 320.6091 345.3723
23770 419.1488 449.4953 459.5091
23771 541.4376 561.4985 634.7948
23772 689.8484 766.0982 905.9451
23773 938.8085 953.0590 974.1027
23774 979.4625 1040.8227 1112.6927
23775 1128.2772 1132.2069 1177.5246
23776 1211.3022 1239.2257 1281.4761
23777 1282.8521 1335.3524 1368.8945
23778 1400.0823 1405.8700 1415.7068
23779 1417.4747 1459.6142 1488.7912
23780 1492.6053 1495.3440 1834.4147
23781 3037.2085 3082.9263 3089.4735
23782 3096.5582 3163.3858 3172.9224
23783 3177.4382 3722.4239 3798.4556
23784 Zero-point correction (Hartree): 0.156271
23785
23786 diHPCARP_I.pmmptmtd
23787 -----
23788 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18193339
23789 Electronic state : 2-A
23790 Cartesian coordinates (Angs):
23791 O -0.329299 0.600437 2.156839
23792 O -1.135870 0.886560 1.177662
23793 C -0.478834 0.847117 -0.111915
23794 C -0.228978 -0.587984 -0.611903
23795 C 0.518494 -1.485537 0.367677
23796 O 1.781755 -0.947486 0.689934
23797 O 2.609896 -1.079803 -0.457121
23798 H 2.667727 -0.161981 -0.768317
23799 C -1.404193 1.607263 -1.049734
23800 H -1.505770 2.641845 -0.725819
23801 H -2.381634 1.130646 -1.049866
23802 H -0.993109 1.585309 -2.056700
23803 C 0.843630 1.593569 0.000646
23804 O 1.655040 1.586953 -0.885586
23805 H 0.978436 2.188733 0.916829
23806 H 0.385225 -0.473753 -1.508836

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23807	O	-1.393863	-1.200228	-1.110107	
23808	O	-2.287918	-1.393458	-0.011650	
23809	H	-2.478567	-2.335748	-0.092062	
23810	H	-0.004146	-1.571410	1.317567	
23811	H	0.633188	-2.474016	-0.081175	
23812	Rotational constants (GHz):		1.1305300	0.8808100	0.7429700
23813	Vibrational harmonic frequencies (cm-1):				
23814		49.4976	86.4304		111.1645
23815		138.7371	168.0727		184.5900
23816		193.9351	208.9827		222.3452
23817		238.2032	258.0621		280.9039
23818		304.3252	311.9859		340.0192
23819		432.3553	451.3066		457.8904
23820		547.2525	562.0876		637.5450
23821		681.8126	773.1511		913.0746
23822		945.7745	954.4738		974.6539
23823		976.0741	1042.2851		1115.2826
23824		1126.0122	1134.3677		1181.3815
23825		1223.9652	1237.9166		1278.8734
23826		1286.1599	1338.7872		1366.8262
23827		1399.0075	1404.5700		1415.2749
23828		1428.2766	1452.9131		1486.9373
23829		1489.6797	1498.4511		1842.2269
23830		3028.0341	3079.0712		3080.5418
23831		3095.9931	3159.2308		3161.3388
23832		3175.1887	3731.2534		3835.2517
23833	Zero-point correction (Hartree): 0.156054				
23834					
23835	diHPCARP_I.pmmmpd				
23836	-----				
23837	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18163056				
23838	Electronic state : 2-A				
23839	Cartesian coordinates (Angs):				
23840	O	-0.438365	1.530845	-1.836540	
23841	O	0.651244	1.477280	-1.127189	
23842	C	0.458241	0.821396	0.150532	
23843	C	0.400850	-0.706567	-0.024730	
23844	C	-0.699347	-1.189727	-0.967283	
23845	O	-1.965698	-0.719063	-0.567979	
23846	O	-2.342620	-1.445717	0.592779	
23847	H	-2.239767	-0.777160	1.290039	
23848	C	1.647432	1.257958	0.993057	
23849	H	1.636318	2.339147	1.123129	
23850	H	2.568816	0.964266	0.495784	
23851	H	1.597326	0.776080	1.966362	
23852	C	-0.821959	1.331806	0.791682	
23853	O	-1.236412	0.866819	1.820565	
23854	H	-1.307008	2.184692	0.293427	
23855	H	0.230454	-1.128985	0.967232	
23856	O	1.607992	-1.210706	-0.555698	
23857	O	2.504355	-1.488766	0.516002	
23858	H	2.602473	-2.445540	0.432878	
23859	H	-0.551723	-0.807707	-1.976003	
23860	H	-0.692162	-2.279537	-0.987903	
23861	Rotational constants (GHz):		1.0681900	0.8511400	0.7373100
23862	Vibrational harmonic frequencies (cm-1):				
23863		61.3191	88.9301		118.9757
23864		140.3092	175.0626		183.4713
23865		204.6973	225.9301		236.0344
23866		265.3362	274.7700		288.7580
23867		295.7675	317.5835		355.2568
23868		400.9790	442.2807		484.5998
23869		533.7750	553.5503		624.5579
23870		668.0962	756.7548		911.8749
23871		951.4571	955.4284		971.7277
23872		1020.7997	1037.4969		1108.1911
23873		1123.7192	1143.6070		1177.7394
23874		1225.7007	1238.1300		1283.4387
23875		1284.3130	1334.7419		1378.9413
23876		1405.4849	1407.8180		1410.3880
23877		1416.4196	1461.2337		1485.4069
23878		1487.5294	1504.3328		1836.4475


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23879          3030.1869          3082.0922          3092.2550
23880          3100.5720          3153.6280          3162.3357
23881          3179.9427          3716.6604          3822.5091
23882 Zero-point correction (Hartree): 0.156281
23883
23884 diHPCARP_I.pmmmppttd
23885 -----
23886 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18014921
23887 Electronic state : 2-A
23888 Cartesian coordinates (Angs):
23889 O      -0.793363      -1.128871      2.002305
23890 O      -0.056087      -1.701833      1.096247
23891 C      -0.125271      -1.035924      -0.188741
23892 C       0.707011      0.252625      -0.198617
23893 C       0.287149      1.282020      0.843630
23894 O      -1.079924      1.613685      0.719850
23895 O      -1.219816      2.426237      -0.437376
23896 H      -1.663374      1.821635      -1.054203
23897 C       0.391094      -2.058603      -1.190804
23898 H      -0.257944      -2.932704      -1.204504
23899 H       1.397391      -2.363702      -0.916584
23900 H       0.400816      -1.610454      -2.182056
23901 C      -1.578881      -0.712771      -0.515285
23902 O      -1.878029      -0.133858      -1.525007
23903 H      -2.328600      -1.096291      0.192309
23904 H       0.590468      0.677507      -1.200104
23905 O       2.053688      -0.136452      0.001968
23906 O       2.866692      0.987245      -0.310855
23907 H       3.327176      0.677212      -1.100391
23908 H       0.399053      0.879450      1.848921
23909 H       0.903113      2.174052      0.738458
23910 Rotational constants (GHz): 0.9819200      0.9235800      0.7146400
23911 Vibrational harmonic frequencies (cm-1):
23912      57.5692      89.1050      105.5978
23913      143.5437      172.6545      177.4236
23914      198.7018      204.8152      220.5551
23915      241.1413      259.0395      277.0765
23916      302.9766      314.2062      340.8273
23917      425.6837      442.8396      453.8288
23918      531.1668      558.0234      601.3456
23919      663.9686      775.8574      911.2744
23920      948.6807      953.5072      972.6365
23921      1020.2621      1054.5670      1107.4721
23922      1128.6210      1141.3003      1169.7357
23923      1227.5060      1241.8139      1280.3875
23924      1283.9299      1340.4699      1374.4828
23925      1400.9607      1404.5074      1414.7629
23926      1423.6744      1457.4446      1487.2797
23927      1491.6490      1501.1613      1838.5440
23928      3034.0303      3069.7025      3083.2121
23929      3101.4548      3157.7258      3161.1331
23930      3179.3792      3725.4893      3823.6648
23931 Zero-point correction (Hartree): 0.155987
23932
23933 diHPCARP_I.pmmmppttd
23934 -----
23935 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18049043
23936 Electronic state : 2-A
23937 Cartesian coordinates (Angs):
23938 O      -0.774169      -1.154889      1.996520
23939 O      -0.024820      -1.710861      1.089619
23940 C      -0.106680      -1.039601      -0.192719
23941 C       0.699819      0.264311      -0.190260
23942 C       0.257029      1.285178      0.850637
23943 O      -1.110626      1.607545      0.727690
23944 O      -1.257255      2.413110      -0.432981
23945 H      -1.677554      1.795740      -1.053882
23946 C       0.433818      -2.042297      -1.202066
23947 H      -0.193017      -2.932457      -1.219995
23948 H       1.449320      -2.319762      -0.933575
23949 H       0.432042      -1.586246      -2.189617
23950 C      -1.567398      -0.751727      -0.518007

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23951	O	-1.881963	-0.150463	-1.509403		
23952	H	-2.307842	-1.184730	0.171100		
23953	H	0.589722	0.687064	-1.192112		
23954	O	2.053014	-0.097089	0.015993		
23955	O	2.850143	0.960243	-0.505921		
23956	H	3.342364	1.235526	0.277090		
23957	H	0.368562	0.882386	1.856391		
23958	H	0.862277	2.186529	0.746958		
23959	Rotational constants (GHz):		0.9799900	0.9213600	0.7138000	
23960	Vibrational harmonic frequencies (cm-1):					
23961		52.2277	82.8160		94.1528	
23962		130.9756	171.3448		178.9613	
23963		198.9803	210.0510		230.1692	
23964		238.9218	258.9155		276.9389	
23965		301.5973	311.9423		341.1440	
23966		431.2455	443.0582		460.6962	
23967		531.8765	559.2732		604.2053	
23968		663.2439	775.2701		911.7357	
23969		950.4086	955.2400		971.4241	
23970		1022.5962	1057.5667		1109.7254	
23971		1131.0234	1136.4048		1171.3083	
23972		1230.4368	1241.5803		1283.2953	
23973		1285.9260	1340.1292		1374.2635	
23974		1401.7932	1409.6132		1416.9370	
23975		1418.8849	1458.7249		1485.8082	
23976		1491.0005	1498.9718		1840.7640	
23977		3032.8164	3082.6372		3084.9201	
23978		3087.7486	3146.9353		3162.8977	
23979		3181.3793	3721.2609		3828.8189	
23980	Zero-point correction (Hartree): 0.155993					
23981						
23982	diHPCARP_I.pmtmmtmmd					
23983	-----					
23984	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18111412					
23985	Electronic state : 2-A					
23986	Cartesian coordinates (Angs):					
23987	O	1.163701	-0.552331	2.040627		
23988	O	1.209013	0.553953	1.358896		
23989	C	1.202856	0.300592	-0.071129		
23990	C	-0.198460	-0.034951	-0.604001		
23991	C	-0.982090	-1.006124	0.272438		
23992	O	-2.232981	-1.317020	-0.313425		
23993	O	-3.149108	-0.279424	0.026253		
23994	H	-3.782676	-0.761729	0.571405		
23995	C	1.765615	1.560682	-0.705731		
23996	H	2.798222	1.711379	-0.392928		
23997	H	1.164664	2.413944	-0.399933		
23998	H	1.723783	1.470036	-1.789180		
23999	C	2.172611	-0.852505	-0.316395		
24000	O	2.065896	-1.614425	-1.231698		
24001	H	3.020827	-0.891532	0.388934		
24002	H	-0.041130	-0.508401	-1.576084		
24003	O	-0.937583	1.116419	-0.932358		
24004	O	-1.235566	1.823105	0.263580		
24005	H	-2.132080	1.498557	0.439880		
24006	H	-0.448147	-1.954907	0.330493		
24007	H	-1.133631	-0.625729	1.281327		
24008	Rotational constants (GHz):		1.3247100	0.7084400	0.6479000	
24009	Vibrational harmonic frequencies (cm-1):					
24010		55.7733	84.8834		90.2422	
24011		138.8604	166.5976		183.7477	
24012		193.0079	205.6663		239.9213	
24013		246.5651	264.6135		292.9782	
24014		319.0497	333.3675		335.1649	
24015		400.2976	474.8700		487.9872	
24016		563.1082	573.6205		613.9256	
24017		698.1222	822.0578		896.7703	
24018		926.3389	957.5187		968.8501	
24019		987.9289	1008.2723		1095.2825	
24020		1117.5574	1147.1408		1175.2380	
24021		1232.7575	1238.5262		1285.7037	
24022		1311.0772	1325.3870		1388.0264	

24023	1396.1048	1403.7892	1414.9043		
24024	1430.1397	1440.7907	1467.6011		
24025	1483.9806	1497.5109	1871.4964		
24026	2991.7605	3078.1903	3093.8289		
24027	3099.0852	3151.2046	3158.7900		
24028	3173.9566	3751.0883	3826.2817		
24029	Zero-point correction (Hartree): 0.156231				
24030					
24031	diHPCARP_I.pmtmptmmd				
24032	-----				
24033	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18284633				
24034	Electronic state : 2-A				
24035	Cartesian coordinates (Angs):				
24036	O	1.237757	-0.498068	2.033007	
24037	O	1.243437	0.593194	1.325779	
24038	C	1.184944	0.306808	-0.096018	
24039	C	-0.227940	-0.068319	-0.562572	
24040	C	-0.973760	-1.018307	0.368096	
24041	O	-2.224661	-1.387930	-0.177798	
24042	O	-3.145930	-0.327213	0.061448	
24043	H	-3.211954	0.068877	-0.818268	
24044	C	1.703496	1.558293	-0.783458	
24045	H	2.745553	1.729224	-0.515900	
24046	H	1.105555	2.412194	-0.474154	
24047	H	1.621480	1.439633	-1.861922	
24048	C	2.161888	-0.838127	-0.355804	
24049	O	2.033788	-1.613781	-1.256466	
24050	H	3.033239	-0.855586	0.321216	
24051	H	-0.101355	-0.567326	-1.526487	
24052	O	-1.003701	1.066385	-0.894781	
24053	O	-1.228882	1.825603	0.284406	
24054	H	-2.042410	1.419067	0.624521	
24055	H	-0.418760	-1.951722	0.460095	
24056	H	-1.117585	-0.601977	1.364672	
24057	Rotational constants (GHz):		1.3206500	0.7143100	0.6522900
24058	Vibrational harmonic frequencies (cm-1):				
24059	61.3418	86.5716	96.7428		
24060	148.1971	176.3940	185.0101		
24061	200.6873	211.4198	243.6862		
24062	260.2386	297.6695	312.3978		
24063	328.7506	337.3494	388.9482		
24064	413.0012	469.4711	542.1500		
24065	564.5748	576.5542	616.9928		
24066	696.7855	828.7881	898.6192		
24067	927.8836	956.3219	970.9617		
24068	989.4915	1008.1651	1100.6400		
24069	1118.3524	1142.7439	1170.5468		
24070	1235.1075	1238.0002	1285.1347		
24071	1308.8609	1323.3225	1388.1224		
24072	1404.0241	1409.8898	1415.2784		
24073	1422.1078	1440.5268	1473.6178		
24074	1484.3062	1499.8244	1871.6672		
24075	2998.2267	3079.4640	3092.5032		
24076	3099.1362	3149.6896	3159.4183		
24077	3175.5350	3730.7420	3799.6928		
24078	Zero-point correction (Hartree): 0.156764				
24079					
24080	diHPCARP_I.pmtmtttd				
24081	-----				
24082	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17918949				
24083	Electronic state : 2-A				
24084	Cartesian coordinates (Angs):				
24085	O	-1.502848	-1.358483	-1.566195	
24086	O	-1.510584	-0.063139	-1.446756	
24087	C	-1.262214	0.346474	-0.075556	
24088	C	0.227863	0.264843	0.266353	
24089	C	0.847596	-1.104733	0.013870	
24090	O	2.142589	-1.205772	0.584786	
24091	O	3.059666	-0.558610	-0.294457	
24092	H	3.692902	-1.264945	-0.466365	
24093	C	-1.799748	1.764454	0.027548	
24094	H	-2.880042	1.770120	-0.113579	

24095	H	-1.330810	2.385257	-0.730801	
24096	H	-1.562040	2.167706	1.010108	
24097	C	-2.097430	-0.554660	0.826772	
24098	O	-1.786048	-0.824419	1.948938	
24099	H	-3.050166	-0.888272	0.379316	
24100	H	0.309136	0.492987	1.331237	
24101	O	0.880247	1.281159	-0.472159	
24102	O	1.903649	1.850481	0.326397	
24103	H	2.658433	1.275986	0.118935	
24104	H	0.272495	-1.877621	0.523831	
24105	H	0.900333	-1.329226	-1.051032	
24106	Rotational constants (GHz):		1.2946400	0.6818200	0.6223800
24107	Vibrational harmonic frequencies (cm-1):				
24108		52.2912	66.0527		88.5704
24109		112.6460	128.2789		164.1975
24110		171.5623	184.0761		207.6493
24111		238.0568	270.3285		294.3309
24112		310.0262	326.2052		343.1822
24113		411.8076	436.3667		525.1419
24114		546.3983	560.5515		589.3184
24115		646.8645	859.3906		898.2287
24116		933.3517	967.0986		971.6546
24117		982.4207	1052.8969		1089.7732
24118		1115.4868	1149.5390		1156.5370
24119		1233.8181	1249.7870		1282.7461
24120		1313.9434	1326.8446		1372.4754
24121		1388.4194	1403.3884		1414.1132
24122		1432.8086	1452.1784		1471.6099
24123		1486.9335	1495.2199		1872.7685
24124		2987.1971	3079.0404		3088.9466
24125		3098.1994	3151.5316		3157.4658
24126		3178.7576	3736.3736		3843.0445
24127	Zero-point correction (Hartree):		0.155754		
24128					
24129	diHPCARP_I.pmtpmtmmd				
24130	-----				
24131	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.18080654		
24132	Electronic state : 2-A				
24133	Cartesian coordinates (Angs):				
24134	O	1.472043	-0.025429	2.028397	
24135	O	1.465660	0.832625	1.050448	
24136	C	1.175232	0.192562	-0.217559	
24137	C	-0.319389	-0.093710	-0.411324	
24138	C	-1.044832	-0.624386	0.827504	
24139	O	-2.440508	-0.452028	0.691999	
24140	O	-2.874241	-1.187867	-0.441786	
24141	H	-2.886971	-0.502202	-1.124877	
24142	C	1.714297	1.137591	-1.278812	
24143	H	2.795808	1.228577	-1.186393	
24144	H	1.256433	2.116222	-1.154524	
24145	H	1.466291	0.753763	-2.266158	
24146	C	1.983096	-1.103974	-0.260015	
24147	O	1.659093	-2.050998	-0.913247	
24148	H	2.926735	-1.072299	0.310859	
24149	H	-0.367846	-0.843864	-1.203446	
24150	O	-1.018102	0.998411	-0.973244	
24151	O	-1.101409	2.031885	-0.002068	
24152	H	-1.944730	1.824466	0.428167	
24153	H	-0.790673	-1.672823	0.991727	
24154	H	-0.805760	-0.053132	1.721873	
24155	Rotational constants (GHz):		1.2473200	0.7301600	0.6643600
24156	Vibrational harmonic frequencies (cm-1):				
24157		48.5947	69.3651		87.4991
24158		130.2249	148.3658		178.6365
24159		182.8977	222.0698		241.4739
24160		260.2760	297.1372		315.0366
24161		339.9370	351.7940		386.8164
24162		416.1095	441.9513		462.3263
24163		547.8560	603.6225		614.2046
24164		737.5842	802.9808		902.6425
24165		935.2251	956.3621		976.4875
24166		991.0479	1009.2255		1086.2445

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24167      1129.5262      1134.3253      1181.3454
24168      1232.0414      1237.3207      1282.3996
24169      1301.7491      1329.4139      1396.4113
24170      1403.0029      1409.2312      1414.7910
24171      1423.0847      1426.2419      1481.3226
24172      1484.6353      1496.2934      1872.2287
24173      2997.0579      3079.0979      3087.8494
24174      3102.5524      3157.3119      3159.6925
24175      3173.6341      3765.3209      3780.5845
24176      Zero-point correction (Hartree): 0.156470
24177
24178      diHPCARP_I.pmtpmtttd
24179      -----
24180      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18016335
24181      Electronic state : 2-A
24182      Cartesian coordinates (Angs):
24183      O      1.762243      -0.813459      1.773400
24184      O      1.752755      0.366713      1.225262
24185      C      1.244157      0.321127      -0.132665
24186      C      -0.281949      0.243411      -0.156052
24187      C      -0.872067      -0.871677      0.698497
24188      O      -2.287462      -0.830050      0.682471
24189      O      -2.727012      -1.160410      -0.625909
24190      H      -2.807309      -0.287250      -1.039057
24191      C      1.776261      1.577368      -0.805595
24192      H      2.862272      1.531772      -0.878643
24193      H      1.489907      2.451946      -0.227901
24194      H      1.351801      1.657325      -1.804398
24195      C      1.865135      -0.891373      -0.821435
24196      O      1.347758      -1.449086      -1.742500
24197      H      2.864510      -1.167167      -0.442836
24198      H      -0.548500      0.085676      -1.203740
24199      O      -0.763915      1.511926      0.259899
24200      O      -2.064376      1.701302      -0.281340
24201      H      -2.621083      1.413696      0.457063
24202      H      -0.519291      -1.848648      0.364086
24203      H      -0.621457      -0.725977      1.748670
24204      Rotational constants (GHz):      1.2570200      0.6983400      0.6445600
24205      Vibrational harmonic frequencies (cm-1):
24206      50.1188      85.3431      90.8644
24207      136.9263      159.2294      174.2936
24208      183.7017      211.9387      224.1697
24209      265.6293      281.1639      301.2691
24210      318.2431      356.2207      393.6956
24211      418.8420      465.2720      500.4901
24212      540.5027      558.2971      586.8964
24213      652.7435      872.7187      901.1521
24214      932.5503      956.9118      976.0505
24215      995.8382      1046.8401      1086.7845
24216      1135.0209      1140.0475      1162.3166
24217      1235.6927      1250.3193      1279.5586
24218      1308.3813      1339.9628      1373.9962
24219      1403.1005      1413.6271      1422.7606
24220      1431.0336      1439.7739      1464.6827
24221      1486.6608      1496.5721      1874.4304
24222      2992.4815      3079.9661      3082.7449
24223      3092.0603      3147.7453      3158.6023
24224      3178.8781      3754.2292      3777.4191
24225      Zero-point correction (Hartree): 0.156389
24226
24227      diHPCARP_I.pmtptmmd
24228      -----
24229      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17939227
24230      Electronic state : 2-A
24231      Cartesian coordinates (Angs):
24232      O      1.404174      -0.064791      2.037066
24233      O      1.540929      0.745771      1.029257
24234      C      1.186041      0.104993      -0.224088
24235      C      -0.332670      0.025112      -0.436722
24236      C      -1.108731      -0.421962      0.797124
24237      O      -2.499984      -0.306096      0.589453
24238      O      -2.853912      -1.165755      -0.486291

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24239	H	-3.320574	-1.872820	-0.023923		
24240	C	1.865515	0.932075	-1.302351		
24241	H	2.948093	0.879026	-1.193317		
24242	H	1.542303	1.966968	-1.216248		
24243	H	1.580119	0.554708	-2.282092		
24244	C	1.810260	-1.287634	-0.202580		
24245	O	1.363441	-2.214000	-0.812328		
24246	H	2.748078	-1.357488	0.375355		
24247	H	-0.481636	-0.709055	-1.230802		
24248	O	-0.861083	1.203591	-0.996857		
24249	O	-0.844795	2.224829	-0.007145		
24250	H	-1.777302	2.249741	0.248139		
24251	H	-0.831136	-1.444860	1.061322		
24252	H	-0.920581	0.229882	1.648014		
24253	Rotational constants (GHz):			1.1823200	0.7562400	0.6577000
24254	Vibrational harmonic frequencies (cm-1):					
24255		42.3757	47.9368			82.2283
24256		104.7229	134.9234			179.1380
24257		181.7051	203.9077			222.3426
24258		241.7950	258.4350			295.0921
24259		318.0072	330.7395			346.8823
24260		368.3604	401.3128			468.8429
24261		553.6474	594.0369			610.6058
24262		721.5605	811.3498			899.0161
24263		934.2000	954.9966			975.7996
24264		987.2060	1003.7832			1089.2584
24265		1133.6395	1144.0996			1180.5230
24266		1232.6285	1239.1885			1284.7385
24267		1308.9737	1324.9978			1388.6886
24268		1400.4162	1404.7041			1407.4395
24269		1416.2502	1430.5852			1478.9315
24270		1485.1397	1496.0609			1871.0704
24271		2993.2554	3075.6751			3078.2413
24272		3110.0904	3153.2595			3159.1258
24273		3172.2807	3796.0609			3820.6886
24274	Zero-point correction (Hartree):			0.155715		
24275	diHPCARP_I.pmtpptpd					
24276	-----					
24277	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17988532					
24278	Electronic state : 2-A					
24279	Cartesian coordinates (Angs):					
24280	O	1.755827	-0.822254	1.762718		
24281	O	1.793985	0.344656	1.188848		
24282	C	1.245192	0.294089	-0.154737		
24283	C	-0.281854	0.278422	-0.130157		
24284	C	-0.892192	-0.816189	0.733446		
24285	O	-2.309124	-0.736320	0.690681		
24286	O	-2.723469	-1.074770	-0.629225		
24287	H	-3.102882	-1.952276	-0.495251		
24288	C	1.797294	1.519142	-0.865036		
24289	H	2.880630	1.448046	-0.954821		
24290	H	1.537252	2.411540	-0.302219		
24291	H	1.356459	1.586877	-1.857730		
24292	C	1.804275	-0.955309	-0.827193		
24293	O	1.225505	-1.547968	-1.688731		
24294	H	2.820087	-1.233131	-0.495368		
24295	H	-0.603859	0.143252	-1.164165		
24296	O	-0.721400	1.543188	0.331559		
24297	O	-1.912893	1.890451	-0.354938		
24298	H	-2.576287	1.358381	0.110021		
24299	H	-0.557280	-1.809309	0.429891		
24300	H	-0.657869	-0.650165	1.784418		
24301	Rotational constants (GHz):			1.2249700	0.7117200	0.6440300
24302	Vibrational harmonic frequencies (cm-1):					
24303		52.2430	76.2087			87.0618
24304		113.8565	138.7692			173.3060
24305		177.6785	196.2075			212.7467
24306		241.6752	273.9603			287.7287
24307		300.6804	320.3922			355.7691
24308		405.6420	439.1944			480.3780
24309		542.1811	558.4512			587.2921

24311	650.6510	868.9823	900.8909	
24312	931.5722	954.5594	973.9829	
24313	994.4781	1051.3007	1080.5109	
24314	1127.5364	1142.8152	1163.7915	
24315	1236.3549	1250.9466	1282.8479	
24316	1305.8111	1331.6072	1369.9584	
24317	1397.4699	1404.7450	1414.8249	
24318	1429.7137	1441.0630	1463.1027	
24319	1486.5246	1496.6712	1873.3418	
24320	2987.2026	3079.7013	3081.8070	
24321	3106.7133	3148.0298	3158.4955	
24322	3178.1221	3765.8488	3819.6555	
24323	Zero-point correction (Hartree): 0.155765			
24324				
24325	diHPCARP_I.ppmmtmpd			
24326	-----			
24327	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17983369			
24328	Electronic state : 2-A			
24329	Cartesian coordinates (Angs):			
24330	O	0.527070	2.215738	-0.971714
24331	O	0.446029	1.755484	0.238254
24332	C	-0.440522	0.603398	0.334090
24333	C	0.141304	-0.532137	-0.553704
24334	C	1.196362	-1.380937	0.145022
24335	O	2.244840	-0.599525	0.673435
24336	O	2.891432	0.037090	-0.423741
24337	H	3.761454	-0.379391	-0.400139
24338	C	-0.527542	0.308039	1.822127
24339	H	-0.975092	1.153044	2.343128
24340	H	0.469668	0.138999	2.220975
24341	H	-1.142704	-0.573393	1.982482
24342	C	-1.804870	1.052562	-0.182943
24343	O	-2.795608	0.386689	-0.062677
24344	H	-1.830510	2.051905	-0.645897
24345	H	0.585961	-0.046146	-1.422777
24346	O	-0.848202	-1.357740	-1.118491
24347	O	-1.504393	-2.076221	-0.078136
24348	H	-2.296569	-1.525135	0.043008
24349	H	0.774285	-1.901078	1.003373
24350	H	1.575763	-2.116485	-0.567141
24351	Rotational constants (GHz): 1.2452200 0.8477800 0.6464100			
24352	Vibrational harmonic frequencies (cm-1):			
24353	67.4677	79.9910	99.4522	
24354	144.7027	171.8492	190.6460	
24355	197.2086	214.3759	223.6801	
24356	243.5833	275.4810	286.2799	
24357	298.6387	325.8226	374.7929	
24358	427.8124	452.6665	514.2839	
24359	558.9675	584.2322	627.1804	
24360	661.8260	782.8583	895.7494	
24361	935.6512	959.7634	976.9572	
24362	993.3979	1036.5091	1104.9899	
24363	1129.2585	1138.4984	1160.8226	
24364	1219.8418	1237.7961	1282.3367	
24365	1292.3816	1341.3851	1371.9929	
24366	1398.7155	1402.2637	1417.1154	
24367	1428.2041	1467.4824	1483.9536	
24368	1492.5261	1516.4413	1852.9872	
24369	3020.2847	3074.6619	3086.5025	
24370	3118.2463	3150.1801	3163.0811	
24371	3186.1848	3697.1381	3828.7945	
24372	Zero-point correction (Hartree): 0.156432			
24373				
24374	diHPCARP_I.ppmmtmpd			
24375	-----			
24376	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18202192			
24377	Electronic state : 2-A			
24378	Cartesian coordinates (Angs):			
24379	O	0.740210	2.139822	-0.939610
24380	O	0.589012	1.673153	0.263662
24381	C	-0.402926	0.603315	0.334173
24382	C	0.095948	-0.563441	-0.564838

24383	C	1.126681	-1.454855	0.117579	
24384	O	2.197559	-0.716672	0.661579	
24385	O	2.918792	-0.152393	-0.428198	
24386	H	2.786836	0.794495	-0.282887	
24387	C	-0.530097	0.301405	1.817426	
24388	H	-0.904082	1.178070	2.344227	
24389	H	0.442041	0.034384	2.224443	
24390	H	-1.224381	-0.521569	1.960817	
24391	C	-1.714181	1.170490	-0.200938	
24392	O	-2.756697	0.589088	-0.089478	
24393	H	-1.648907	2.163329	-0.674897	
24394	H	0.543628	-0.104641	-1.447423	
24395	O	-0.949310	-1.330302	-1.107536	
24396	O	-1.641703	-1.992070	-0.053974	
24397	H	-2.409450	-1.404682	0.046389	
24398	H	0.688246	-1.980867	0.964208	
24399	H	1.490630	-2.185015	-0.606850	
24400	Rotational constants (GHz):		1.2591000	0.8515200	0.6498800
24401	Vibrational harmonic frequencies (cm-1):				
24402		74.8344	93.4594		104.6219
24403		155.0986	171.5049		184.6213
24404		197.9143	212.2597		233.1707
24405		271.2173	282.8281		299.2638
24406		323.2726	333.7118		369.9345
24407		424.7726	445.7661		506.1943
24408		534.3004	588.0199		625.6979
24409		660.7109	779.1595		888.9545
24410		936.6806	959.9708		977.5877
24411		992.6864	1035.0143		1108.4253
24412		1128.3546	1143.3838		1155.7333
24413		1218.6091	1234.2995		1279.8517
24414		1290.5381	1345.7078		1376.8980
24415		1401.3603	1406.2739		1418.2865
24416		1426.6740	1461.2625		1484.4612
24417		1491.8220	1515.4119		1855.4983
24418		3012.1143	3083.9311		3088.3839
24419		3114.8332	3151.2376		3165.0828
24420		3190.8969	3711.9819		3799.6341
24421	Zero-point correction (Hartree):		0.156565		
24422	diHPCARP_I.ppmptpmd				
24423	-----				
24425	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17977357		
24426	Electronic state : 2-A				
24427	Cartesian coordinates (Angs):				
24428	O	-0.590285	-1.812415	-1.294361	
24429	O	-0.681555	-1.588078	-0.014941	
24430	C	0.344718	-0.659084	0.429587	
24431	C	0.021844	0.743842	-0.131847	
24432	C	-1.250291	1.356065	0.460144	
24433	O	-2.362265	0.498390	0.487868	
24434	O	-2.766936	0.295876	-0.860353	
24435	H	-2.591443	-0.647604	-0.982819	
24436	C	0.332012	-0.722029	1.946860	
24437	H	0.697541	-1.685526	2.300641	
24438	H	-0.686565	-0.584535	2.305937	
24439	H	0.970628	0.068681	2.336793	
24440	C	1.657913	-1.257898	-0.065803	
24441	O	2.655134	-0.644109	-0.315758	
24442	H	1.636950	-2.360804	-0.120086	
24443	H	-0.047548	0.681071	-1.217271	
24444	O	1.034245	1.659691	0.230246	
24445	O	1.886446	1.923930	-0.869315	
24446	H	2.538572	1.210492	-0.772437	
24447	H	-1.076028	1.620066	1.504101	
24448	H	-1.477553	2.266502	-0.095599	
24449	Rotational constants (GHz):		1.2174700	0.8201800	0.6532200
24450	Vibrational harmonic frequencies (cm-1):				
24451		33.5335	63.6803		97.0090
24452		138.6038	155.9721		168.1319
24453		210.2808	232.8074		251.5567
24454		266.4131	281.4662		314.3615


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24455      320.9381      335.6013      376.7018
24456      403.8464      446.8405      504.1272
24457      547.4259      571.1028      619.4925
24458      684.4809      757.9330      900.0469
24459      947.2092      968.6639      972.6739
24460      1021.9530      1041.8431      1104.6598
24461      1130.4329      1146.1434      1166.1882
24462      1221.1937      1254.5670      1277.8670
24463      1292.8943      1327.6995      1371.2165
24464      1400.4718      1405.3288      1422.9312
24465      1431.2690      1468.6900      1480.4366
24466      1492.0000      1511.7391      1870.2020
24467      2988.5390      3072.9364      3081.9404
24468      3117.2751      3136.6591      3149.9086
24469      3166.2605      3716.3005      3793.7760
24470 Zero-point correction (Hartree): 0.156360
24471
24472 diHPCARP_I.ppmmttptd
24473 -----
24474 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17980783
24475 Electronic state : 2-A
24476 Cartesian coordinates (Angs):
24477 O      -0.692994      -1.662864      -1.395411
24478 O      -0.533687      -1.647703      -0.105093
24479 C       0.406190      -0.626945      0.338185
24480 C      -0.075952      0.758615      -0.167451
24481 C      -1.304129      1.282174      0.577089
24482 O      -2.347787      0.344382      0.654245
24483 O      -2.888615      0.208289      -0.653098
24484 H      -2.620856      -0.690623      -0.893697
24485 C       0.466655      -0.737703      1.844553
24486 H       0.926910      -1.678121      2.139611
24487 H      -0.535743      -0.682376      2.262913
24488 H       1.075992      0.078008      2.229217
24489 C       1.752241      -0.969408      -0.296569
24490 O       2.794067      -0.687099      0.222462
24491 H       1.695330      -1.497253      -1.263158
24492 H      -0.283236      0.691215      -1.234733
24493 O       0.910531      1.737718      0.063120
24494 O       1.800366      1.752158      -1.046787
24495 H       2.628570      1.474704      -0.631070
24496 H      -1.049857      1.509031      1.612817
24497 H      -1.642188      2.195971      0.087749
24498 Rotational constants (GHz): 1.2865800      0.7879100      0.6571700
24499 Vibrational harmonic frequencies (cm-1):
24500      45.6828      67.2668      87.2682
24501      145.9107      157.5902      172.8912
24502      193.0985      210.2711      239.4623
24503      249.2067      276.4190      282.2255
24504      338.4803      344.3854      378.0987
24505      384.2001      425.0030      470.4772
24506      505.6142      547.6345      599.4684
24507      670.4998      765.7269      882.3643
24508      931.8675      953.8006      1004.7332
24509      1028.6856      1032.9850      1113.8872
24510      1132.6161      1141.2538      1161.6142
24511      1207.5359      1245.7123      1284.3900
24512      1305.2468      1339.2620      1372.9365
24513      1397.5488      1407.8239      1423.4198
24514      1426.1978      1431.3369      1482.3122
24515      1491.3084      1509.1837      1858.1290
24516      3008.1221      3083.9185      3086.6440
24517      3119.9755      3141.4474      3165.1828
24518      3173.5185      3777.5856      3796.2309
24519 Zero-point correction (Hartree): 0.155999
24520
24521 diHPCARP_I.pppmtmpd
24522 -----
24523 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18068651
24524 Electronic state : 2-A
24525 Cartesian coordinates (Angs):
24526 O       2.429104      -1.461169      -0.877454

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24527	O	1.783673	-1.383099	0.246257	
24528	C	0.959128	-0.180741	0.334818	
24529	C	-0.126696	-0.304617	-0.768610	
24530	C	-1.233315	-1.300967	-0.433046	
24531	O	-2.095504	-0.921957	0.615363	
24532	O	-3.161522	-0.160033	0.074426	
24533	H	-2.794209	0.737981	0.096724	
24534	C	0.477567	-0.170395	1.777553	
24535	H	1.332818	-0.082114	2.446724	
24536	H	-0.054983	-1.091240	2.001128	
24537	H	-0.199494	0.662528	1.936797	
24538	C	1.879192	1.011687	0.097248	
24539	O	1.506340	2.148378	0.193300	
24540	H	2.929122	0.766064	-0.127774	
24541	H	0.392504	-0.695660	-1.647612	
24542	O	-0.586286	0.942228	-1.242028	
24543	O	-1.168164	1.692985	-0.184845	
24544	H	-0.411170	2.241869	0.088200	
24545	H	-1.823324	-1.491406	-1.329869	
24546	H	-0.767636	-2.236487	-0.112251	
24547	Rotational constants (GHz): 1.3479300 0.7792900 0.6325500				
24548	Vibrational harmonic frequencies (cm-1):				
24549		80.7718	94.5387	99.5788	
24550		171.6710	177.8070	201.1892	
24551		214.7248	234.5307	256.0629	
24552		282.7578	288.3537	301.2949	
24553		320.5710	350.1130	440.3324	
24554		459.5896	512.1689	528.4864	
24555		549.4115	579.4680	658.2713	
24556		713.9620	833.8249	885.3693	
24557		894.1609	962.4307	971.4186	
24558		987.3080	1017.7124	1047.6832	
24559		1132.9495	1140.7955	1169.1875	
24560		1218.9732	1237.4932	1280.7841	
24561		1323.3561	1352.1740	1390.8815	
24562		1406.8031	1411.0017	1424.4404	
24563		1450.8240	1462.1803	1465.5457	
24564		1483.7173	1501.9596	1852.2783	
24565		3021.1342	3066.9463	3084.4829	
24566		3085.0933	3124.7921	3164.0137	
24567		3196.3320	3654.5454	3737.8328	
24568	Zero-point correction (Hartree): 0.157094				
24569					
24570	diHPCARP_I.pppmtpm				
24571	-----				
24572	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17935167				
24573	Electronic state : 2-A				
24574	Cartesian coordinates (Angs):				
24575	O	2.127644	-1.348959	-1.296470	
24576	O	1.425919	-1.626530	-0.235797	
24577	C	0.880870	-0.419556	0.361706	
24578	C	-0.230982	0.114127	-0.560596	
24579	C	-1.339994	-0.901353	-0.828976	
24580	O	-2.194434	-1.055135	0.286638	
24581	O	-3.239362	-0.098231	0.198697	
24582	H	-2.784837	0.722444	0.442546	
24583	C	0.418916	-0.819857	1.751871	
24584	H	1.275807	-1.075847	2.374970	
24585	H	-0.245158	-1.678771	1.688292	
24586	H	-0.125045	0.007090	2.202271	
24587	C	2.055083	0.542844	0.492131	
24588	O	1.985852	1.732154	0.361972	
24589	H	3.002978	0.050125	0.770675	
24590	H	0.223539	0.415127	-1.505007	
24591	O	-0.813329	1.253515	0.059370	
24592	O	-0.492279	2.432237	-0.655896	
24593	H	0.394108	2.621973	-0.302567	
24594	H	-1.930085	-0.585699	-1.688650	
24595	H	-0.914746	-1.886075	-1.027462	
24596	Rotational constants (GHz): 1.2363600 0.7804400 0.6077700				
24597	Vibrational harmonic frequencies (cm-1):				
24598		50.3286	64.6931	79.8240	

24599	117.9963	137.4954	182.4850		
24600	196.7092	226.2517	239.5497		
24601	258.1304	278.3968	290.1172		
24602	328.0008	368.5619	412.8013		
24603	453.7217	471.0126	511.8357		
24604	549.1526	573.9130	648.8564		
24605	705.5825	796.5783	902.0084		
24606	916.0092	963.0324	973.9326		
24607	1002.6976	1044.6151	1071.1425		
24608	1122.6416	1145.7982	1147.8159		
24609	1223.7430	1260.3816	1275.1634		
24610	1307.8734	1350.5938	1366.4529		
24611	1399.1458	1411.0062	1423.1531		
24612	1455.4085	1472.5601	1477.5597		
24613	1489.3576	1494.8228	1865.9693		
24614	2995.5641	3076.6114	3085.2311		
24615	3108.1918	3139.9162	3155.6883		
24616	3175.7441	3685.7904	3758.0692		
24617	Zero-point correction (Hartree): 0.156478				
24618					
24619	diHPCARP_I.pppmtpd				
24620	-----				
24621	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17772105				
24622	Electronic state : 2-A				
24623	Cartesian coordinates (Angs):				
24624	O	1.874140	-1.623979	-1.274179	
24625	O	1.652945	-1.424994	-0.009090	
24626	C	1.018304	-0.141541	0.271682	
24627	C	-0.216638	-0.002171	-0.633336	
24628	C	-1.250380	-1.115215	-0.494693	
24629	O	-1.943710	-1.114754	0.736910	
24630	O	-2.910554	-0.068688	0.707634	
24631	H	-2.504328	0.584608	1.294056	
24632	C	0.759369	-0.129583	1.757675	
24633	H	1.706488	-0.170691	2.291065	
24634	H	0.134145	-0.970280	2.044665	
24635	H	0.263563	0.801454	2.024056	
24636	C	2.034304	0.935290	-0.138021	
24637	O	2.406904	1.793743	0.600632	
24638	H	2.400219	0.842350	-1.176267	
24639	H	0.122883	0.009846	-1.672318	
24640	O	-0.742720	1.271281	-0.304642	
24641	O	-1.706356	1.609354	-1.286442	
24642	H	-2.514347	1.233092	-0.900802	
24643	H	-1.967720	-1.060527	-1.314720	
24644	H	-0.755855	-2.086234	-0.536161	
24645	Rotational constants (GHz): 1.2839700			0.7190300	0.6261200
24646	Vibrational harmonic frequencies (cm-1):				
24647	18.9540	71.0377	77.7954		
24648	122.7641	160.0575	176.6180		
24649	187.1082	211.4661	235.1779		
24650	256.5247	272.3016	288.3565		
24651	305.9346	350.7743	379.2842		
24652	404.5329	466.5840	479.0724		
24653	555.9046	563.0029	653.9981		
24654	739.7407	806.9573	871.7827		
24655	897.7987	934.7700	975.5151		
24656	1016.9155	1047.7964	1054.0990		
24657	1117.7118	1139.7331	1178.3925		
24658	1197.1746	1265.1209	1289.9361		
24659	1323.5999	1363.4471	1390.1482		
24660	1398.3532	1406.8595	1416.5144		
24661	1434.5578	1455.9318	1476.3052		
24662	1489.0083	1491.8609	1883.6834		
24663	2986.3878	3074.8417	3086.6220		
24664	3092.2681	3137.8654	3167.8318		
24665	3184.6304	3725.7259	3793.9725		
24666	Zero-point correction (Hartree): 0.156171				
24667					
24668	diHPCARP_I.pptmptmmd				
24669	-----				
24670	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17784293				

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24671 Electronic state : 2-A
24672 Cartesian coordinates (Angs):
24673 O -1.685062 2.081020 -0.858573
24674 O -1.671263 1.501349 0.303039
24675 C -1.096526 0.152428 0.280040
24676 C 0.313245 0.253927 -0.331324
24677 C 1.340266 0.843627 0.619595
24678 O 2.576679 1.086565 -0.019864
24679 O 3.258071 -0.158552 -0.150174
24680 H 3.168103 -0.329853 -1.097482
24681 C -1.193779 -0.330821 1.706403
24682 H -2.239313 -0.375437 2.003245
24683 H -0.664146 0.343637 2.376764
24684 H -0.769243 -1.327911 1.778704
24685 C -1.969129 -0.681680 -0.668238
24686 O -2.495705 -1.697981 -0.333145
24687 H -2.080765 -0.259076 -1.681350
24688 H 0.237442 0.898269 -1.209719
24689 O 0.722451 -0.979214 -0.896937
24690 O 0.988799 -1.915366 0.137224
24691 H 1.934022 -1.757691 0.293150
24692 H 0.999725 1.826440 0.949797
24693 H 1.497943 0.214165 1.495472
24694 Rotational constants (GHz): 1.3730900 0.7063900 0.5685300
24695 Vibrational harmonic frequencies (cm-1):
24696 34.0099 71.7490 98.5085
24697 129.0919 153.2706 173.9600
24698 205.3106 214.0605 233.7735
24699 262.5010 274.9543 287.4777
24700 315.4877 324.6051 383.7888
24701 409.3434 465.8775 507.3468
24702 540.3579 565.5994 658.7667
24703 676.9896 811.5172 878.1383
24704 888.1680 954.4928 979.2105
24705 1005.8634 1013.5808 1100.6767
24706 1118.7213 1139.8387 1157.8380
24707 1205.9430 1259.4758 1293.3672
24708 1312.6095 1335.4896 1385.3706
24709 1396.4855 1410.4175 1425.2171
24710 1429.8291 1448.0207 1478.3943
24711 1488.7863 1498.2776 1882.0595
24712 2996.9302 3084.4386 3089.9323
24713 3098.5219 3138.1896 3163.9812
24714 3187.4387 3726.2357 3803.2620
24715 Zero-point correction (Hartree): 0.156222
24716
24717 diHPCARP_I.pptmptmpd
24718 -----
24719 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18016140
24720 Electronic state : 2-A
24721 Cartesian coordinates (Angs):
24722 O 1.896257 -1.887807 -1.039042
24723 O 1.700345 -1.538364 0.196208
24724 C 1.106146 -0.212413 0.311622
24725 C -0.299180 -0.281339 -0.342326
24726 C -1.351827 -0.903216 0.564100
24727 O -2.542708 -1.120296 -0.158481
24728 O -3.327052 0.060888 -0.095095
24729 H -2.904310 0.629794 -0.755160
24730 C 1.129156 0.083386 1.802799
24731 H 2.157321 0.122370 2.158990
24732 H 0.604256 -0.698536 2.347468
24733 H 0.646143 1.036859 1.994787
24734 C 2.015164 0.764222 -0.427055
24735 O 1.859922 1.952145 -0.372646
24736 H 2.845632 0.310985 -0.991376
24737 H -0.203157 -0.898779 -1.237622
24738 O -0.725880 0.953730 -0.878054
24739 O -0.877161 1.901197 0.174101
24740 H -0.039465 2.388131 0.088997
24741 H -1.012799 -1.888535 0.891335
24742 H -1.560179 -0.278081 1.431816

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24743 Rotational constants (GHz): 1.3297400 0.7337200 0.5831000
24744 Vibrational harmonic frequencies (cm-1):
24745 72.9018 92.1875 99.9820
24746 131.8518 172.0173 195.1843
24747 202.8315 223.8265 240.5660
24748 254.2135 287.8671 295.7977
24749 322.5471 328.6489 418.1821
24750 433.0623 475.5126 520.8614
24751 561.3549 568.6129 618.9721
24752 682.6845 824.9415 895.2789
24753 900.7455 964.0697 984.2435
24754 995.7580 1007.1101 1101.8594
24755 1128.2685 1149.6955 1156.2709
24756 1221.9775 1233.2041 1280.5306
24757 1311.0096 1326.5362 1391.4802
24758 1405.2419 1415.4394 1421.9632
24759 1438.5137 1462.0045 1470.0822
24760 1488.8620 1505.2899 1854.3082
24761 3016.8854 3077.0330 3086.4542
24762 3101.7215 3140.1786 3159.8667
24763 3187.2290 3699.8996 3775.2857
24764 Zero-point correction (Hartree): 0.156690
24765
24766 diHPCARP_I.pptmptpm
24767 -----
24768 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17892672
24769 Electronic state : 2-A
24770 Cartesian coordinates (Angs):
24771 O 1.807912 -1.589830 -1.364959
24772 O 1.501142 -1.632788 -0.100512
24773 C 1.074562 -0.330067 0.374150
24774 C -0.313762 -0.030630 -0.232460
24775 C -1.325192 -1.131645 0.075738
24776 O -2.548308 -0.864721 -0.569146
24777 O -3.356465 -0.076307 0.291180
24778 H -2.971853 0.805740 0.182521
24779 C 1.071702 -0.415767 1.892010
24780 H 2.088491 -0.491556 2.276110
24781 H 0.518478 -1.296139 2.213286
24782 H 0.598712 0.476449 2.296409
24783 C 2.162129 0.649375 -0.043034
24784 O 1.992442 1.824690 -0.206011
24785 H 3.165169 0.196742 -0.125284
24786 H -0.223793 0.074516 -1.314226
24787 O -0.831234 1.177707 0.299300
24788 O -0.685641 2.236302 -0.633280
24789 H 0.238332 2.500236 -0.482949
24790 H -0.969291 -2.081280 -0.324431
24791 H -1.499650 -1.232733 1.147563
24792 Rotational constants (GHz): 1.2681500 0.7252700 0.5759900
24793 Vibrational harmonic frequencies (cm-1):
24794 46.0496 58.8750 63.8696
24795 117.5092 137.1833 178.2144
24796 204.4551 220.0406 243.4445
24797 260.4402 278.4736 295.4770
24798 315.8762 337.4232 395.0331
24799 430.0629 463.0049 513.7445
24800 556.7336 563.6993 584.2916
24801 663.9663 830.3106 887.5825
24802 910.6687 969.0717 977.1313
24803 1004.6914 1053.5538 1113.8038
24804 1134.6275 1135.9406 1159.9932
24805 1215.6768 1254.4217 1272.9634
24806 1311.2800 1334.4117 1362.5475
24807 1406.2269 1411.4259 1422.1942
24808 1450.2594 1469.7368 1477.4329
24809 1490.7073 1504.5130 1865.0184
24810 2998.2448 3076.8087 3082.4330
24811 3108.0093 3139.6177 3152.9354
24812 3172.6796 3693.0768 3777.0464
24813 Zero-point correction (Hartree): 0.156180
24814

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24815 diHPCARP_I.pptptpmd
24816 -----
24817 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17733304
24818 Electronic state : 2-A
24819 Cartesian coordinates (Angs):
24820 O 0.311555 -2.042604 -1.338640
24821 O 0.645349 -1.930514 -0.086742
24822 C 0.912595 -0.553684 0.294693
24823 C -0.365965 0.280532 0.032108
24824 C -1.518413 -0.165392 0.919387
24825 O -2.748153 0.364441 0.491002
24826 O -3.091082 -0.318074 -0.712033
24827 H -3.227532 0.422515 -1.315237
24828 C 1.315463 -0.585216 1.753578
24829 H 2.257073 -1.115805 1.878446
24830 H 0.550947 -1.080553 2.348748
24831 H 1.443110 0.437583 2.101114
24832 C 2.060422 -0.057076 -0.576489
24833 O 2.772440 0.847744 -0.243154
24834 H 2.192430 -0.590261 -1.532453
24835 H -0.651788 0.172165 -1.013354
24836 O -0.140949 1.641549 0.324985
24837 O 0.339739 2.288570 -0.845579
24838 H 1.263826 2.453658 -0.611722
24839 H -1.571690 -1.255387 0.959124
24840 H -1.392180 0.232208 1.926958
24841 Rotational constants (GHz): 1.2063500 0.7458200 0.6045100
24842 Vibrational harmonic frequencies (cm-1):
24843 29.0531 44.8173 63.5955
24844 112.9408 155.3703 165.8217
24845 189.8941 193.8064 207.5390
24846 227.1499 254.5947 267.7690
24847 280.5076 305.0781 345.7101
24848 423.2004 437.0724 471.8156
24849 498.4864 564.4266 585.8421
24850 676.8632 819.7065 887.6387
24851 907.9715 957.6757 981.9365
24852 1007.0391 1050.5701 1110.3817
24853 1128.8568 1142.6369 1172.3341
24854 1209.0152 1241.2537 1278.9380
24855 1307.1215 1345.0938 1369.5468
24856 1400.3218 1406.3928 1419.9936
24857 1421.9214 1433.9768 1469.8224
24858 1489.0316 1503.7956 1856.8124
24859 3011.8610 3074.7333 3085.2998
24860 3123.3664 3137.3966 3162.7760
24861 3173.9218 3795.2217 3830.8741
24862 Zero-point correction (Hartree): 0.155409
24863
24864 diHPCARP_I.ptmmmtmpd
24865 -----
24866 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18023070
24867 Electronic state : 2-A
24868 Cartesian coordinates (Angs):
24869 O 2.602185 -0.010352 -0.883477
24870 O 1.606572 -0.790991 -1.179577
24871 C 0.494898 -0.715710 -0.241829
24872 C -0.251026 0.617456 -0.483823
24873 C -1.386538 0.911680 0.500002
24874 O -2.445079 -0.016880 0.435712
24875 O -2.987601 0.043160 -0.880982
24876 H -3.870527 0.391220 -0.707535
24877 C -0.376140 -1.913108 -0.586583
24878 H 0.231160 -2.816699 -0.584206
24879 H -0.823189 -1.782400 -1.570379
24880 H -1.165751 -2.005432 0.152344
24881 C 1.039652 -0.866718 1.176184
24882 O 0.317882 -1.055331 2.111510
24883 H 2.137460 -0.838887 1.275340
24884 H -0.658276 0.576636 -1.496038
24885 O 0.614206 1.725822 -0.532659
24886 O 1.250563 1.848465 0.733499

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24887	H	2.141120	1.542075	0.502017	
24888	H	-1.042848	0.860449	1.530897	
24889	H	-1.744041	1.920289	0.281654	
24890	Rotational constants (GHz):		1.2673700	0.7605800	0.7013900
24891	Vibrational harmonic frequencies (cm-1):				
24892		42.4908	75.1559		127.5783
24893		163.1176	166.6741		181.8191
24894		198.5860	215.7328		226.0779
24895		236.9004	266.5013		280.2456
24896		317.8943	338.3669		351.5353
24897		435.4238	463.7213		485.4505
24898		507.4763	545.9240		634.1172
24899		692.7503	792.6030		895.8433
24900		930.4163	954.7961		977.3527
24901		994.3381	1054.3061		1101.4036
24902		1120.1175	1128.2968		1170.8289
24903		1208.6223	1233.7004		1277.3291
24904		1300.5626	1340.9863		1375.9336
24905		1390.6597	1404.2774		1418.5552
24906		1420.3561	1433.4030		1484.7320
24907		1489.8073	1497.1316		1863.3365
24908		2999.7274	3074.2003		3083.9924
24909		3103.3261	3158.7816		3163.0790
24910		3194.1342	3755.7523		3828.0485
24911	Zero-point correction (Hartree): 0.156224				
24912					
24913	diHPCARP_I.ptppmttptd				
24914	-----				
24915	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18032620				
24916	Electronic state : 2-A				
24917	Cartesian coordinates (Angs):				
24918	O	2.505138	1.283689	0.361774	
24919	O	2.296668	0.348276	-0.518226	
24920	C	1.064200	-0.380956	-0.259404	
24921	C	-0.108168	0.463094	-0.787304	
24922	C	-1.321005	-0.334524	-1.255422	
24923	O	-1.856180	-1.229096	-0.311770	
24924	O	-2.450826	-0.460343	0.727279	
24925	H	-1.743491	-0.508125	1.395978	
24926	C	1.241504	-1.701087	-0.995844	
24927	H	2.151548	-2.190529	-0.651886	
24928	H	1.333036	-1.519738	-2.066320	
24929	H	0.389380	-2.348899	-0.803397	
24930	C	1.040487	-0.679436	1.238256	
24931	O	0.053330	-0.906867	1.875352	
24932	H	2.044673	-0.751467	1.687099	
24933	H	0.262776	1.006234	-1.665863	
24934	O	-0.391798	1.388967	0.247879	
24935	O	-1.480845	2.200634	-0.142983	
24936	H	-2.222453	1.709826	0.247283	
24937	H	-2.089439	0.358110	-1.598804	
24938	H	-1.032027	-0.960041	-2.100216	
24939	Rotational constants (GHz):		1.2878100	0.8207400	0.7158400
24940	Vibrational harmonic frequencies (cm-1):				
24941		51.4184	111.3387		130.7645
24942		158.8030	160.2241		192.1109
24943		201.4680	240.3265		272.7816
24944		290.0246	305.7819		322.6756
24945		350.7384	365.3703		377.1235
24946		479.9673	507.1436		528.9568
24947		563.1730	616.4088		621.5863
24948		713.6832	837.2049		879.7568
24949		911.1039	951.4344		975.3267
24950		988.1835	1050.1537		1064.4801
24951		1133.4326	1134.2775		1177.1754
24952		1216.5070	1266.8604		1284.1015
24953		1304.3858	1360.8608		1368.1441
24954		1402.9069	1407.9180		1433.2638
24955		1447.9012	1471.1572		1481.6934
24956		1503.8256	1505.6592		1871.6248
24957		3009.0412	3026.8889		3073.6233
24958		3093.2868	3136.1953		3149.5313

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24959          3170.1524          3675.7821          3730.4042
24960 Zero-point correction (Hartree): 0.157321
24961
24962 diHPCARP_I.pttmtmpd
24963 -----
24964 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18014768
24965 Electronic state : 2-A
24966 Cartesian coordinates (Angs):
24967 O      1.973018      1.771327      -0.269315
24968 O      2.018165      0.627994      -0.885469
24969 C      1.145002      -0.382836      -0.314119
24970 C      -0.315974      -0.041596      -0.675554
24971 C      -1.343526      -1.004499      -0.083667
24972 O      -2.616691      -0.709352      -0.616774
24973 O      -3.239275      0.263855      0.207071
24974 H      -2.826331      1.086320      -0.093322
24975 C      1.577053      -1.683183      -0.973410
24976 H      2.652267      -1.810813      -0.862464
24977 H      1.329859      -1.673348      -2.033495
24978 H      1.080751      -2.518270      -0.486603
24979 C      1.393548      -0.467422      1.191836
24980 O      0.982614      -1.386465      1.836929
24981 H      2.006682      0.337605      1.628190
24982 H      -0.398497      -0.073619      -1.765267
24983 O      -0.655513      1.299685      -0.390715
24984 O      -0.510299      1.514748      1.007748
24985 H      0.297356      2.052431      1.009591
24986 H      -1.123499      -2.028185      -0.385593
24987 H      -1.371363      -0.949251      1.002641
24988 Rotational constants (GHz):      1.3483400      0.7331100      0.6454800
24989 Vibrational harmonic frequencies (cm-1):
24990      72.4369      83.2586      122.4570
24991      139.3006      176.5473      184.7395
24992      203.5672      222.1122      237.4194
24993      265.7398      291.2712      310.3819
24994      327.2636      346.4905      397.2813
24995      416.5300      479.4883      489.8413
24996      509.8577      560.6453      638.0179
24997      669.6334      837.6177      891.6086
24998      917.3011      956.6075      993.3267
24999      999.7168      1004.4211      1110.6487
25000      1122.8552      1130.7577      1165.5085
25001      1209.5486      1226.4841      1275.5424
25002      1302.1141      1323.3047      1387.6313
25003      1399.1246      1406.6469      1416.3184
25004      1430.6095      1435.9950      1463.8559
25005      1491.9484      1504.3762      1865.4949
25006      3009.3521      3081.9291      3084.7455
25007      3100.7869      3159.3741      3160.8527
25008      3180.3471      3752.7398      3780.4162
25009 Zero-point correction (Hartree): 0.156565
25010
25011 diHPCARP_I.pttpptmtd
25012 -----
25013 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17944532
25014 Electronic state : 2-A
25015 Cartesian coordinates (Angs):
25016 O      -2.406214      -0.923985      -0.932924
25017 O      -1.798090      0.170340      -1.280255
25018 C      -0.820202      0.637050      -0.312856
25019 C      0.424817      -0.275747      -0.373816
25020 C      1.477862      0.071305      0.677094
25021 O      2.734537      -0.440702      0.292524
25022 O      3.161532      0.326404      -0.831391
25023 H      3.965467      0.731763      -0.485563
25024 C      -0.484584      2.049651      -0.765943
25025 H      -1.401785      2.621728      -0.894064
25026 H      0.054025      2.024641      -1.711515
25027 H      0.124276      2.541104      -0.012755
25028 C      -1.458234      0.674984      1.073400
25029 O      -0.919694      1.226982      1.988689
25030 H      -2.450483      0.204477      1.166031

```


25031	H	0.866754	-0.155943	-1.365280	
25032	O	0.104010	-1.644240	-0.333717	
25033	O	-0.542724	-1.912630	0.903757	
25034	H	-1.451895	-2.040100	0.592345	
25035	H	1.547894	1.143164	0.856692	
25036	H	1.240926	-0.431648	1.613377	
25037	Rotational constants (GHz):			1.2605500	0.7139600 0.6575500
25038	Vibrational harmonic frequencies (cm-1):				
25039		47.1606	71.4966		120.3315
25040		147.8594	157.4923		175.1845
25041		189.4174	196.6097		219.4254
25042		237.9167	271.6442		289.1999
25043		316.6183	335.3346		353.4694
25044		384.2335	469.8635		489.9603
25045		511.2210	565.5322		647.9489
25046		673.3802	849.3203		896.5346
25047		920.8499	955.3112		987.1185
25048		991.5476	1005.4111		1095.1062
25049		1123.6060	1139.8428		1164.0650
25050		1207.9047	1222.3243		1276.5371
25051		1299.5459	1329.0864		1387.8507
25052		1391.3966	1400.9498		1417.0112
25053		1425.5281	1430.9769		1462.9172
25054		1488.8188	1503.4915		1860.7976
25055		3005.8964	3083.8791		3100.1293
25056		3103.7202	3158.6041		3160.3083
25057		3185.2224	3761.1781		3834.4108
25058	Zero-point correction (Hartree): 0.156051				
25059	diHPCARP_I.pttpttmpd				
25060	-----				
25061	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17949053				
25062	Electronic state : 2-A				
25063	Cartesian coordinates (Angs):				
25064	O	-2.321127	-1.124717	-0.882856	
25065	O	-1.800989	-0.006854	-1.292890	
25066	C	-0.868462	0.590767	-0.352646	
25067	C	0.443049	-0.225374	-0.362239	
25068	C	1.465902	0.271914	0.655085	
25069	O	2.737600	-0.272909	0.394633	
25070	O	3.211439	0.364377	-0.793535	
25071	H	3.593785	-0.388231	-1.259734	
25072	C	-0.643247	1.998557	-0.882466	
25073	H	-1.602886	2.481911	-1.056796	
25074	H	-0.086314	1.967795	-1.817214	
25075	H	-0.093159	2.581085	-0.149151	
25076	C	-1.516629	0.657652	1.028344	
25077	O	-1.029385	1.303083	1.910158	
25078	H	-2.469424	0.116408	1.145946	
25079	H	0.870093	-0.134051	-1.363195	
25080	O	0.230091	-1.609696	-0.235535	
25081	O	-0.395108	-1.852584	1.017721	
25082	H	-1.292226	-2.065731	0.717871	
25083	H	1.526651	1.359833	0.673712	
25084	H	1.209640	-0.085717	1.650518	
25085	Rotational constants (GHz):			1.2647000	0.7107200 0.6558400
25086	Vibrational harmonic frequencies (cm-1):				
25087		37.3207	74.5725		126.7794
25088		150.9016	161.4327		164.3329
25089		172.2873	192.0878		219.0650
25090		237.8181	275.5499		286.7196
25091		314.7133	335.9421		352.9722
25092		384.2194	467.0563		474.5223
25093		511.5351	566.1382		650.7286
25094		672.7896	844.1527		895.8225
25095		920.7027	957.8666		987.1507
25096		993.0868	1005.0096		1102.7029
25097		1125.8150	1136.6979		1165.1814
25098		1208.7272	1224.2016		1276.1182
25099		1299.6886	1327.0795		1387.8565
25100		1399.2241	1412.0064		1418.6130
25101		1428.9335	1433.3889		1466.0886
25102					

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25103      1491.0034      1504.3850      1862.8168
25104      3010.1152      3083.5782      3099.1779
25105      3101.5323      3158.7902      3163.7098
25106      3184.0827      3755.8505      3841.3729
25107 Zero-point correction (Hartree): 0.156059
25108
25109 diHPCARP_I.tmmmpmpd
25110 -----
25111 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20901343
25112 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09326400
25113 T1 diagnostic: 0.020213
25114 E(MP2/Aug-CC-pVTZ) (Hartree): -721.04792499
25115 E(MP3/Aug-CC-pVTZ) (Hartree): -721.07035089
25116 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05100303
25117 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07218263
25118 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.53922702
25119 E(UHF/Aug-CC-pVTZ) (Hartree): -718.53418766
25120 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18336945
25121 Electronic state : 2-A
25122 Cartesian coordinates (Angs):
25123 O      -1.710073      -1.653756      -1.426895
25124 O      -1.278782      -0.495754      -1.022591
25125 C      -0.538647      -0.604162      0.224862
25126 C      0.035619      0.788833      0.535866
25127 C      0.870324      1.353574      -0.610037
25128 O      1.906878      0.458328      -0.955130
25129 O      2.877473      0.497989      0.080487
25130 H      2.777155      -0.377747      0.489225
25131 C      -1.452590      -1.105641      1.329692
25132 H      -1.886540      -2.062604      1.050477
25133 H      -2.243272      -0.382514      1.518927
25134 H      -0.864203      -1.230504      2.236788
25135 C      0.608919      -1.585009      0.007951
25136 O      1.398278      -1.822228      0.883221
25137 H      0.652488      -2.069678      -0.978310
25138 H      0.678012      0.655097      1.409468
25139 O      -0.938090      1.702920      0.986388
25140 O      -1.677587      2.188945      -0.127209
25141 H      -2.436396      1.591179      -0.161255
25142 H      0.278615      1.456306      -1.516308
25143 H      1.277609      2.323328      -0.325178
25144 Rotational constants (GHz):      1.0830800      0.9056600      0.6710700
25145 Vibrational harmonic frequencies (cm-1):
25146      47.0620      111.5834      118.1274
25147      133.0552      170.7481      182.7149
25148      186.9795      205.7523      228.5085
25149      232.8251      261.9754      286.7124
25150      315.2631      342.1871      374.2251
25151      403.7946      428.7794      473.9315
25152      520.3868      583.1728      626.9312
25153      704.8105      753.9643      900.2708
25154      945.3712      967.9794      977.1827
25155      982.7300      1037.9474      1111.2135
25156      1124.7345      1133.4865      1180.3765
25157      1212.0226      1237.5682      1269.7932
25158      1287.7735      1333.7819      1377.2567
25159      1398.0915      1405.7875      1414.0459
25160      1416.9989      1463.9702      1485.8240
25161      1489.2131      1497.6934      1835.1991
25162      3038.5726      3084.2908      3097.8887
25163      3099.8051      3165.9817      3170.8567
25164      3173.9577      3721.6774      3797.5204
25165 Zero-point correction (Hartree): 0.156124
25166
25167 diHPCARP_I.tmmmpmpd
25168 -----
25169 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18325967
25170 Electronic state : 2-A
25171 Cartesian coordinates (Angs):
25172 O      -1.177281      -2.342443      -1.154478
25173 O      -0.842008      -1.088566      -1.179830
25174 C      -0.559967      -0.573717      0.148984

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25175	C	-0.105484	0.878008	-0.050139			
25176	C	1.001262	0.994983	-1.097662			
25177	O	2.076218	0.133329	-0.793948			
25178	O	2.792150	0.708136	0.288858			
25179	H	2.548145	0.128267	1.029921			
25180	C	-1.795327	-0.696107	1.025543			
25181	H	-2.077408	-1.741742	1.122941			
25182	H	-2.612573	-0.134400	0.579297			
25183	H	-1.573085	-0.285931	2.008416			
25184	C	0.580290	-1.392823	0.736773			
25185	O	1.121750	-1.072333	1.762315			
25186	H	0.853861	-2.303724	0.183341			
25187	H	0.257256	1.241251	0.912480			
25188	O	-1.154233	1.704463	-0.507453			
25189	O	-1.867101	2.205289	0.619247			
25190	H	-1.707245	3.153533	0.534163			
25191	H	0.642443	0.671904	-2.073735			
25192	H	1.348007	2.025774	-1.155503			
25193	Rotational constants (GHz):				1.0136100	0.8843100	0.6774200
25194	Vibrational harmonic frequencies (cm-1):						
25195		62.6265	86.8495			116.5531	
25196		144.0882	179.0021			187.1718	
25197		196.6358	207.5881			212.9516	
25198		253.4012	270.7674			286.2121	
25199		319.7481	345.3074			390.0226	
25200		401.7437	418.5744			435.7365	
25201		522.7113	596.9311			625.0795	
25202		655.6117	756.2892			906.4213	
25203		953.1553	969.8868			981.6991	
25204		1021.4057	1038.4651			1106.2713	
25205		1121.3007	1147.3295			1178.1730	
25206		1208.8946	1250.9469			1279.1044	
25207		1296.0055	1335.9282			1386.7224	
25208		1401.5624	1407.8044			1409.8397	
25209		1415.5617	1466.5770			1482.9491	
25210		1486.9963	1507.4930			1833.5246	
25211		3034.2418	3086.5465			3097.5081	
25212		3106.4773	3156.9774			3171.8453	
25213		3176.0561	3706.4868			3822.8984	
25214	Zero-point correction (Hartree):				0.156338		
25215	diHPCARP_I.tmmpttmd						
25216	-----						
25217	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18219560						
25218	Electronic state : 2-A						
25219	Cartesian coordinates (Angs):						
25220	O	2.628575	-0.325049	-1.241967			
25221	O	1.359104	-0.574913	-1.131812			
25222	C	0.866163	-0.266521	0.198031			
25223	C	-0.644996	-0.499106	0.169496			
25224	C	-1.324923	0.249917	-0.972367			
25225	O	-1.017091	1.629073	-0.926501			
25226	O	-1.759658	2.200258	0.140907			
25227	H	-1.068292	2.379104	0.799827			
25228	C	1.579468	-1.120569	1.234432			
25229	H	2.645554	-0.907486	1.221131			
25230	H	1.413582	-2.173101	1.020628			
25231	H	1.180325	-0.878033	2.217732			
25232	C	1.139528	1.210743	0.471519			
25233	O	0.739290	1.748158	1.469380			
25234	H	1.750890	1.731471	-0.280007			
25235	H	-1.035423	-0.154319	1.130790			
25236	O	-0.849246	-1.893699	0.042140			
25237	O	-2.230588	-2.134927	0.278357			
25238	H	-2.199274	-2.638887	1.100936			
25239	H	-0.939733	-0.096948	-1.930391			
25240	H	-2.402152	0.100213	-0.931340			
25241	Rotational constants (GHz):				0.9936300	0.9071100	0.6482000
25242	Vibrational harmonic frequencies (cm-1):						
25243		59.5762	85.4361			116.4754	
25244		124.5267	173.1733			187.8668	
25245		194.3784	207.4295			216.2527	

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25247      229.1574      258.1555      277.5166
25248      315.1812      325.6623      380.1728
25249      407.6770      420.6411      451.8499
25250      498.3945      581.2703      621.4550
25251      658.7356      772.6931      905.8202
25252      954.5284      969.0832      974.9768
25253      1019.2259      1052.7760      1104.6912
25254      1126.8100      1138.8385      1174.2459
25255      1216.0564      1248.9548      1276.6987
25256      1292.8843      1345.9672      1384.1319
25257      1396.6022      1404.8736      1412.2986
25258      1425.3228      1463.0823      1487.2225
25259      1490.3173      1502.4005      1836.7871
25260      3036.6285      3078.7520      3087.1799
25261      3103.3854      3161.4890      3168.2164
25262      3179.8804      3717.3968      3823.2145
25263 Zero-point correction (Hartree): 0.156110
25264
25265 diHPCARP_I.tmmptttd
25266 -----
25267 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18221721
25268 Electronic state : 2-A
25269 Cartesian coordinates (Angs):
25270 O      2.635275      -0.315192      -1.239931
25271 O      1.367694      -0.572970      -1.126398
25272 C      0.870236      -0.255224      0.200470
25273 C      -0.637595      -0.504818      0.167477
25274 C      -1.326483      0.237359      -0.973276
25275 O      -1.043476      1.620797      -0.934867
25276 O      -1.788203      2.182480      0.135275
25277 H      -1.097958      2.358201      0.796785
25278 C      1.586394      -1.092275      1.248396
25279 H      2.651533      -0.874468      1.232639
25280 H      1.421615      -2.147859      1.050829
25281 H      1.183846      -0.838582      2.227322
25282 C      1.130966      1.226594      0.459528
25283 O      0.717402      1.773308      1.446682
25284 H      1.747192      1.742873      -0.291417
25285 H      -1.033313      -0.172959      1.130136
25286 O      -0.827177      -1.900895      0.041672
25287 O      -2.155061      -2.174823      0.477506
25288 H      -2.525850      -2.608977      -0.300376
25289 H      -0.936912      -0.104146      -1.932042
25290 H      -2.402882      0.074454      -0.928960
25291 Rotational constants (GHz): 0.9889000 0.9077800 0.6475800
25292 Vibrational harmonic frequencies (cm-1):
25293      58.5865      77.7897      110.7032
25294      121.7029      175.1548      185.8769
25295      191.7484      202.7260      215.1754
25296      225.6224      257.5833      276.7982
25297      313.7814      323.8898      379.3592
25298      407.3168      426.6230      450.5099
25299      497.5409      582.5411      621.5230
25300      659.6641      771.8122      905.3690
25301      955.7829      968.7843      975.0811
25302      1020.7031      1055.0858      1106.2949
25303      1128.1624      1136.3223      1174.5534
25304      1213.8205      1251.2004      1279.5094
25305      1294.7454      1345.9292      1380.5746
25306      1397.3034      1406.8741      1416.2657
25307      1419.2580      1464.4990      1486.6093
25308      1489.1789      1500.7376      1837.7785
25309      3033.8088      3087.5016      3089.4052
25310      3093.5147      3149.7431      3169.5174
25311      3182.4728      3711.4110      3830.7369
25312 Zero-point correction (Hartree): 0.156038
25313
25314 diHPCARP_I.tmmmtmpd
25315 -----
25316 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17880679
25317 Electronic state : 2-A
25318 Cartesian coordinates (Angs):

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25319	O	1.588481	-1.540009	1.605652		
25320	O	1.130245	-0.411159	1.151922		
25321	C	0.577025	-0.560290	-0.184489		
25322	C	-0.085214	0.775732	-0.559741		
25323	C	-0.970464	1.338318	0.548716		
25324	O	-1.946356	0.394702	0.935233		
25325	O	-2.847645	0.246659	-0.159311		
25326	H	-3.674353	0.547090	0.237295		
25327	C	1.671464	-0.950688	-1.161280		
25328	H	2.136601	-1.879644	-0.840649		
25329	H	2.425010	-0.169341	-1.235818		
25330	H	1.221193	-1.097675	-2.140947		
25331	C	-0.486136	-1.663974	-0.134393		
25332	O	-1.007012	-2.062220	-1.133487		
25333	H	-0.715920	-2.062930	0.865074		
25334	H	-0.696919	0.569281	-1.441193		
25335	O	0.829407	1.747943	-1.019081		
25336	O	1.568743	2.245125	0.089682		
25337	H	2.366921	1.700090	0.078486		
25338	H	-0.394154	1.525753	1.451243		
25339	H	-1.435328	2.264465	0.208751		
25340	Rotational constants (GHz):			1.0363400	0.9111700	0.6805100
25341	Vibrational harmonic frequencies (cm-1):					
25342		35.5552	93.9801			95.4695
25343		123.2705	136.9239			143.0740
25344		155.7452	182.5700			199.9491
25345		215.3541	234.0392			245.6851
25346		293.9954	312.3332			349.1941
25347		377.9994	410.3607			477.6679
25348		515.7962	583.1546			624.6631
25349		707.1746	759.1204			891.9431
25350		939.9914	968.2347			975.5813
25351		983.0348	1034.6531			1104.5189
25352		1122.3871	1124.7954			1182.4946
25353		1207.3352	1233.7859			1271.0374
25354		1289.4500	1333.4052			1376.0547
25355		1392.0143	1400.7910			1406.8800
25356		1414.5254	1423.3026			1482.1293
25357		1487.5387	1499.3665			1867.2359
25358		3028.0810	3084.7914			3089.1966
25359		3100.6432	3164.8335			3168.9940
25360		3173.9331	3798.7607			3831.1696
25361	Zero-point correction (Hartree):			0.155202		
25362	diHPCARP_I.tmmmtmtd					
25363	-----					
25364	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17856107					
25365	Electronic state : 2-A					
25366	Cartesian coordinates (Angs):					
25367	O	1.284048	-1.701705	1.675736		
25368	O	0.928122	-0.533687	1.234168		
25369	C	0.537443	-0.592194	-0.163774		
25370	C	-0.018101	0.787789	-0.551734		
25371	C	-0.878342	1.406723	0.546131		
25372	O	-1.902745	0.519028	0.938709		
25373	O	-2.807068	0.413770	-0.159623		
25374	H	-3.626858	0.723156	0.244071		
25375	C	1.720966	-0.996532	-1.024046		
25376	H	2.068237	-1.983341	-0.727864		
25377	H	2.522438	-0.270781	-0.914346		
25378	H	1.397278	-1.028930	-2.062539		
25379	C	-0.581584	-1.631416	-0.289122		
25380	O	-1.053558	-1.906670	-1.352480		
25381	H	-0.902459	-2.105031	0.651367		
25382	H	-0.624796	0.628452	-1.445985		
25383	O	0.966308	1.690810	-0.999725		
25384	O	1.853314	1.939631	0.095178		
25385	H	1.929999	2.899943	0.051224		
25386	H	-0.293912	1.570690	1.448605		
25387	H	-1.299576	2.350214	0.195023		
25388	Rotational constants (GHz):			1.0350300	0.9062300	0.6967400
25389	Vibrational harmonic frequencies (cm-1):					
25390						

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25391      48.6871      87.0223      97.2390
25392      118.4479     129.4682     138.4000
25393      150.1930     155.4767     194.1879
25394      216.3584     233.0454     244.4042
25395      288.0200     308.2709     339.7235
25396      375.6381     413.0587     475.9683
25397      509.8854     583.0832     626.8367
25398      703.3754     760.4440     894.8950
25399      942.3848     972.1089     977.3482
25400      982.2573     1040.5609    1104.9167
25401      1120.2041     1130.1447    1182.9172
25402      1208.0951     1238.9479    1275.9423
25403      1293.9968     1337.5255    1373.6898
25404      1388.6400     1397.8531    1409.0520
25405      1410.0590     1434.3640    1484.3436
25406      1489.5582     1502.8665    1866.4660
25407      3023.0297     3080.5226    3089.4896
25408      3103.8429     3163.2593    3171.6093
25409      3182.3073     3833.6783    3841.4798
25410 Zero-point correction (Hartree): 0.155247
25411
25412 diHPCARP_I.tmpmmtmmd
25413 -----
25414 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17792676
25415 Electronic state : 2-A
25416 Cartesian coordinates (Angs):
25417 O      -1.197692     -0.491913      2.206436
25418 O      -0.292149     -0.364656      1.285484
25419 C      -0.881383     -0.247128     -0.043637
25420 C       0.220590     -0.034779     -1.090797
25421 C       1.113510      1.199085     -0.881895
25422 O       1.377680      1.592007      0.443158
25423 O       2.284520      0.665685      1.021924
25424 H       1.687128      0.150192      1.585999
25425 C      -1.702110     -1.491853     -0.343475
25426 H      -2.491680     -1.607034      0.394447
25427 H      -1.050282     -2.362267     -0.328034
25428 H      -2.145804     -1.389174     -1.332006
25429 C      -1.779934      0.989825     -0.025044
25430 O      -2.193655      1.480512     -1.035175
25431 H      -2.027931      1.382945      0.974152
25432 H      -0.328424      0.157123     -2.016807
25433 O       0.927188     -1.210809     -1.419251
25434 O       1.538820     -1.762213     -0.264115
25435 H       2.326692     -1.208210     -0.151118
25436 H       2.047501      1.048419     -1.428811
25437 H       0.601064      2.068209     -1.296416
25438 Rotational constants (GHz):      1.1231500      0.8328200      0.8011900
25439 Vibrational harmonic frequencies (cm-1):
25440      43.4596      52.2927      116.9873
25441      134.8771     143.7990     188.0400
25442      195.6324     201.7624     225.8398
25443      252.5716     254.5746     264.4695
25444      316.9081     326.7659     391.9782
25445      398.3062     457.5813     503.1559
25446      556.9202     594.0546     650.1323
25447      721.5840     772.9568     867.8393
25448      939.7257     964.3652     971.0510
25449      1001.9256     1032.0656     1067.5967
25450      1127.3029     1136.0020     1174.7019
25451      1210.7920     1244.2356     1282.7927
25452      1311.3368     1363.6434     1382.5889
25453      1397.4967     1403.4685     1415.7464
25454      1431.0528     1455.5937     1473.1877
25455      1486.1780     1501.5461     1863.1954
25456      3013.5596     3065.8556     3082.8864
25457      3087.5375     3126.1098     3170.2225
25458      3178.9779     3745.8720     3754.2196
25459 Zero-point correction (Hartree): 0.156044
25460
25461 diHPCARP_I.tmpmmtttd
25462 -----

```

```

25463 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18017382
25464 Electronic state : 2-A
25465 Cartesian coordinates (Angs):
25466 O -1.658400 -1.208740 -1.691937
25467 O -0.601701 -0.647186 -1.189229
25468 C -0.953137 0.308675 -0.148323
25469 C 0.371588 0.746152 0.496745
25470 C 1.060488 -0.333327 1.324484
25471 O 1.210534 -1.573168 0.671055
25472 O 2.131420 -1.391901 -0.397931
25473 H 1.530418 -1.274309 -1.149983
25474 C -1.710690 1.475163 -0.757386
25475 H -2.578954 1.105422 -1.297869
25476 H -1.062083 2.028817 -1.431354
25477 H -2.046073 2.124869 0.048707
25478 C -1.804940 -0.421960 0.886265
25479 O -2.309685 0.161439 1.800491
25480 H -1.899062 -1.511766 0.746743
25481 H 0.143632 1.576323 1.174540
25482 O 1.140856 1.215235 -0.600768
25483 O 2.429746 1.578095 -0.149073
25484 H 2.922335 0.758674 -0.315974
25485 H 2.024680 0.031720 1.677767
25486 H 0.443088 -0.558163 2.195839
25487 Rotational constants (GHz): 1.2314300 0.7554500 0.7247100
25488 Vibrational harmonic frequencies (cm-1):
25489 55.5982 64.1071 97.3411
25490 102.7277 140.1800 188.7028
25491 208.8851 222.1168 231.2865
25492 247.9090 282.1259 306.2349
25493 334.4722 358.9643 394.6620
25494 452.3230 460.0610 481.6971
25495 514.6578 599.3579 644.8599
25496 740.6360 804.7511 864.3580
25497 928.5407 956.9574 978.7857
25498 994.4432 1047.9840 1057.8998
25499 1126.9207 1152.7277 1165.5600
25500 1220.8092 1244.6432 1288.3954
25501 1298.3565 1363.6932 1381.3496
25502 1397.9739 1406.9996 1415.8432
25503 1431.5043 1443.6608 1491.1756
25504 1493.5311 1501.1058 1867.2678
25505 3007.7832 3052.4113 3086.9870
25506 3089.7356 3134.5878 3169.3354
25507 3179.3341 3735.3087 3756.4319
25508 Zero-point correction (Hartree): 0.156433
25509
25510 diHPCARP_I.tmppppttd
25511 -----
25512 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18017383
25513 Electronic state : 2-A
25514 Cartesian coordinates (Angs):
25515 O 1.658163 -1.208153 1.692570
25516 O 0.601583 -0.646818 1.189409
25517 C 0.953212 0.308693 0.148250
25518 C -0.371493 0.746160 -0.496923
25519 C -1.060469 -0.333435 -1.324436
25520 O -1.210483 -1.573143 -0.670667
25521 O -2.131542 -1.391658 0.398099
25522 H -1.530771 -1.273952 1.150308
25523 C 1.710908 1.475242 0.756895
25524 H 2.579224 1.105616 1.297395
25525 H 1.062450 2.029182 1.430780
25526 H 2.046282 2.124703 -0.049412
25527 C 1.804846 -0.422403 -0.886197
25528 O 2.309470 0.160595 -1.800731
25529 H 1.898916 -1.512153 -0.746158
25530 H -0.143512 1.576242 -1.174824
25531 O -1.140704 1.215326 0.600549
25532 O -2.429561 1.577993 0.148782
25533 H -2.922103 0.758571 0.315732
25534 H -2.024734 0.031530 -1.677618

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25535      H      -0.443179      -0.558420      -2.195821
25536 Rotational constants (GHz):      1.2314600      0.7554500      0.7247900
25537 Vibrational harmonic frequencies (cm-1):
25538      55.5556      64.0639      97.3514
25539      102.6220      140.1036      188.7254
25540      208.8277      222.1330      231.3036
25541      247.9249      282.1015      306.2292
25542      334.4706      358.9611      394.6729
25543      452.1572      459.9700      481.7437
25544      514.6006      599.3583      644.8590
25545      740.6412      804.7496      864.3910
25546      928.5529      956.9792      978.7861
25547      994.4527      1048.0335      1057.9845
25548      1126.9142      1152.7859      1165.5752
25549      1220.8213      1244.6207      1288.4450
25550      1298.3446      1363.6849      1381.3521
25551      1398.0002      1406.9800      1415.8301
25552      1431.4446      1443.6776      1491.1881
25553      1493.5307      1501.1243      1867.3241
25554      3007.7235      3052.3756      3086.9187
25555      3089.7520      3134.6142      3169.2300
25556      3179.2626      3735.4570      3756.4983
25557 Zero-point correction (Hartree): 0.156432
25558
25559 diHPCARP_I.tmtmmtmmd
25560 -----
25561 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17917703
25562 Electronic state : 2-A
25563 Cartesian coordinates (Angs):
25564 O      -2.291428      -1.097369      1.517264
25565 O      -1.105795      -0.721674      1.145519
25566 C      -1.120118      -0.046235      -0.145888
25567 C      0.326855      0.314176      -0.504138
25568 C      1.123075      0.789759      0.706675
25569 O      2.425532      1.201136      0.341163
25570 O      3.243448      0.037052      0.257743
25571 H      3.882743      0.207805      0.960184
25572 C      -1.774914      -0.924458      -1.198931
25573 H      -2.821221      -1.091699      -0.955996
25574 H      -1.248986      -1.875269      -1.246803
25575 H      -1.699597      -0.426075      -2.163763
25576 C      -1.953934      1.221917      0.035375
25577 O      -1.815841      2.191344      -0.651966
25578 H      -2.717427      1.161712      0.830074
25579 H      0.269474      1.132177      -1.225552
25580 O      0.984637      -0.694898      -1.230408
25581 O      1.162971      -1.824785      -0.387994
25582 H      2.073663      -1.679513      -0.089073
25583 H      0.649209      1.683653      1.117864
25584 H      1.178172      0.029811      1.483938
25585 Rotational constants (GHz):      1.3551300      0.6770500      0.5934800
25586 Vibrational harmonic frequencies (cm-1):
25587      52.1520      79.8817      82.4692
25588      114.8450      156.3970      162.3737
25589      194.5786      199.5469      238.1844
25590      248.9708      263.6928      281.1328
25591      299.7499      329.5311      375.7019
25592      393.5411      455.4009      484.1346
25593      510.8265      568.4700      656.5548
25594      693.7951      796.1525      891.0234
25595      939.4117      959.6657      979.1246
25596      994.1192      1008.1859      1092.6620
25597      1121.5580      1146.8036      1172.0393
25598      1202.2472      1251.6171      1278.2928
25599      1319.3064      1327.2402      1394.1648
25600      1397.2795      1400.4927      1409.9276
25601      1429.8393      1441.7993      1471.5472
25602      1482.0072      1501.1370      1865.6161
25603      2998.1650      3081.8586      3085.8111
25604      3101.6462      3145.8769      3169.2229
25605      3177.4702      3763.4245      3826.7240
25606 Zero-point correction (Hartree): 0.155976

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25607
25608 diHPCARP_I.tmtmptmmd
25609 -----
25610 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18107258
25611 Electronic state : 2-A
25612 Cartesian coordinates (Angs):
25613 O -2.344857 -1.086063 1.457740
25614 O -1.143258 -0.718801 1.131881
25615 C -1.105181 -0.041572 -0.157222
25616 C 0.354122 0.315887 -0.454758
25617 C 1.118970 0.770826 0.783424
25618 O 2.423147 1.205312 0.458905
25619 O 3.241850 0.051296 0.290909
25620 H 3.323632 0.013786 -0.672039
25621 C -1.725821 -0.911363 -1.237799
25622 H -2.781349 -1.071823 -1.033238
25623 H -1.206987 -1.866524 -1.270831
25624 H -1.613938 -0.408780 -2.196955
25625 C -1.937335 1.232821 -0.006386
25626 O -1.767213 2.199651 -0.689790
25627 H -2.729406 1.177826 0.759895
25628 H 0.329285 1.139695 -1.171738
25629 O 1.039581 -0.695605 -1.165275
25630 O 1.136424 -1.849064 -0.342388
25631 H 1.968260 -1.682749 0.129560
25632 H 0.629732 1.649163 1.208758
25633 H 1.166856 -0.003994 1.547177
25634 Rotational constants (GHz): 1.3562700 0.6833700 0.5964300
25635 Vibrational harmonic frequencies (cm-1):
25636 54.3454 82.0892 87.8020
25637 117.4779 156.4553 176.1814
25638 193.8949 202.8831 237.0234
25639 264.4098 272.0729 303.2447
25640 312.6431 375.8797 380.3414
25641 404.8348 460.9113 499.2659
25642 532.9411 573.0439 657.6174
25643 693.8986 801.1821 893.1662
25644 940.4981 958.5222 980.3995
25645 996.4194 1007.7235 1096.6892
25646 1122.2058 1143.2975 1167.7179
25647 1200.8475 1253.0876 1277.4515
25648 1314.3385 1327.2543 1395.4770
25649 1398.0842 1409.0158 1411.1204
25650 1422.6134 1439.9369 1478.2437
25651 1481.5227 1502.8411 1865.9980
25652 3001.5918 3085.8742 3085.9896
25653 3099.2894 3142.3488 3168.8160
25654 3178.0475 3740.2560 3797.4088
25655 Zero-point correction (Hartree): 0.156338
25656
25657 diHPCARP_I.tmtmptmmd
25658 -----
25659 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17938265
25660 Electronic state : 2-A
25661 Cartesian coordinates (Angs):
25662 O 2.602060 -0.982023 -1.186195
25663 O 1.333445 -0.794743 -0.983616
25664 C 1.084496 0.046837 0.177489
25665 C -0.429149 0.206931 0.340814
25666 C -1.166617 0.410739 -0.986938
25667 O -2.536363 0.101396 -0.852273
25668 O -3.095412 0.982376 0.110239
25669 H -3.047915 0.446947 0.915532
25670 C 1.734151 -0.554802 1.413317
25671 H 2.814301 -0.583702 1.295201
25672 H 1.351933 -1.561874 1.563867
25673 H 1.479761 0.058428 2.275965
25674 C 1.718878 1.408262 -0.113486
25675 O 1.389199 2.403614 0.461930
25676 H 2.522650 1.395664 -0.869037
25677 H -0.566629 1.084982 0.974575
25678 O -1.027374 -0.820854 1.101889

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25679	O	-0.981392	-2.028502	0.355182	
25680	H	-1.827884	-1.997342	-0.115654	
25681	H	-1.031963	1.438417	-1.332303	
25682	H	-0.818108	-0.279430	-1.752573	
25683	Rotational constants (GHz):		1.3248800	0.6996000	0.5972100
25684	Vibrational harmonic frequencies (cm-1):				
25685		47.3634	62.0804		70.2184
25686		121.6216	128.7003		152.8794
25687		180.5705	210.0009		233.6495
25688		250.0392	268.1144		323.4436
25689		343.2299	372.1852		386.9982
25690		399.0499	441.5921		460.9355
25691		483.3861	604.6946		655.3016
25692		727.0620	791.7264		891.4318
25693		946.7105	953.9726		986.2762
25694		992.5034	1010.7650		1084.2846
25695		1130.5390	1137.5354		1181.7017
25696		1201.0373	1252.9775		1278.8319
25697		1305.3379	1335.6947		1396.3550
25698		1399.6930	1408.2656		1410.1775
25699		1423.5263	1428.4266		1482.6027
25700		1490.7152	1501.2633		1865.8599
25701		3000.6279	3074.9588		3085.5201
25702		3106.1139	3152.9942		3168.8586
25703		3177.7887	3765.2317		3777.0674
25704	Zero-point correction (Hartree):		0.156101		
25705					
25706	diHPCARP_I.tmtpmttpd				
25707	-----				
25708	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17926285		
25709	Electronic state : 2-A				
25710	Cartesian coordinates (Angs):				
25711	O	-2.838277	-0.495082	1.319100	
25712	O	-1.551417	-0.557185	1.154891	
25713	C	-1.153450	-0.093361	-0.163821	
25714	C	0.373661	-0.132949	-0.198221	
25715	C	0.999245	0.562002	1.006219	
25716	O	2.406734	0.447865	1.008626	
25717	O	2.909415	1.178985	-0.098905	
25718	H	2.961402	0.494920	-0.783991	
25719	C	-1.794863	-0.951154	-1.242587	
25720	H	-2.877283	-0.864328	-1.189047	
25721	H	-1.499211	-1.988478	-1.113179	
25722	H	-1.454325	-0.595054	-2.213206	
25723	C	-1.623736	1.355019	-0.313862	
25724	O	-1.298465	2.027084	-1.247077	
25725	H	-2.291987	1.722940	0.483247	
25726	H	0.667101	0.366782	-1.124122	
25727	O	0.761557	-1.494735	-0.262720	
25728	O	2.070101	-1.559075	-0.815299	
25729	H	2.610049	-1.643501	-0.016230	
25730	H	0.710509	1.616829	1.033114	
25731	H	0.691406	0.069688	1.928113	
25732	Rotational constants (GHz):		1.3484600	0.6445200	0.5867100
25733	Vibrational harmonic frequencies (cm-1):				
25734		34.0820	51.5936		86.0713
25735		124.1580	143.6825		161.7817
25736		186.4130	201.7467		218.5492
25737		243.7338	261.8676		288.7466
25738		344.1127	360.9301		389.4584
25739		406.5155	446.4307		476.9813
25740		497.2508	558.7598		619.3358
25741		669.2452	840.0942		898.7978
25742		951.2895	954.8006		984.7670
25743		995.5975	1045.3509		1083.9845
25744		1139.8270	1142.7151		1162.9274
25745		1214.0275	1254.2917		1281.6281
25746		1310.4076	1342.7269		1387.5462
25747		1396.2703	1407.9965		1421.5956
25748		1430.5071	1438.7663		1472.0444
25749		1487.4183	1499.4505		1869.8968
25750		2998.8868	3058.0518		3088.1086

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25751          3094.9612              3141.5867              3169.5744
25752          3183.5055              3750.6021              3784.2789
25753 Zero-point correction (Hartree): 0.155954
25754
25755 diHPCARP_I.tpmptmpd
25756 -----
25757 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18137003
25758 Electronic state : 2-A
25759 Cartesian coordinates (Angs):
25760 O      -0.013965      2.784094      -0.102709
25761 O      0.475628      1.609650      -0.364207
25762 C     -0.406898      0.541811      0.096975
25763 C      0.198035     -0.733595     -0.548490
25764 C      1.325078     -1.363643      0.261367
25765 O      2.316829     -0.426703      0.614368
25766 O      2.952634     -0.001950     -0.585615
25767 H      2.637113      0.909800     -0.656531
25768 C     -0.475946      0.572565      1.612299
25769 H     -0.903543      1.519865      1.933805
25770 H      0.520653      0.466288      2.032904
25771 H     -1.109038     -0.238731      1.960741
25772 C     -1.777357      0.805321     -0.522875
25773 O     -2.772215      0.264825     -0.130363
25774 H     -1.793976      1.515409     -1.366061
25775 H      0.586340     -0.439569     -1.526435
25776 O     -0.782147     -1.690617     -0.877768
25777 O     -1.379423     -2.174838      0.319669
25778 H     -2.197994     -1.651741      0.343586
25779 H      0.949178     -1.746692      1.208831
25780 H      1.755063     -2.185074     -0.313499
25781 Rotational constants (GHz): 1.1579400      0.8972200      0.6092800
25782 Vibrational harmonic frequencies (cm-1):
25783      73.8053          97.8733          103.1207
25784      147.3549         156.3721         180.0991
25785      191.8135         215.2958         236.5321
25786      249.1662         277.3039         304.7347
25787      331.7607         371.7828         377.9795
25788      400.4385         462.2883         495.1923
25789      511.0151         593.5717         617.6138
25790      691.0589         775.5809         878.9526
25791      947.3165         973.6698         978.3772
25792      994.0077        1032.4733        1105.5219
25793     1128.5559        1137.7983        1155.6584
25794     1224.4175        1246.6094        1279.4993
25795     1287.0012        1341.9607        1376.7465
25796     1398.3531        1408.9472        1423.2529
25797     1427.8565        1464.0418        1482.5872
25798     1491.3198        1510.3306        1860.3665
25799     3008.7614        3085.2615        3090.3743
25800     3093.1669        3152.2872        3172.5111
25801     3187.8743        3719.1528        3789.8211
25802 Zero-point correction (Hartree): 0.156548
25803
25804 diHPCARP_I.tppmtmpd
25805 -----
25806 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17967451
25807 Electronic state : 2-A
25808 Cartesian coordinates (Angs):
25809 O      2.919825     -1.329983      0.037547
25810 O      1.749540     -1.262855     -0.520318
25811 C      0.949550     -0.174594      0.032107
25812 C     -0.280038     -0.152543     -0.913151
25813 C     -1.305939     -1.249171     -0.635587
25814 O     -2.024114     -1.117669      0.568268
25815 O     -3.169131     -0.316913      0.328684
25816 H     -2.823119      0.575685      0.488549
25817 C      0.690673     -0.453628      1.503043
25818 H      1.640923     -0.476418      2.032351
25819 H      0.185245     -1.408565      1.621314
25820 H      0.057760      0.323065      1.920901
25821 C      1.763338      1.104578     -0.143520
25822 O      1.441630      2.147240      0.355289

```

25823	H	2.671001	1.015076	-0.761837	
25824	H	0.110414	-0.348191	-1.917137	
25825	O	-0.827750	1.141305	-1.066690	
25826	O	-1.273339	1.641318	0.186117	
25827	H	-0.497707	2.151799	0.480085	
25828	H	-2.008302	-1.297955	-1.468194	
25829	H	-0.775000	-2.201892	-0.564557	
25830	Rotational constants (GHz):		1.4173800	0.7522600	0.5984800
25831	Vibrational harmonic frequencies (cm-1):				
25832		73.5141	85.3365		100.9086
25833		152.3786	171.2723		190.2304
25834		216.2970	232.2022		246.6778
25835		273.7840	277.8852		308.1745
25836		329.6740	362.2854		409.3314
25837		472.9398	511.7183		524.1334
25838		544.6984	572.4658		663.1417
25839		730.5501	829.2815		873.9762
25840		904.1041	961.7579		981.9502
25841		994.5422	1021.1467		1046.9160
25842		1128.7553	1142.0261		1160.9911
25843		1218.7865	1250.5634		1283.9992
25844		1322.6541	1360.4903		1381.9762
25845		1407.2065	1408.5992		1422.8039
25846		1453.2269	1462.1237		1470.0267
25847		1480.1833	1500.9830		1854.7108
25848		3014.6695	3063.7256		3073.0100
25849		3095.3452	3125.1606		3174.9030
25850		3193.7379	3664.1764		3728.1552
25851	Zero-point correction (Hartree): 0.156980				
25852					
25853	diHPCARP_I.ttmmttd				
25854	-----				
25855	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17836066				
25856	Electronic state : 2-A				
25857	Cartesian coordinates (Angs):				
25858	O	2.742346	-1.047614	-0.913219	
25859	O	1.605256	-0.500931	-1.219771	
25860	C	0.705302	-0.469976	-0.077149	
25861	C	-0.482612	0.371103	-0.565143	
25862	C	-1.596049	0.538318	0.471515	
25863	O	-2.415661	-0.607414	0.563657	
25864	O	-3.069371	-0.771301	-0.690530	
25865	H	-3.985184	-0.578265	-0.455928	
25866	C	0.288290	-1.884654	0.282368	
25867	H	1.180891	-2.491034	0.420403	
25868	H	-0.332171	-2.310296	-0.504410	
25869	H	-0.276856	-1.867204	1.210373	
25870	C	1.459845	0.175401	1.086573	
25871	O	1.082078	0.082045	2.218208	
25872	H	2.383664	0.709349	0.813205	
25873	H	-0.899052	-0.122199	-1.445772	
25874	O	-0.081486	1.623790	-1.072254	
25875	O	0.384342	2.383479	0.047824	
25876	H	1.084703	2.899329	-0.369634	
25877	H	-1.199678	0.668281	1.478216	
25878	H	-2.185008	1.414465	0.193246	
25879	Rotational constants (GHz):		1.1926800	0.7219100	0.6546400
25880	Vibrational harmonic frequencies (cm-1):				
25881		37.9275	62.7013		104.4131
25882		128.6363	148.3403		166.0863
25883		188.8375	209.8996		213.4954
25884		230.6939	252.4691		271.3917
25885		285.9911	310.4435		352.9646
25886		387.4632	433.2895		452.3383
25887		517.9320	533.0036		634.0351
25888		702.4633	801.3298		891.3675
25889		929.1146	967.2260		981.8941
25890		995.6340	1055.3928		1096.5131
25891		1113.6553	1123.9149		1177.8157
25892		1191.6181	1261.2345		1277.6614
25893		1303.6591	1331.5232		1366.5147
25894		1392.3036	1403.5126		1414.8258

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25895      1421.5465              1438.5686              1481.3957
25896      1483.8116              1501.6595              1862.9353
25897      3013.1673              3075.2808              3084.4521
25898      3103.9280              3147.4284              3165.7109
25899      3181.5025              3827.1630              3839.3845
25900      Zero-point correction (Hartree): 0.155666
25901
25902      diHPCARP_I.ttpmptmmd
25903      -----
25904      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18241022
25905      Electronic state : 2-A
25906      Cartesian coordinates (Angs):
25907      O      3.083684      -0.225887      0.093884
25908      O      2.130614      0.464992      -0.451144
25909      C      0.841570      -0.202918      -0.309557
25910      C      -0.145112      0.841613      -0.853689
25911      C      -1.562171      0.379795      -1.181649
25912      O      -2.331013      0.001233      -0.055169
25913      O      -2.346166      -1.413806      0.050859
25914      H      -1.636498      -1.578088      0.701785
25915      C      0.852269      -1.470633      -1.145831
25916      H      1.703561      -2.082626      -0.856884
25917      H      0.932864      -1.220571      -2.203413
25918      H      -0.062152      -2.033536      -0.975768
25919      C      0.686555      -0.531717      1.178448
25920      O      -0.086255      -1.359256      1.583478
25921      H      1.375100      -0.002669      1.848365
25922      H      0.291863      1.190104      -1.795520
25923      O      -0.163890      2.018616      -0.066696
25924      O      -0.483981      1.685094      1.274795
25925      H      -1.424098      1.444529      1.234525
25926      H      -2.075361      1.244868      -1.605731
25927      H      -1.567905      -0.426745      -1.913746
25928      Rotational constants (GHz):      1.3152300      0.8101500      0.7137100
25929      Vibrational harmonic frequencies (cm-1):
25930      84.2201      94.9515      130.3128
25931      154.6438      179.0790      189.0485
25932      217.3453      230.9274      250.4167
25933      282.0255      303.9399      318.4244
25934      329.2797      397.2171      422.4300
25935      454.3976      474.5831      515.3187
25936      568.5407      610.2168      655.1355
25937      734.5190      838.2262      880.9997
25938      914.7144      934.2737      993.0865
25939      999.3804      1016.2559      1072.9247
25940      1121.1432      1135.7597      1161.0866
25941      1200.4273      1264.4016      1281.4958
25942      1314.5077      1347.5396      1371.7335
25943      1404.1210      1407.8540      1426.3362
25944      1455.7636      1467.5849      1494.0593
25945      1501.9288      1510.9106      1836.6956
25946      3062.9253      3067.8691      3079.2366
25947      3081.5240      3138.1986      3160.7337
25948      3179.3376      3583.5204      3731.1433
25949      Zero-point correction (Hartree): 0.157273
25950
25951      diHPCARP_I.ttpmtpd
25952      -----
25953      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18246030
25954      Electronic state : 2-A
25955      Cartesian coordinates (Angs):
25956      O      3.207443      0.459932      0.169459
25957      O      2.093353      0.907465      -0.320706
25958      C      1.025706      -0.083105      -0.222180
25959      C      -0.225911      0.681652      -0.676346
25960      C      -1.314359      -0.158214      -1.331362
25961      O      -1.746675      -1.283748      -0.607759
25962      O      -2.421586      -0.827349      0.558442
25963      H      -1.763838      -1.055204      1.236873
25964      C      1.376545      -1.285034      -1.079626
25965      H      2.347374      -1.669665      -0.776298
25966      H      1.422077      -0.997308      -2.129387

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25967	H	0.621870	-2.055375	-0.937350	
25968	C	0.925252	-0.478656	1.255961	
25969	O	0.160088	-1.310919	1.652241	
25970	H	1.617661	0.048883	1.929438	
25971	H	0.093085	1.419083	-1.423173	
25972	O	-0.638914	1.360360	0.503004	
25973	O	-1.838901	2.061095	0.260793	
25974	H	-2.493976	1.398260	0.534525	
25975	H	-2.160015	0.486125	-1.573632	
25976	H	-0.926089	-0.569330	-2.263467	
25977	Rotational constants (GHz):		1.3878000	0.7496400	0.6719400
25978	Vibrational harmonic frequencies (cm-1):				
25979		58.5419	92.7929		133.5557
25980		142.5557	155.7321		196.3602
25981		205.7460	230.3595		247.7494
25982		268.9420	287.5520		324.3154
25983		340.2853	363.5902		409.4926
25984		469.7667	470.3840		519.1763
25985		546.0172	580.1233		652.0722
25986		723.9612	815.4681		865.5151
25987		906.3181	966.1374		979.7317
25988		989.1240	1052.3161		1066.9975
25989		1128.3933	1136.2721		1168.0265
25990		1216.6528	1269.9512		1286.0262
25991		1303.6489	1362.1990		1377.8223
25992		1397.3229	1409.3654		1427.0494
25993		1442.4900	1453.3047		1478.7189
25994		1497.1165	1506.3290		1860.4118
25995		3028.9266	3037.6468		3078.1906
25996		3091.8829	3136.9262		3160.5169
25997		3175.1198	3726.1356		3735.7207
25998	Zero-point correction (Hartree): 0.157086				
25999					
26000	diHPCARP_I.ttpttmmdd				
26001	-----				
26002	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18156555				
26003	Electronic state : 2-A				
26004	Cartesian coordinates (Angs):				
26005	O	3.089537	0.020288	0.249396	
26006	O	2.113800	0.565551	-0.408870	
26007	C	0.881349	-0.202044	-0.266092	
26008	C	-0.160288	0.690129	-0.958308	
26009	C	-1.469849	0.001461	-1.372872	
26010	O	-1.986108	-1.013067	-0.548436	
26011	O	-2.505452	-0.432496	0.640799	
26012	H	-1.945907	-0.879258	1.299274	
26013	C	1.046034	-1.539349	-0.966890	
26014	H	1.936067	-2.033847	-0.584811	
26015	H	1.154233	-1.391224	-2.041116	
26016	H	0.178129	-2.160693	-0.762206	
26017	C	0.666866	-0.398864	1.240080	
26018	O	-0.059192	-1.243352	1.689021	
26019	H	1.268607	0.259545	1.880616	
26020	H	0.309409	1.016748	-1.891945	
26021	O	-0.353136	1.925323	-0.300563	
26022	O	-0.738399	1.708985	1.044439	
26023	H	-1.646698	1.368076	0.968291	
26024	H	-2.219361	0.781382	-1.532391	
26025	H	-1.307547	-0.518590	-2.317517	
26026	Rotational constants (GHz):		1.3535300	0.7914800	0.7429500
26027	Vibrational harmonic frequencies (cm-1):				
26028		87.9560	118.5522		145.8817
26029		160.2757	173.7370		187.2498
26030		226.1831	236.7314		243.3677
26031		253.3502	265.5454		312.3370
26032		352.3438	389.5647		419.7486
26033		433.2756	446.1479		519.6128
26034		596.5386	618.7597		639.0235
26035		721.5455	782.7683		878.7065
26036		908.1240	959.7769		992.3726
26037		1014.0212	1035.6126		1063.8542
26038		1120.6593	1136.5157		1169.6217

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26039      1208.0281      1268.3782      1279.6874
26040      1310.6881      1355.6094      1381.4779
26041      1400.1443      1409.3428      1429.0819
26042      1445.1806      1463.2528      1487.4986
26043      1492.0051      1504.1144      1842.6281
26044      3054.9380      3060.5389      3067.5629
26045      3079.7401      3126.3070      3159.9874
26046      3182.7631      3684.8164      3710.8643
26047 Zero-point correction (Hartree): 0.157226
26048
26049 diHPCARP_I.tttmtmmd
26050 -----
26051 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18110599
26052 Electronic state : 2-A
26053 Cartesian coordinates (Angs):
26054 O      -3.115499      -0.735078      -0.484512
26055 O      -1.909801      -0.674944      -0.961598
26056 C      -1.096713      0.266697      -0.213426
26057 C       0.323370      0.048650      -0.755694
26058 C       1.323810      1.029502      -0.146676
26059 O       2.631441      0.807863      -0.637536
26060 O       3.219140      -0.250389      0.112312
26061 H       3.926442      0.215566      0.575165
26062 C      -1.597447      1.677627      -0.468276
26063 H      -2.671959      1.707704      -0.301741
26064 H      -1.382540      1.981926      -1.492210
26065 H      -1.124082      2.362934      0.231232
26066 C      -1.214072      -0.084648      1.273475
26067 O      -0.916826      0.703225      2.125203
26068 H      -1.595963      -1.091278      1.494961
26069 H       0.290288      0.197363      -1.838376
26070 O       0.734728      -1.294212      -0.648676
26071 O       0.848618      -1.628159      0.725310
26072 H       1.793871      -1.466472      0.874313
26073 H       1.080625      2.042308      -0.466863
26074 H       1.315225      0.996533      0.943063
26075 Rotational constants (GHz): 1.5531600 0.6361000 0.6177900
26076 Vibrational harmonic frequencies (cm-1):
26077      57.6710      80.1917      120.9069
26078     136.8549     165.9285     184.3353
26079     189.1384     235.8374     245.5330
26080     264.2320     281.2499     294.8083
26081     315.1092     333.6918     382.9215
26082     403.2616     448.0593     496.8471
26083     503.0352     605.0993     640.4428
26084     694.2545     820.0668     879.5890
26085     925.4038     960.1765     990.7595
26086    1006.0953    1009.9527    1092.8479
26087    1122.3509    1142.0198    1172.4037
26088    1200.6778    1258.8420    1277.9843
26089    1311.8484    1325.8249    1387.3168
26090    1395.7511    1398.3961    1416.8096
26091    1428.3733    1442.7018    1474.4226
26092    1488.1349    1507.8084    1856.8850
26093    3042.0696    3076.8546    3084.2125
26094    3092.9705    3146.6900    3159.1867
26095    3170.3174    3725.4131    3822.0560
26096 Zero-point correction (Hartree): 0.156493
26097
26098 diHPCARP_I.tttmptmmd
26099 -----
26100 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18264158
26101 Electronic state : 2-A
26102 Cartesian coordinates (Angs):
26103 O      -3.072129      -0.792505      -0.564962
26104 O      -1.846022      -0.722756      -0.985479
26105 C      -1.086522      0.255728      -0.228211
26106 C       0.356965      0.059093      -0.708733
26107 C       1.327870      1.058965      -0.087188
26108 O       2.640779      0.880015      -0.577010
26109 O       3.228312      -0.224967      0.104355
26110 H       3.233041      -0.896811      -0.591414

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26111	C	-1.603972	1.649429	-0.539741	
26112	H	-2.685028	1.660220	-0.420294	
26113	H	-1.351001	1.934259	-1.560555	
26114	H	-1.174925	2.360487	0.162574	
26115	C	-1.260131	-0.057816	1.262073	
26116	O	-0.993377	0.752094	2.102394	
26117	H	-1.654662	-1.057161	1.494760	
26118	H	0.362809	0.182926	-1.795211	
26119	O	0.794417	-1.278266	-0.554039	
26120	O	0.841326	-1.585617	0.829921	
26121	H	1.735093	-1.287328	1.070164	
26122	H	1.062593	2.070107	-0.393237	
26123	H	1.320362	1.016923	1.002570	
26124	Rotational constants (GHz):			1.5422600	0.6403700 0.6208900
26125	Vibrational harmonic frequencies (cm-1):				
26126		59.6178	84.1523		119.1092
26127		134.0275	166.6872		176.8886
26128		198.9045	237.2390		246.5642
26129		265.4072	283.1079		316.6571
26130		333.6525	370.0441		386.1658
26131		408.7756	450.4264		493.3321
26132		578.0583	609.1285		638.3481
26133		695.4642	826.0205		880.1783
26134		926.6800	957.4082		989.9152
26135		1006.5486	1011.6360		1097.1676
26136		1122.4651	1136.1724		1168.0942
26137		1196.9705	1261.8461		1276.9983
26138		1308.5305	1323.9286		1385.6672
26139		1398.4919	1408.3107		1416.4984
26140		1421.9664	1441.3298		1480.5408
26141		1488.1528	1508.4342		1858.9143
26142		3039.9358	3076.9062		3082.9995
26143		3095.6425	3148.7656		3159.7281
26144		3171.8581	3695.5787		3798.5417
26145	Zero-point correction (Hartree):			0.156785	
26146	diHPCARP_I.tttptmmd				
26147	-----				
26148	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18265567				
26149	Electronic state : 2-A				
26150	Cartesian coordinates (Angs):				
26151	O	-3.009789	-0.959312	0.563877	
26152	O	-1.741139	-1.227266	0.493693	
26153	C	-1.038503	-0.229748	-0.292116	
26154	C	0.440984	-0.559359	-0.086755	
26155	C	1.355703	0.312805	-0.957612	
26156	O	2.639683	0.414590	-0.381649	
26157	O	3.203479	-0.888162	-0.343692	
26158	H	2.980656	-1.171933	0.555113	
26159	C	-1.436910	-0.357885	-1.751271	
26160	H	-2.520766	-0.311562	-1.829549	
26161	H	-1.084411	-1.303291	-2.161975	
26162	H	-1.017315	0.471718	-2.316346	
26163	C	-1.415966	1.150540	0.257125	
26164	O	-1.297158	2.140912	-0.404316	
26165	H	-1.806085	1.159886	1.285299	
26166	H	0.576154	-1.615402	-0.331459	
26167	O	0.834097	-0.510372	1.271850	
26168	O	0.788815	0.838665	1.709940	
26169	H	1.676826	1.153061	1.478118	
26170	H	1.422209	-0.094691	-1.966987	
26171	H	0.996987	1.341662	-1.006057	
26172	Rotational constants (GHz):			1.4996200	0.6398400 0.6256200
26173	Vibrational harmonic frequencies (cm-1):				
26174		63.7784	91.9583		114.8347
26175		126.8763	152.2474		178.7963
26176		195.0085	241.0894		247.6148
26177		276.8770	290.4356		310.9210
26178		355.1705	378.6926		400.1963
26179		419.6128	455.1005		487.9484
26180		494.9635	604.3212		674.1556
26181		731.9873	800.3617		878.9584
26182					

26183	935.5966	960.6626	990.5423			
26184	1000.3118	1012.8149	1084.4066			
26185	1125.1388	1138.3300	1179.0496			
26186	1200.8478	1270.2384	1278.0618			
26187	1304.4887	1327.3444	1389.7394			
26188	1398.7565	1405.5816	1418.1852			
26189	1423.6720	1429.8639	1485.6619			
26190	1492.1814	1505.2858	1861.6394			
26191	3037.7100	3078.3114	3083.6087			
26192	3092.2370	3140.9885	3160.8735			
26193	3170.8610	3749.4917	3773.5980			
26194	Zero-point correction (Hartree): 0.156916					
26195						
26196						
26197						
26198	(2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)					
26199	=====					
26200						
26201	diHPCARP_Ib.mmmmpmpd					
26202	-----					
26203	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20867822					
26204	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09276229					
26205	T1 diagnostic: 0.020361					
26206	E(MP2/Aug-CC-pVTZ) (Hartree): -721.04757901					
26207	E(MP3/Aug-CC-pVTZ) (Hartree): -721.07004318					
26208	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05076294					
26209	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07191418					
26210	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.53760896					
26211	E(UHF/Aug-CC-pVTZ) (Hartree): -718.53239354					
26212	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18365819					
26213	Electronic state : 2-A					
26214	Cartesian coordinates (Angs):					
26215	O	-2.373957	0.449740	1.215166		
26216	O	-0.974640	0.652897	1.245013		
26217	C	-0.425330	0.761854	-0.060358		
26218	C	0.063297	-0.583832	-0.618686		
26219	C	0.779176	-1.431307	0.427724		
26220	O	1.880301	-0.726995	0.953063		
26221	O	2.899749	-0.725184	-0.035372		
26222	H	2.874882	0.192652	-0.353495		
26223	C	-1.329974	1.503216	-1.038814		
26224	H	-1.639380	2.453375	-0.606756		
26225	H	-2.218121	0.919168	-1.259668		
26226	H	-0.775738	1.685932	-1.957965		
26227	C	0.809521	1.636859	0.165843		
26228	O	1.677911	1.767240	-0.654456		
26229	H	0.810911	2.181277	1.123315		
26230	H	0.729297	-0.374981	-1.455480		
26231	O	-0.986398	-1.364260	-1.231359		
26232	O	-1.867061	-1.788421	-0.377893		
26233	H	-2.438159	-0.506987	1.072047		
26234	H	0.126649	-1.614709	1.278981		
26235	H	1.102273	-2.376596	-0.008530		
26236	Rotational constants (GHz):			1.2497800	0.8353700	0.6715300
26237	Vibrational harmonic frequencies (cm-1):					
26238		52.3334	85.3203			104.2284
26239		140.1963	183.7021			188.9342
26240		210.5456	233.3624			252.9626
26241		255.9632	275.0152			287.9584
26242		331.6702	360.3007			418.8707
26243		457.3340	462.8850			485.6657
26244		490.9905	577.2854			634.7513
26245		684.7211	780.1742			916.6761
26246		948.2586	956.2718			980.9902
26247		1016.7438	1030.6754			1071.6421
26248		1118.5733	1134.4736			1185.1583
26249		1223.8878	1242.2535			1266.5515
26250		1286.8511	1349.1392			1382.9831
26251		1394.3492	1408.0229			1426.2362
26252		1459.2881	1464.1614			1480.6634
26253		1486.7548	1502.7714			1841.0525
26254		3022.3367	3083.2748			3092.4813

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26255          3129.3997          3160.3267          3161.9068
26256          3182.5228          3720.8199          3759.6466
26257 Zero-point correction (Hartree): 0.156834
26258
26259 diHPCARP_Ib.mmmmpmpd
26260 -----
26261 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18143003
26262 Electronic state : 2-A
26263 Cartesian coordinates (Angs):
26264 O          1.824869          -0.350768          1.729350
26265 O          0.736336          -1.125456          1.252334
26266 C          0.466737          -0.756913          -0.094993
26267 C          0.079939          0.722557          -0.235741
26268 C          -0.815134          1.182851          0.905570
26269 O          -1.968537          0.370036          0.967423
26270 O          -2.820991          0.755489          -0.101003
26271 H          -2.710691          0.023908          -0.730295
26272 C          1.591569          -1.164335          -1.036755
26273 H          1.776008          -2.234912          -0.949762
26274 H          2.499465          -0.618364          -0.789412
26275 H          1.315714          -0.929431          -2.062941
26276 C          -0.766962          -1.597355          -0.412349
26277 O          -1.438651          -1.421266          -1.392977
26278 H          -0.975459          -2.406862          0.305546
26279 H          -0.414685          0.849015          -1.198245
26280 O          1.232106          1.583997          -0.240580
26281 O          1.693551          1.780233          -1.439907
26282 H          2.513092          -1.018743          1.837804
26283 H          -0.314676          1.049340          1.863452
26284 H          -1.095131          2.227089          0.772327
26285 Rotational constants (GHz):      1.1305600      0.8094600      0.7390800
26286 Vibrational harmonic frequencies (cm-1):
26287      65.8560          78.3410          109.1218
26288      124.4862          151.6643          177.2115
26289      191.8134          202.1520          229.6539
26290      237.7194          266.6594          279.1871
26291      303.0491          364.5720          372.3019
26292      417.5785          435.0081          453.3931
26293      498.0063          534.8388          629.7364
26294      685.1611          765.9940          917.6711
26295      951.1543          954.9395          983.2542
26296      1031.0387          1057.0412          1068.5487
26297      1115.5017          1143.2126          1188.6096
26298      1218.4786          1253.6663          1280.8165
26299      1287.4227          1343.0021          1378.7890
26300      1398.5528          1405.1379          1410.5355
26301      1417.2528          1460.5484          1486.3551
26302      1488.2302          1506.2784          1844.6527
26303      3012.8016          3074.7364          3097.2033
26304      3126.0790          3154.1927          3159.8782
26305      3167.5831          3724.4718          3821.1201
26306 Zero-point correction (Hartree): 0.156060
26307
26308 diHPCARP_Ib.mmmmpppd
26309 -----
26310 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18132956
26311 Electronic state : 2-A
26312 Cartesian coordinates (Angs):
26313 O          2.239760          -0.602782          1.416024
26314 O          0.876416          -0.957614          1.270843
26315 C          0.440089          -0.734514          -0.065380
26316 C          0.038718          0.734066          -0.274891
26317 C          -0.885505          1.252548          0.821863
26318 O          -2.032491          0.446550          0.949334
26319 O          -2.872110          0.723461          -0.160916
26320 H          -2.762918          -0.075878          -0.704215
26321 C          1.436876          -1.229625          -1.106196
26322 H          1.694199          -2.267310          -0.897429
26323 H          2.345023          -0.635347          -1.085849
26324 H          0.980404          -1.160156          -2.091555
26325 C          -0.810416          -1.601560          -0.180771
26326 O          -1.537497          -1.554933          -1.137328

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26327	H	-0.965966	-2.310290	0.647771		
26328	H	-0.398873	0.854885	-1.264743		
26329	O	1.208321	1.574419	-0.202369		
26330	O	1.760950	1.777682	-1.362149		
26331	H	2.200057	0.339520	1.630820		
26332	H	-0.390638	1.189140	1.791173		
26333	H	-1.166645	2.285677	0.618763		
26334	Rotational constants (GHz):			1.1909300	0.7981500	0.6901900
26335	Vibrational harmonic frequencies (cm-1):					
26336		47.7714	81.9424			103.0599
26337		134.7851	158.4837			183.3173
26338		202.2988	217.2319			242.8945
26339		258.8642	269.2525			299.8745
26340		327.7211	352.4450			370.9283
26341		412.3886	446.9592			459.8634
26342		501.5254	534.9104			629.4858
26343		681.5345	763.3354			920.0469
26344		955.1386	958.7244			980.1300
26345		1023.7431	1045.3044			1062.2000
26346		1123.3824	1143.9282			1186.0757
26347		1218.1693	1249.6745			1279.9976
26348		1291.7500	1331.1468			1365.8968
26349		1397.1700	1409.7792			1416.5062
26350		1433.1331	1471.3937			1478.6183
26351		1483.4701	1503.9698			1838.3634
26352		3020.7119	3083.4809			3088.6212
26353		3129.0562	3146.9483			3160.7506
26354		3186.2837	3702.2182			3790.5578
26355	Zero-point correction (Hartree):			0.156185		
26356	diHPCARP_Ib.mmmpttmd					
26357	-----					
26358	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18102246					
26359	Electronic state : 2-A					
26360	Cartesian coordinates (Angs):					
26361	O	2.063426	-0.290910	1.485278		
26362	O	0.969516	-1.129821	1.150488		
26363	C	0.538293	-0.813807	-0.167363		
26364	C	0.076335	0.636834	-0.312363		
26365	C	-0.717871	1.110859	0.896292		
26366	O	-1.831627	0.266230	1.099784		
26367	O	-2.797804	0.583176	0.108413		
26368	H	-2.729916	-0.172385	-0.497754		
26369	C	1.569845	-1.201250	-1.219771		
26370	H	1.808686	-2.261031	-1.136392		
26371	H	2.473658	-0.611784	-1.086406		
26372	H	1.167272	-1.007196	-2.212718		
26373	C	-0.686275	-1.713099	-0.323155		
26374	O	-1.458500	-1.605053	-1.237027		
26375	H	-0.788374	-2.497017	0.444146		
26376	H	-0.526172	0.712044	-1.217706		
26377	O	1.219479	1.495754	-0.500257		
26378	O	0.870921	2.615403	-1.060902		
26379	H	2.789102	-0.924322	1.546447		
26380	H	-0.119726	1.024933	1.802338		
26381	H	-1.039793	2.141305	0.749987		
26382	Rotational constants (GHz):			1.0483800	0.8802000	0.7018800
26383	Vibrational harmonic frequencies (cm-1):					
26384		61.7412	81.7625			96.6558
26385		113.9950	151.5648			168.2868
26386		173.4450	188.6724			224.2970
26387		235.7809	250.0451			264.8296
26388		299.2811	338.7158			366.4971
26389		415.1938	440.8970			461.4933
26390		479.7285	538.4575			612.4462
26391		681.3148	799.6449			916.9594
26392		951.5185	954.2098			985.2298
26393		1034.9741	1063.8596			1071.8851
26394		1108.8001	1129.5895			1184.3441
26395		1227.5603	1258.1285			1278.8411
26396		1289.0493	1344.6436			1383.8351
26397		1396.1459	1405.0893			1409.7317

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26399      1417.8938      1457.3103      1484.1341
26400      1490.7898      1504.2601      1847.1559
26401      3020.7643      3075.5421      3097.7137
26402      3119.9178      3153.0957      3161.4350
26403      3170.2452      3729.9469      3823.9391
26404      Zero-point correction (Hartree): 0.155811
26405
26406      diHPCARP_Ib.mmmmpptpd
26407      -----
26408      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18122986
26409      Electronic state : 2-A
26410      Cartesian coordinates (Angs):
26411      O      2.452774      -0.575367      1.160174
26412      O      1.089862      -0.959309      1.164254
26413      C      0.515894      -0.790571      -0.127277
26414      C      0.038059      0.649012      -0.338103
26415      C      -0.817697      1.170318      0.812336
26416      O      -1.931416      0.340858      1.041635
26417      O      -2.849958      0.555187      -0.018831
26418      H      -2.761232      -0.265030      -0.533539
26419      C      1.425382      -1.268930      -1.253837
26420      H      1.783019      -2.273959      -1.035978
26421      H      2.280926      -0.609857      -1.362824
26422      H      0.852851      -1.283592      -2.179472
26423      C      -0.706109      -1.706302      -0.096278
26424      O      -1.508200      -1.733871      -0.991278
26425      H      -0.767538      -2.375422      0.776061
26426      H      -0.487535      0.727974      -1.289344
26427      O      1.213784      1.486649      -0.411068
26428      O      0.950015      2.642057      -0.946718
26429      H      2.413800      0.378990      1.314258
26430      H      -0.249188      1.137796      1.742144
26431      H      -1.133163      2.192295      0.602316
26432      Rotational constants (GHz):      1.0942600      0.8669000      0.6555300
26433      Vibrational harmonic frequencies (cm-1):
26434      44.3336      86.4919      100.3644
26435      126.3091      155.9575      178.2042
26436      195.1336      213.1798      230.8914
26437      252.3267      262.3363      285.7602
26438      327.6321      336.4070      349.7337
26439      440.5961      451.5462      458.3666
26440      482.4402      540.9428      621.3619
26441      675.2214      791.1389      921.6518
26442      950.6595      959.4954      980.8757
26443      1021.6383      1061.3837      1067.8206
26444      1105.8570      1138.5481      1180.8003
26445      1227.6318      1251.7364      1284.8319
26446      1287.4224      1329.6531      1376.7419
26447      1395.3980      1406.0198      1412.4593
26448      1434.3691      1467.9119      1477.6933
26449      1488.8433      1502.2588      1840.3213
26450      3025.2254      3084.6868      3087.0345
26451      3125.1510      3146.9175      3161.6125
26452      3185.6050      3705.2144      3786.3378
26453      Zero-point correction (Hartree): 0.156024
26454
26455      diHPCARP_Ib.mmpmptmpd
26456      -----
26457      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17936128
26458      Electronic state : 2-A
26459      Cartesian coordinates (Angs):
26460      O      0.674010      -0.672066      1.870129
26461      O      -0.290763      0.263217      1.429388
26462      C      -0.948533      -0.221522      0.264293
26463      C      -0.045953      -0.386022      -0.967193
26464      C      0.997582      0.691745      -1.221399
26465      O      1.792337      1.050092      -0.103989
26466      O      1.286704      2.254882      0.451975
26467      H      0.711125      1.910752      1.154158
26468      C      -1.730020      -1.493574      0.578689
26469      H      -2.466544      -1.285282      1.353917
26470      H      -1.046926      -2.258776      0.937107

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26471	H	-2.238868	-1.852307	-0.314591		
26472	C	-1.965794	0.884615	-0.019978		
26473	O	-2.404932	1.112564	-1.109031		
26474	H	-2.300375	1.432025	0.878865		
26475	H	-0.722718	-0.396511	-1.823276		
26476	O	0.537403	-1.716516	-1.008156		
26477	O	1.728318	-1.777680	-0.498522		
26478	H	1.449155	-0.425579	1.331708		
26479	H	1.685615	0.322531	-1.982128		
26480	H	0.501234	1.585755	-1.596578		
26481	Rotational constants (GHz):			1.0766100	0.9294800	0.7792700
26482	Vibrational harmonic frequencies (cm-1):					
26483		50.1026	80.6354	92.6417		
26484		132.2368	182.1754	184.4991		
26485		216.7643	237.8046	247.7656		
26486		262.0150	279.9564	301.8178		
26487		331.7376	365.7732	449.8039		
26488		465.6554	499.9524	518.7936		
26489		533.7845	603.4586	656.8918		
26490		700.3675	842.6417	889.7254		
26491		918.1679	942.4070	968.1444		
26492		991.0732	1038.5172	1067.4738		
26493		1093.0753	1137.6680	1165.8980		
26494		1210.4555	1255.6333	1268.8707		
26495		1317.5172	1365.7237	1394.3429		
26496		1398.5155	1405.6759	1414.7968		
26497		1456.8892	1464.7114	1483.2399		
26498		1485.1873	1504.1408	1869.9265		
26499		2988.9475	3077.2874	3089.7216		
26500		3109.1916	3144.0939	3153.9822		
26501		3177.7895	3661.2288	3746.1656		
26502	Zero-point correction (Hartree): 0.156951					
26503						
26504	diHPCARP_Ib.mmpmptppd					
26505	-----					
26506	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18023923					
26507	Electronic state : 2-A					
26508	Cartesian coordinates (Angs):					
26509	O	0.465863	-0.624958	2.011526		
26510	O	0.426678	0.613148	1.325783		
26511	C	-0.612683	0.601557	0.349628		
26512	C	-0.371936	-0.393070	-0.792396		
26513	C	1.045913	-0.469820	-1.334131		
26514	O	2.006203	-0.825696	-0.349094		
26515	O	2.791459	0.308811	-0.019010		
26516	H	2.263669	0.712927	0.689756		
26517	C	-1.973300	0.428384	1.014089		
26518	H	-2.127464	1.232990	1.732502		
26519	H	-2.005878	-0.522563	1.539398		
26520	H	-2.762773	0.449667	0.265393		
26521	C	-0.556456	2.023955	-0.206063		
26522	O	-0.829827	2.303619	-1.336558		
26523	H	-0.280365	2.788187	0.541897		
26524	H	-1.043648	-0.121837	-1.606904		
26525	O	-0.723987	-1.735389	-0.383642		
26526	O	-1.972875	-2.010067	-0.611854		
26527	H	1.053403	-1.147998	1.436580		
26528	H	1.076751	-1.251313	-2.094017		
26529	H	1.328965	0.478168	-1.788558		
26530	Rotational constants (GHz):			1.0333600	0.8913400	0.7543300
26531	Vibrational harmonic frequencies (cm-1):					
26532		46.7544	77.9741	85.1678		
26533		114.1952	173.7692	185.9245		
26534		196.7867	228.9044	238.1577		
26535		264.0000	291.6722	304.2812		
26536		330.6485	399.1101	427.9089		
26537		447.8895	477.8465	494.7682		
26538		528.5433	607.1575	673.5060		
26539		685.1257	818.8788	909.1405		
26540		919.3956	940.6659	978.9461		
26541		985.0293	1043.2572	1062.0366		
26542		1115.6093	1130.0308	1164.9933		

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26543      1210.6647      1261.6764      1287.2464
26544      1305.4212      1346.4298      1363.8484
26545      1397.5494      1402.1157      1415.7912
26546      1459.8303      1471.1049      1479.6986
26547      1480.7463      1503.8360      1870.2049
26548      2990.4212      3078.4862      3088.1212
26549      3119.1718      3148.4931      3157.0921
26550      3177.2031      3675.0392      3705.3817
26551 Zero-point correction (Hartree): 0.156610
26552
26553 diHPCARP_Ib.mmpmpttpd
26554 -----
26555 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18070309
26556 Electronic state : 2-A
26557 Cartesian coordinates (Angs):
26558 O      0.383774      0.354461      2.123649
26559 O     -0.390210      1.015652      1.139835
26560 C     -0.984111      0.062866      0.261493
26561 C      0.022485     -0.718489     -0.581691
26562 C      1.188467      0.060252     -1.169499
26563 O      1.969059      0.729924     -0.190240
26564 O      1.699170      2.122041     -0.239040
26565 H      0.947988      2.198447      0.372149
26566 C     -1.940586     -0.850684      1.022215
26567 H     -2.725705     -0.253493      1.484765
26568 H     -1.396738     -1.381905      1.798000
26569 H     -2.390818     -1.569171      0.338846
26570 C     -1.830641      0.944969     -0.655446
26571 O     -2.069458      0.675307     -1.795909
26572 H     -2.246715      1.839450     -0.159128
26573 H     -0.526440     -1.178106     -1.404461
26574 O      0.538599     -1.802506      0.235418
26575 O      1.078865     -2.725962     -0.498887
26576 H      1.244488      0.276407      1.673804
26577 H      1.847527     -0.656932     -1.659739
26578 H      0.834341      0.780486     -1.905289
26579 Rotational constants (GHz): 0.9649200 0.9132500 0.7605700
26580 Vibrational harmonic frequencies (cm-1):
26581      47.9329      76.1020      83.2183
26582     136.5615     168.5481     177.0440
26583     198.2245     227.4506     238.2052
26584     261.2791     282.3580     294.4412
26585     322.5353     406.7025     411.5099
26586     450.7382     494.4304     502.7708
26587     539.7303     619.4171     663.5732
26588     703.7034     816.6028     902.7087
26589     912.2489     950.1030     981.3929
26590     985.4444     1053.0196    1062.9862
26591    1099.5873     1125.3576    1164.6549
26592    1218.9630     1263.1817    1290.1889
26593    1299.7090     1343.2905    1368.3443
26594    1395.4033     1403.9487    1418.7303
26595    1458.2503     1472.8677    1482.2007
26596    1487.0768     1505.7398    1871.4348
26597    2987.9173     3076.5316    3091.9639
26598    3111.1294     3149.3314    3152.3636
26599    3180.1522     3684.2498    3708.9357
26600 Zero-point correction (Hartree): 0.156698
26601
26602 diHPCARP_Ib.mppmmtmd
26603 -----
26604 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17920222
26605 Electronic state : 2-A
26606 Cartesian coordinates (Angs):
26607 O      0.050603      2.026130      0.898839
26608 O     -0.888910      1.548268     -0.048594
26609 C     -1.160714      0.179873      0.199186
26610 C      0.007050     -0.751545     -0.126012
26611 C      0.871762     -0.303407     -1.297345
26612 O      1.673737      0.825792     -0.983574
26613 O      2.923196      0.379795     -0.478388
26614 H      2.740396      0.222627      0.459508

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26615	C	-1.723006	-0.043427	1.599972	
26616	H	-2.647255	0.521630	1.716426	
26617	H	-1.006139	0.298822	2.340600	
26618	H	-1.926437	-1.102015	1.756999	
26619	C	-2.299003	-0.092202	-0.787493	
26620	O	-2.454430	-1.130807	-1.360743	
26621	H	-2.998284	0.754703	-0.896210	
26622	H	-0.401018	-1.740766	-0.332690	
26623	O	0.846642	-0.881244	1.049814	
26624	O	1.529783	-1.988314	1.023333	
26625	H	0.861305	1.985929	0.364417	
26626	H	1.523889	-1.113756	-1.618003	
26627	H	0.232042	0.000112	-2.126407	
26628	Rotational constants (GHz):			1.2413000	0.7537100 0.6942200
26629	Vibrational harmonic frequencies (cm-1):				
26630		56.1165	67.1049		88.9373
26631		92.6829	141.1461		170.6300
26632		192.2290	212.5500		235.5922
26633		257.4288	278.2823		292.0655
26634		322.0626	388.0564		405.5779
26635		413.1216	454.6967		490.7065
26636		528.3702	546.8982		661.9081
26637		708.1436	827.1550		889.4929
26638		917.7352	963.6905		972.7688
26639		999.9849	1041.9001		1061.9904
26640		1094.5291	1122.7444		1176.8744
26641		1218.8306	1262.4829		1282.9737
26642		1301.5583	1349.1745		1379.0664
26643		1393.4995	1400.4624		1413.1838
26644		1428.6139	1467.3372		1471.3957
26645		1486.2183	1504.5538		1869.5081
26646		2994.7525	3075.9140		3093.1871
26647		3121.0097	3150.3033		3151.4189
26648		3180.1828	3711.7575		3777.6953
26649	Zero-point correction (Hartree):			0.156187	
26650	diHPCARP_Ib.mmpmtpd				
26651	-----				
26652	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17953964				
26653	Electronic state : 2-A				
26654	Cartesian coordinates (Angs):				
26655	O	-0.296512	-0.768303	2.029197	
26656	O	0.638671	-1.217241	1.063345	
26657	C	1.072009	-0.122370	0.274332	
26658	C	-0.010138	0.404192	-0.676883	
26659	C	-0.940171	-0.678449	-1.210442	
26660	O	-1.866950	-1.125911	-0.232064	
26661	O	-3.041272	-0.332553	-0.309526	
26662	H	-2.791146	0.471224	0.170537	
26663	C	1.713447	0.969701	1.122218	
26664	H	2.544023	0.545804	1.685689	
26665	H	0.983941	1.367835	1.822427	
26666	H	2.076283	1.776093	0.487143	
26667	C	2.187973	-0.759823	-0.556235	
26668	O	2.417152	-0.478292	-1.696536	
26669	H	2.796143	-1.488456	0.007225	
26670	H	0.487528	0.915071	-1.499951	
26671	O	-0.852567	1.380841	-0.019163	
26672	O	-0.405871	2.595129	-0.137178	
26673	H	-1.126623	-1.022497	1.592754	
26674	H	-1.496608	-0.321601	-2.075061	
26675	H	-0.353474	-1.552335	-1.493308	
26676	Rotational constants (GHz):			1.1799500	0.7647800 0.7181800
26677	Vibrational harmonic frequencies (cm-1):				
26678		54.5372	79.7443		93.2390
26679		109.1129	146.0754		169.7090
26680		189.3635	218.5408		241.7464
26681		259.9810	293.1239		295.3048
26682		322.9337	403.3671		422.1062
26683		438.5076	453.4397		500.4296
26684		514.4828	545.8773		673.0510
26685		683.6533	815.4804		901.2025

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26687      917.6066      966.0862      968.6553
26688      1012.6846     1022.7667     1061.9999
26689      1104.3555     1124.0806     1176.9728
26690      1211.1934     1261.9550     1289.3381
26691      1307.9084     1349.0928     1373.8871
26692      1394.8871     1398.9483     1411.4051
26693      1446.7607     1469.5279     1473.0850
26694      1481.9408     1504.5420     1867.8934
26695      2994.6806     3077.6560     3096.3880
26696      3128.6297     3152.5502     3154.9147
26697      3176.1185     3723.5949     3762.6185
26698 Zero-point correction (Hartree): 0.156487
26699
26700 diHPCARP_Ib.mmpmtpd
26701 -----
26702 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17957753
26703 Electronic state : 2-A
26704 Cartesian coordinates (Angs):
26705 O      0.258978      1.931540      1.528629
26706 O      0.538157      0.558919      1.316974
26707 C      0.940507      0.297123     -0.029903
26708 C     -0.281132     -0.001234     -0.916418
26709 C     -0.940854     -1.355750     -0.672635
26710 O     -0.810718     -1.823325      0.646755
26711 O     -1.702399     -1.080918      1.466721
26712 H     -1.086268     -0.460162      1.885353
26713 C      1.799446      1.416082     -0.606756
26714 H      2.586232      1.684109      0.096072
26715 H      1.198281      2.298939     -0.807858
26716 H      2.246505      1.062659     -1.534239
26717 C      1.811819     -0.951852      0.077061
26718 O      2.091589     -1.608009     -0.884160
26719 H      2.195102     -1.169996      1.087284
26720 H     -0.006662      0.074747     -1.968319
26721 O     -1.207966      1.086038     -0.654814
26722 O     -2.175354      1.118989     -1.517965
26723 H     -0.632177      2.026755      1.158909
26724 H     -1.990220     -1.306143     -0.966238
26725 H     -0.427809     -2.103000     -1.276174
26726 Rotational constants (GHz):      1.0259800      0.9099500      0.7752400
26727 Vibrational harmonic frequencies (cm-1):
26728      67.0112      78.3491      109.8815
26729      121.9762     156.7098     176.9638
26730      194.7171     205.4539     242.4299
26731      265.5126     280.9832     336.6329
26732      343.2297     357.0531     423.8560
26733      424.3959     453.8988     466.6599
26734      505.3674     553.9936     672.4720
26735      698.5075     839.8590     877.9793
26736      929.3571     957.7401     966.9038
26737      990.7383     1047.6664     1060.9341
26738      1101.6932     1140.6714     1160.5260
26739      1215.8546     1257.0203     1294.4963
26740      1302.9448     1352.3550     1356.9680
26741      1392.5992     1404.9513     1414.3406
26742      1447.1439     1455.6211     1470.0282
26743      1492.0834     1498.7312     1865.1512
26744      3012.6249     3081.9430     3091.2642
26745      3117.1750     3151.6069     3162.7273
26746      3172.0728     3756.6783     3768.4174
26747 Zero-point correction (Hartree): 0.156612
26748
26749 diHPCARP_Ib.mmpmtpd
26750 -----
26751 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17815742
26752 Electronic state : 2-A
26753 Cartesian coordinates (Angs):
26754 O      0.129930      1.932842      1.017290
26755 O     -0.821802      1.552909      0.040871
26756 C     -1.150270      0.184867      0.213007
26757 C     -0.008358     -0.776612     -0.116740
26758 C      0.873471     -0.362400     -1.284128

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26759	O	1.622740	0.821789	-1.065472	
26760	O	2.780959	0.480277	-0.306095	
26761	H	3.484798	0.675489	-0.937694	
26762	C	-1.757559	-0.080337	1.588187	
26763	H	-2.663681	0.513097	1.706767	
26764	H	-1.046438	0.202907	2.358578	
26765	H	-2.001778	-1.136611	1.694015	
26766	C	-2.269877	0.005989	-0.812727	
26767	O	-2.435613	-0.985026	-1.463445	
26768	H	-2.948330	0.874301	-0.877170	
26769	H	-0.454654	-1.740969	-0.364005	
26770	O	0.790344	-0.978288	1.071852	
26771	O	1.528031	-2.039883	0.961655	
26772	H	0.955241	1.826551	0.515941	
26773	H	1.554131	-1.176372	-1.530671	
26774	H	0.239570	-0.144395	-2.144588	
26775	Rotational constants (GHz):		1.2253800	0.7626000	0.7110700
26776	Vibrational harmonic frequencies (cm-1):				
26777		54.8857	59.6793		84.5541
26778		90.2626	142.0135		168.4859
26779		188.2511	208.1262		228.8235
26780		247.7513	252.1421		274.8873
26781		297.3574	324.7963		392.0078
26782		406.5965	454.3372		478.6060
26783		517.3331	551.7036		664.4843
26784		712.5377	833.5159		873.8656
26785		917.3792	961.4796		973.2907
26786		994.9728	1043.4124		1064.8187
26787		1099.5403	1126.3762		1175.8250
26788		1221.4449	1268.0214		1290.3766
26789		1311.6533	1353.2771		1380.8481
26790		1394.5321	1399.8977		1408.2602
26791		1421.6705	1442.3069		1462.7194
26792		1484.8680	1503.0683		1867.9835
26793		2994.8407	3076.0001		3088.7389
26794		3107.7526	3145.5828		3150.6099
26795		3180.8624	3730.4602		3820.4208
26796	Zero-point correction (Hartree):		0.155759		
26797	diHPCARP_Ib.mtmmptppd				
26798	-----				
26799	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17751466				
26800	Electronic state : 2-A				
26802	Cartesian coordinates (Angs):				
26803	O	1.564003	-1.404671	1.502443	
26804	O	1.930526	-0.338731	0.646450	
26805	C	0.792578	0.463050	0.360794	
26806	C	-0.301376	-0.379748	-0.314698	
26807	C	-1.542851	0.391340	-0.759708	
26808	O	-2.476723	0.510027	0.285128	
26809	O	-3.015098	-0.802368	0.475979	
26810	H	-3.312324	-0.739005	1.391233	
26811	C	0.253730	1.158440	1.599202	
26812	H	1.075211	1.659438	2.108105	
26813	H	-0.190774	0.429559	2.273562	
26814	H	-0.494932	1.896452	1.320243	
26815	C	1.363521	1.474077	-0.635330	
26816	O	0.788507	2.480728	-0.936854	
26817	H	2.343545	1.205816	-1.063893	
26818	H	-0.604424	-1.181111	0.356434	
26819	O	0.249455	-0.997782	-1.501223	
26820	O	0.912122	-2.082304	-1.234009	
26821	H	1.475090	-2.125332	0.858640	
26822	H	-1.312272	1.417638	-1.040968	
26823	H	-1.995059	-0.125600	-1.608229	
26824	Rotational constants (GHz):		1.0468000	0.7903300	0.6742400
26825	Vibrational harmonic frequencies (cm-1):				
26826		40.8465	50.8520		69.4770
26827		101.3341	110.0677		160.9221
26828		181.2603	194.4715		200.5893
26829		215.8919	232.1076		265.6609
26830		309.4858	342.7920		381.3841

26831	406.6180	462.4294	492.9720		
26832	512.4067	532.9731	611.0867		
26833	663.0201	778.9180	913.1000		
26834	918.7019	968.2519	985.3556		
26835	1035.6940	1057.5460	1071.6857		
26836	1123.2877	1131.6865	1183.0172		
26837	1209.6984	1253.5064	1290.5485		
26838	1304.4494	1342.9677	1362.7858		
26839	1401.0723	1417.2084	1419.0458		
26840	1444.4536	1446.9540	1484.0541		
26841	1486.1353	1499.3419	1866.1997		
26842	3002.6541	3078.3792	3082.2902		
26843	3135.0531	3151.8395	3162.7152		
26844	3171.2259	3742.2936	3845.6055		
26845	Zero-point correction (Hartree): 0.155613				
26846					
26847	diHPCARP_Ib.mtptmtpd				
26848	-----				
26849	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18083228				
26850	Electronic state : 2-A				
26851	Cartesian coordinates (Angs):				
26852	O	2.607163	-0.819595	-0.685161	
26853	O	1.669983	-1.040347	0.354502	
26854	C	0.364430	-0.691302	-0.092680	
26855	C	0.331641	0.795753	-0.491999	
26856	C	-1.031104	1.356955	-0.853002	
26857	O	-2.008430	1.103190	0.136991	
26858	O	-2.925805	0.140387	-0.360535	
26859	H	-2.726069	-0.631317	0.197255	
26860	C	-0.098872	-1.576904	-1.230746	
26861	H	0.013199	-2.617751	-0.935664	
26862	H	0.509472	-1.391385	-2.113841	
26863	H	-1.145650	-1.393759	-1.462915	
26864	C	-0.432669	-0.929848	1.197551	
26865	O	-1.434308	-1.589193	1.239550	
26866	H	0.006469	-0.482283	2.101921	
26867	H	1.019332	0.945218	-1.324893	
26868	O	0.825474	1.598869	0.609509	
26869	O	2.121362	1.659078	0.644820	
26870	H	2.983618	0.029934	-0.405005	
26871	H	-0.939861	2.440685	-0.941956	
26872	H	-1.364585	0.953620	-1.807054	
26873	Rotational constants (GHz): 1.3224900			0.8092100	0.6491800
26874	Vibrational harmonic frequencies (cm-1):				
26875	65.2519	87.3108	114.1111		
26876	163.5719	173.0559	184.5486		
26877	203.2965	209.7887	231.2560		
26878	245.6380	285.1464	300.9920		
26879	320.8998	383.8795	432.5337		
26880	451.7497	473.8916	501.8543		
26881	517.4268	560.6272	648.9009		
26882	683.9113	795.7795	882.3005		
26883	912.2391	932.9019	983.4132		
26884	1016.2716	1043.4797	1055.4234		
26885	1116.4953	1145.0502	1169.7233		
26886	1214.7601	1251.8621	1296.4108		
26887	1310.8555	1355.3766	1366.7495		
26888	1403.3290	1405.3083	1423.9562		
26889	1446.2568	1467.4564	1474.9113		
26890	1495.9542	1498.2528	1855.2608		
26891	3034.0150	3084.6367	3087.5434		
26892	3112.2898	3146.6207	3167.8315		
26893	3173.7990	3683.9623	3737.4770		
26894	Zero-point correction (Hartree): 0.156710				
26895					
26896	diHPCARP_Ib.mtptmtpd				
26897	-----				
26898	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18019022				
26899	Electronic state : 2-A				
26900	Cartesian coordinates (Angs):				
26901	O	1.682346	-1.755907	1.049316	
26902	O	1.987085	-0.714773	0.139715	

26903	C	1.038030	0.330504	0.280852	
26904	C	-0.368596	-0.180119	-0.072456	
26905	C	-1.447732	0.880859	-0.173581	
26906	O	-2.729421	0.300543	-0.231267	
26907	O	-2.989986	-0.208880	1.078383	
26908	H	-3.459679	-1.023431	0.864004	
26909	C	1.062353	0.935841	1.678652	
26910	H	2.098468	1.069353	1.984493	
26911	H	0.571511	0.272586	2.388108	
26912	H	0.568186	1.904569	1.678477	
26913	C	1.514377	1.351906	-0.750542	
26914	O	0.983544	2.417784	-0.880154	
26915	H	2.378336	1.043279	-1.362190	
26916	H	-0.658041	-0.934109	0.657653	
26917	O	-0.325346	-0.829864	-1.365938	
26918	O	0.046650	-2.070223	-1.291547	
26919	H	1.214858	-2.372716	0.463588	
26920	H	-1.389444	1.576566	0.662994	
26921	H	-1.353781	1.440519	-1.102738	
26922	Rotational constants (GHz):		1.0992000	0.7626200	0.6385600
26923	Vibrational harmonic frequencies (cm-1):				
26924		40.6244	62.1462		83.8235
26925		108.9352	154.5141		163.3680
26926		175.6366	185.4033		193.2816
26927		220.8641	246.7873		258.4429
26928		297.3524	327.5172		366.2697
26929		433.2453	461.8200		490.5021
26930		519.4510	541.1193		604.2137
26931		664.7106	834.6216		870.0704
26932		918.2682	965.4451		989.3833
26933		1002.9417	1058.2935		1081.6219
26934		1108.7330	1146.0758		1179.3849
26935		1201.1476	1260.6901		1291.3537
26936		1304.7306	1330.2297		1371.6599
26937		1396.9649	1413.3296		1416.7775
26938		1431.9407	1450.0691		1460.1604
26939		1490.8565	1502.7734		1867.3917
26940		3003.2393	3081.5327		3100.7824
26941		3134.6149	3159.3186		3161.1372
26942		3172.5553	3732.8987		3841.7435
26943	Zero-point correction (Hartree):		0.155673		
26944	diHPCARP_Ib.mttpptppd				
26945	-----				
26947	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.18041897		
26948	Electronic state : 2-A				
26949	Cartesian coordinates (Angs):				
26950	O	1.736881	-1.670843	1.101544	
26951	O	2.012777	-0.630252	0.182362	
26952	C	1.011622	0.368931	0.285570	
26953	C	-0.361132	-0.212163	-0.093989	
26954	C	-1.481011	0.800432	-0.249488	
26955	O	-2.736283	0.157554	-0.259364	
26956	O	-2.946176	-0.353657	1.054274	
26957	H	-3.738806	0.128714	1.318246	
26958	C	0.972611	0.991433	1.675828	
26959	H	1.993557	1.172726	2.007038	
26960	H	0.491982	0.315378	2.380167	
26961	H	0.438290	1.938253	1.650898	
26962	C	1.461199	1.399496	-0.747954	
26963	O	0.879643	2.435044	-0.905819	
26964	H	2.354475	1.127958	-1.334460	
26965	H	-0.640021	-0.963066	0.643720	
26966	O	-0.255789	-0.883563	-1.372254	
26967	O	0.188606	-2.097463	-1.266485	
26968	H	1.299150	-2.312398	0.518731	
26969	H	-1.442385	1.551609	0.538237	
26970	H	-1.413244	1.297494	-1.216438	
26971	Rotational constants (GHz):		1.0952800	0.7642100	0.6426900
26972	Vibrational harmonic frequencies (cm-1):				
26973		53.9684	62.9053		89.0954
26974		113.6716	157.5590		168.4070

26975	187.8414	194.2113	198.4763			
26976	221.8731	252.6122	261.7265			
26977	300.3454	329.6166	372.3220			
26978	445.0602	462.3244	510.0249			
26979	531.6904	545.7451	606.5537			
26980	666.0582	836.8403	872.8731			
26981	920.2786	966.0209	989.1138			
26982	1004.5094	1058.5633	1084.4254			
26983	1101.8138	1153.3587	1180.5166			
26984	1201.4047	1260.5735	1296.7717			
26985	1308.9769	1335.4392	1373.4422			
26986	1393.6944	1399.8691	1417.2794			
26987	1431.6391	1453.1366	1460.4195			
26988	1491.6340	1503.1166	1865.8334			
26989	3005.8366	3081.8884	3100.7417			
26990	3133.0047	3157.3871	3161.2360			
26991	3172.4196	3729.2718	3830.7588			
26992	Zero-point correction (Hartree): 0.155977					
26993						
26994	diHPCARP_Ib.pmmptmmd					
26995	-----					
26996	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18315940					
26997	Electronic state : 2-A					
26998	Cartesian coordinates (Angs):					
26999	O	-1.154557	0.101207	1.930651		
27000	O	-1.445080	0.957502	0.836855		
27001	C	-0.405624	0.889759	-0.116638		
27002	C	-0.172835	-0.513886	-0.721337		
27003	C	0.518097	-1.581030	0.132533		
27004	O	1.722865	-1.107653	0.678080		
27005	O	2.659759	-0.999559	-0.384162		
27006	H	2.769702	-0.035673	-0.451638		
27007	C	-0.855747	1.855773	-1.210613		
27008	H	-1.087345	2.823711	-0.770778		
27009	H	-1.745922	1.468049	-1.701092		
27010	H	-0.054332	1.978602	-1.935112		
27011	C	0.890080	1.414970	0.497054		
27012	O	1.858517	1.670395	-0.170738		
27013	H	0.855457	1.600200	1.581524		
27014	H	0.420759	-0.364764	-1.623356		
27015	O	-1.418868	-1.041423	-1.221582		
27016	O	-2.209641	-1.441411	-0.269143		
27017	H	-1.728557	-0.650468	1.717535		
27018	H	-0.082558	-1.868274	0.988009		
27019	H	0.705011	-2.457378	-0.490768		
27020	Rotational constants (GHz):			1.1742700	0.8850700	0.7198200
27021	Vibrational harmonic frequencies (cm-1):					
27022	60.9275	113.8295	139.7592			
27023	158.1366	161.6904	202.4503			
27024	209.6896	232.7462	250.4618			
27025	270.3555	282.9650	295.2098			
27026	302.8420	340.9262	428.7026			
27027	446.1331	470.8832	496.0499			
27028	524.7189	564.0777	631.2466			
27029	691.6852	774.8174	924.0725			
27030	951.1282	964.4429	978.9403			
27031	1005.4801	1049.1713	1060.8470			
27032	1114.5083	1142.4388	1187.6208			
27033	1226.8812	1241.0997	1255.7760			
27034	1295.5990	1359.9161	1381.0818			
27035	1401.4767	1409.0165	1416.1570			
27036	1432.8173	1469.0766	1486.1274			
27037	1491.6045	1505.2773	1833.5013			
27038	3032.1255	3084.9020	3086.5414			
27039	3119.6110	3165.8910	3175.8116			
27040	3194.6460	3701.8603	3752.4277			
27041	Zero-point correction (Hartree): 0.157076					
27042						
27043	diHPCARP_Ib.pmmptmpd					
27044	-----					
27045	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17985984					
27046	Electronic state : 2-A					

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27047 Cartesian coordinates (Angs):
27048 O -0.329862 0.583267 2.111552
27049 O -1.291586 0.808800 1.075687
27050 C -0.615282 0.763839 -0.164077
27051 C -0.173203 -0.638429 -0.607378
27052 C 0.666375 -1.438755 0.383769
27053 O 1.865586 -0.767755 0.687866
27054 O 2.701654 -0.835827 -0.459766
27055 H 2.629032 0.067621 -0.806687
27056 C -1.626263 1.353107 -1.150655
27057 H -1.811801 2.399885 -0.915049
27058 H -2.561692 0.803225 -1.076660
27059 H -1.239719 1.274283 -2.164626
27060 C 0.565283 1.724522 -0.135977
27061 O 1.473488 1.693841 -0.920438
27062 H 0.474164 2.525707 0.616800
27063 H 0.389434 -0.513652 -1.532800
27064 O -1.316534 -1.414888 -1.014750
27065 O -1.997146 -1.862505 0.001883
27066 H -0.652353 1.193039 2.785941
27067 H 0.148288 -1.556583 1.329971
27068 H 0.878388 -2.418699 -0.047256
27069 Rotational constants (GHz): 1.0963400 0.8914000 0.7412600
27070 Vibrational harmonic frequencies (cm-1):
27071 46.1729 83.8493 104.0987
27072 132.9629 146.2856 174.1280
27073 189.5755 213.7994 232.2228
27074 240.6377 266.0643 285.3808
27075 300.9309 309.2263 343.0692
27076 434.1689 467.8260 469.6695
27077 538.5768 572.5038 619.1046
27078 681.1982 777.4169 933.3010
27079 954.8365 964.9485 973.1534
27080 1016.3096 1042.7135 1054.4630
27081 1120.0582 1133.0307 1192.3071
27082 1219.9626 1242.0912 1254.4724
27083 1290.4792 1360.5889 1388.6092
27084 1398.6506 1411.9699 1418.4214
27085 1422.6024 1457.3323 1486.5551
27086 1494.7194 1505.0722 1852.0082
27087 3003.4229 3079.8953 3086.5900
27088 3122.9507 3159.8035 3172.8282
27089 3187.9753 3741.6924 3839.5277
27090 Zero-point correction (Hartree): 0.156310
27091
27092 diHPCARP_Ib.pmmmpptppd
27093 -----
27094 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18080426
27095 Electronic state : 2-A
27096 Cartesian coordinates (Angs):
27097 O -0.401504 1.570304 -1.715037
27098 O 0.845274 1.415090 -1.029539
27099 C 0.603849 0.725527 0.184387
27100 C 0.332939 -0.772864 -0.004384
27101 C -0.793465 -1.136032 -0.967137
27102 O -2.019671 -0.572658 -0.569921
27103 O -2.460507 -1.280680 0.580637
27104 H -2.245644 -0.653705 1.290383
27105 C 1.876833 0.961491 0.999527
27106 H 1.972347 2.019575 1.239236
27107 H 2.741920 0.652873 0.416524
27108 H 1.839653 0.379575 1.917662
27109 C -0.519747 1.403646 0.951732
27110 O -1.133745 0.881289 1.841072
27111 H -0.666475 2.465692 0.691209
27112 H 0.152080 -1.212947 0.975278
27113 O 1.512733 -1.398900 -0.547201
27114 O 2.283513 -1.898142 0.373000
27115 H -0.333832 2.488616 -2.002946
27116 H -0.594977 -0.738208 -1.959858
27117 H -0.876272 -2.222495 -1.016328
27118 Rotational constants (GHz): 1.0539700 0.8633000 0.7326400

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27119 Vibrational harmonic frequencies (cm-1):
27120      59.4352      83.9785      98.8226
27121      125.4969     167.3044     184.6021
27122      198.0327     213.8146     232.3081
27123      250.5191     280.7833     281.2092
27124      288.6396     324.5573     366.4401
27125      407.9677     479.4361     493.4437
27126      535.6404     543.0885     626.2116
27127      655.0089     759.7602     930.7941
27128      954.3144     964.0772     972.6419
27129     1033.4824     1042.8747    1056.8193
27130     1121.9252     1134.6509    1192.2864
27131     1225.9959     1251.7970    1283.6216
27132     1292.5929     1337.1186    1383.7914
27133     1397.2561     1411.5195    1413.0580
27134     1416.6562     1460.1801    1482.5767
27135     1490.8714     1504.8312    1853.1500
27136     2997.4058     3079.4611    3087.4249
27137     3129.1143     3158.7314    3162.3090
27138     3174.3392     3723.5686    3834.2552
27139 Zero-point correction (Hartree): 0.156310
27140
27141 diHPCARP_Ib.pmmpttpd
27142 -----
27143 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18052666
27144 Electronic state : 2-A
27145 Cartesian coordinates (Angs):
27146 O      -0.082216     -1.423912      1.875273
27147 O       1.075180     -1.309905      1.041065
27148 C       0.667687     -0.785462     -0.210518
27149 C       0.342289      0.708176     -0.178687
27150 C      -0.685994      1.160181      0.854106
27151 O      -1.925341      0.520417      0.672898
27152 O      -2.519563      1.062903     -0.498480
27153 H      -2.361794      0.354235     -1.142915
27154 C       1.855368     -1.066961     -1.134555
27155 H       1.981978     -2.140557     -1.265757
27156 H       2.759891     -0.654328     -0.694501
27157 H       1.680865     -0.603407     -2.103504
27158 C      -0.495536     -1.598472     -0.756714
27159 O      -1.235548     -1.213634     -1.619430
27160 H      -0.548929     -2.627360     -0.361979
27161 H       0.025327      1.012640     -1.176113
27162 O       1.578808      1.394877      0.110375
27163 O       1.540356      2.633089     -0.281426
27164 H       0.066491     -2.292085      2.269036
27165 H      -0.361161      0.893189      1.857377
27166 H      -0.798947      2.242226      0.774365
27167 Rotational constants (GHz):  0.9704000    0.9315400    0.7157400
27168 Vibrational harmonic frequencies (cm-1):
27169      58.8011      82.5740      91.9681
27170     123.3291     165.6716     184.5255
27171     198.8836     217.0460     222.8174
27172     239.1460     267.7084     281.7471
27173     291.3922     328.1323     353.0539
27174     433.5280     453.4258     477.1759
27175     539.8767     558.7843     609.5148
27176     646.6440     787.4813     932.3615
27177     956.0137     964.2484     974.3299
27178     1029.5993     1051.1638    1070.8324
27179     1106.6871     1133.6331    1182.9556
27180     1231.3117     1257.6627    1284.7357
27181     1293.6785     1334.5107    1389.2962
27182     1396.8413     1408.5973    1412.7301
27183     1418.1908     1459.8115    1487.3025
27184     1490.6018     1503.6035    1855.6093
27185     2999.5753     3079.4529    3089.5501
27186     3119.7498     3159.0324    3163.1995
27187     3173.8968     3730.3295    3834.1286
27188 Zero-point correction (Hartree): 0.156256
27189
27190 diHPCARP_Ib.pmpmtmmd

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27191 -----
27192 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18145724
27193 Electronic state : 2-A
27194 Cartesian coordinates (Angs):
27195 O -0.491170 -1.624126 -1.379441
27196 O -0.625289 -0.211834 -1.483130
27197 C -1.052865 0.296871 -0.236179
27198 C 0.033900 0.451374 0.840532
27199 C 0.947525 -0.734250 1.123068
27200 O 1.720201 -1.220136 0.041810
27201 O 2.955365 -0.533963 -0.020538
27202 H 2.733325 0.228685 -0.576829
27203 C -1.698587 1.640584 -0.569103
27204 H -2.595148 1.475004 -1.163974
27205 H -1.004075 2.244572 -1.148932
27206 H -1.960581 2.172312 0.343998
27207 C -2.160370 -0.615890 0.290406
27208 O -2.349131 -0.840126 1.451370
27209 H -2.809856 -1.014819 -0.506815
27210 H -0.498112 0.637212 1.775082
27211 O 0.772715 1.682764 0.656315
27212 O 1.432644 1.721669 -0.459825
27213 H 0.466241 -1.714109 -1.234487
27214 H 1.619147 -0.487974 1.945059
27215 H 0.308767 -1.567003 1.422059
27216 Rotational constants (GHz): 1.2840100 0.8075500 0.7075300
27217 Vibrational harmonic frequencies (cm-1):
27218 52.6672 67.0695 104.0344
27219 116.5237 170.9434 205.1143
27220 222.9768 233.5826 237.1234
27221 259.3790 289.2394 307.5532
27222 315.0918 358.9528 444.8966
27223 449.8272 486.4638 518.3783
27224 578.5439 617.6760 627.3375
27225 684.2163 832.8930 911.0499
27226 940.7667 957.7846 968.7581
27227 993.4735 1040.8913 1055.9313
27228 1086.5329 1139.7273 1177.4113
27229 1226.3309 1253.0879 1270.6213
27230 1330.2905 1363.2978 1398.0529
27231 1400.7286 1407.7279 1415.4153
27232 1441.8872 1452.0273 1461.1361
27233 1484.2590 1508.4268 1865.1134
27234 3006.8723 3078.3934 3084.1126
27235 3108.0646 3139.2560 3159.3039
27236 3166.9652 3677.3696 3747.6109
27237 Zero-point correction (Hartree): 0.156964
27238
27239 diHPCARP_Ib.pmpmpmpmd
27240 -----
27241 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18187625
27242 Electronic state : 2-A
27243 Cartesian coordinates (Angs):
27244 O -0.516467 -1.969224 -1.043374
27245 O -0.690791 -0.612097 -1.434572
27246 C -1.038718 0.152443 -0.295178
27247 C 0.148823 0.536811 0.600224
27248 C 1.027347 -0.592437 1.121037
27249 O 1.777777 -1.244406 0.108956
27250 O 2.993111 -0.551327 -0.106313
27251 H 2.733046 0.155697 -0.714716
27252 C -1.734120 1.387612 -0.861443
27253 H -2.654161 1.087450 -1.360280
27254 H -1.086447 1.871181 -1.590097
27255 H -1.960621 2.094397 -0.065732
27256 C -2.073270 -0.619626 0.515784
27257 O -2.139929 -0.583858 1.711231
27258 H -2.791630 -1.182379 -0.104468
27259 H -0.245792 1.089315 1.452061
27260 O 1.017018 1.434501 -0.131542
27261 O 0.741599 2.687742 0.075066
27262 H 0.451094 -2.027718 -0.974636

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27263	H	1.720013	-0.209630	1.869053	
27264	H	0.395594	-1.357782	1.570646	
27265	Rotational constants (GHz):		1.1255700	0.8514800	0.6702400
27266	Vibrational harmonic frequencies (cm-1):				
27267		56.1031	70.6178		100.1744
27268		117.1043	147.9677		175.8741
27269		199.6806	237.7265		245.0648
27270		268.8593	286.4444		310.8748
27271		317.5302	352.8847		370.4924
27272		430.6593	496.4182		505.9951
27273		555.7816	602.8006		646.0658
27274		668.4012	822.3203		896.4145
27275		935.6958	956.8752		977.8468
27276		1011.1581	1035.6635		1055.5415
27277		1103.8734	1132.5193		1173.7292
27278		1238.1311	1252.6548		1289.6040
27279		1313.7362	1345.2424		1372.1154
27280		1397.0293	1404.2247		1414.4677
27281		1442.9365	1453.0391		1471.6361
27282		1482.9478	1504.0443		1863.5671
27283		2998.7448	3078.6419		3096.7702
27284		3127.4641	3153.6036		3158.1513
27285		3167.8573	3707.9393		3779.0983
27286	Zero-point correction (Hartree): 0.156690				
27287					
27288	diHPCARP_Ib.pmpmttmd				
27289	-----				
27290	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18223384				
27291	Electronic state : 2-A				
27292	Cartesian coordinates (Angs):				
27293	O	1.139271	1.928462	-0.637654	
27294	O	0.740042	0.709974	-1.256914	
27295	C	0.933132	-0.377094	-0.354530	
27296	C	-0.310182	-0.704241	0.477189	
27297	C	-0.981770	0.420913	1.250020	
27298	O	-1.210501	1.616022	0.526784	
27299	O	-2.135304	1.364197	-0.516877	
27300	H	-1.557471	1.078006	-1.243356	
27301	C	1.333437	-1.562720	-1.231980	
27302	H	2.313569	-1.377058	-1.668030	
27303	H	0.611154	-1.685513	-2.035172	
27304	H	1.364340	-2.477245	-0.641618	
27305	C	2.121355	-0.070409	0.551895	
27306	O	2.140231	-0.327562	1.721200	
27307	H	2.989316	0.352966	0.021947	
27308	H	-0.038004	-1.468910	1.205842	
27309	O	-1.253581	-1.318340	-0.440133	
27310	O	-2.209213	-1.926520	0.189741	
27311	H	0.310118	2.202275	-0.200877	
27312	H	-1.926686	0.046942	1.645331	
27313	H	-0.329727	0.719976	2.071196	
27314	Rotational constants (GHz):		1.1481300	0.8744500	0.7105900
27315	Vibrational harmonic frequencies (cm-1):				
27316		51.2925	70.4440		99.9942
27317		116.8787	159.6579		192.9819
27318		220.4816	224.8505		264.6960
27319		273.2083	301.3821		316.4968
27320		344.1423	382.2060		397.3779
27321		438.3152	450.9949		524.3816
27322		565.4295	623.5596		672.7510
27323		715.4933	840.9829		870.4810
27324		934.0251	955.0379		971.0884
27325		998.3602	1047.0525		1051.8581
27326		1096.5696	1130.0312		1167.2532
27327		1241.3174	1248.7461		1292.8700
27328		1311.7380	1347.6969		1370.0221
27329		1398.2538	1408.2899		1421.8802
27330		1449.5286	1466.9908		1480.9166
27331		1488.3407	1502.2328		1864.5906
27332		3014.9589	3078.4454		3088.4986
27333		3111.2509	3145.8889		3158.0047
27334		3170.0599	3584.2753		3732.1200


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27335 Zero-point correction (Hartree): 0.156844
27336
27337 diHPCARP_Ib.pmppttmd
27338 -----
27339 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17957537
27340 Electronic state : 2-A
27341 Cartesian coordinates (Angs):
27342 O -0.878343 -1.991081 -0.733398
27343 O -0.866560 -0.705327 -1.342149
27344 C -1.067814 0.275463 -0.342307
27345 C 0.182133 0.664970 0.452651
27346 C 0.979856 -0.422512 1.154993
27347 O 1.513342 -1.444234 0.330254
27348 O 2.575451 -0.903146 -0.441655
27349 H 3.342360 -1.330710 -0.039100
27350 C -1.629487 1.482476 -1.093413
27351 H -2.613283 1.239184 -1.491265
27352 H -0.968997 1.733236 -1.919893
27353 H -1.708519 2.339482 -0.426698
27354 C -2.158954 -0.218215 0.601643
27355 O -2.172054 -0.002808 1.780088
27356 H -2.972214 -0.756834 0.086529
27357 H -0.143975 1.348662 1.238969
27358 O 1.028882 1.426684 -0.439851
27359 O 1.930397 2.090148 0.213198
27360 H 0.071133 -2.136809 -0.579134
27361 H 1.791357 0.050984 1.708028
27362 H 0.318813 -0.942164 1.849267
27363 Rotational constants (GHz): 1.1916700 0.8191500 0.6806400
27364 Vibrational harmonic frequencies (cm-1):
27365 46.7030 58.7615 91.4795
27366 114.0381 159.6445 166.1316
27367 196.2229 218.2330 222.5696
27368 248.9680 265.9626 286.7204
27369 313.9294 320.3221 362.4770
27370 415.3382 458.8596 534.5212
27371 562.7453 622.9604 625.1157
27372 709.3895 832.5857 871.3031
27373 937.1444 960.5687 971.3396
27374 1001.9911 1053.1662 1056.2778
27375 1099.7548 1134.2026 1173.1730
27376 1242.9453 1262.1586 1293.9189
27377 1320.2116 1355.1976 1378.3353
27378 1398.7852 1404.5368 1414.3941
27379 1430.0572 1460.1075 1468.5174
27380 1487.1691 1502.7558 1864.2185
27381 3002.4866 3078.4235 3086.4855
27382 3098.9404 3145.5627 3158.1804
27383 3169.5981 3667.6386 3812.2595
27384 Zero-point correction (Hartree): 0.156272
27385
27386 diHPCARP_Ib.pmptmtpmd
27387 -----
27388 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18021269
27389 Electronic state : 2-A
27390 Cartesian coordinates (Angs):
27391 O 0.507023 -1.893089 -1.021812
27392 O -0.416772 -0.884762 -1.415624
27393 C -1.020828 -0.342938 -0.257527
27394 C -0.172349 0.691638 0.497726
27395 C 1.239145 0.305593 0.894836
27396 O 2.037180 0.190248 -0.274277
27397 O 3.335069 -0.191683 0.161528
27398 H 3.859549 0.573974 -0.105347
27399 C -2.325509 0.273703 -0.754841
27400 H -2.971642 -0.512375 -1.141817
27401 H -2.112379 0.977524 -1.556921
27402 H -2.828710 0.800969 0.053085
27403 C -1.388022 -1.491685 0.677261
27404 O -1.368996 -1.411834 1.872162
27405 H -1.723185 -2.398839 0.146265
27406 H -0.708928 0.931601 1.414977

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27407	O	-0.073931	1.910422	-0.271377		
27408	O	-0.985720	2.775083	0.061084		
27409	H	1.339903	-1.391351	-1.018300		
27410	H	1.656832	1.086396	1.531963		
27411	H	1.223115	-0.640843	1.437899		
27412	Rotational constants (GHz):		1.0589800	0.8328400	0.6356300	
27413	Vibrational harmonic frequencies (cm-1):					
27414		51.6325	73.7656		95.4306	
27415		106.7541	132.8080		165.3692	
27416		184.6498	220.7394		233.4096	
27417		264.8324	276.2715		292.4656	
27418		301.7052	329.7407		357.0229	
27419		376.3914	439.6521		512.6603	
27420		556.9523	594.4153		648.4042	
27421		692.8246	809.4061		926.6935	
27422		936.1177	961.5723		989.2753	
27423		1034.3216	1053.5425		1061.9185	
27424		1105.6993	1134.7251		1180.1972	
27425		1236.4142	1248.2611		1279.4033	
27426		1297.5934	1348.8334		1376.1309	
27427		1400.9190	1405.8318		1413.5063	
27428		1421.1671	1453.9254		1480.8269	
27429		1505.4969	1515.7837		1864.4338	
27430		3001.5411	3073.4991		3079.1324	
27431		3124.4820	3127.8693		3159.5704	
27432		3168.1428	3687.6830		3821.9697	
27433	Zero-point correction (Hartree):		0.156268			
27434	diHPCARP_Ib.pmpmttmd					
27435	-----					
27437	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.18107084			
27438	Electronic state : 2-A					
27439	Cartesian coordinates (Angs):					
27440	O	-0.306701	-1.987707	-0.917255		
27441	O	-0.830368	-0.747718	-1.378775		
27442	C	-1.182343	0.040899	-0.258993		
27443	C	-0.014266	0.752262	0.428894		
27444	C	1.183527	-0.070990	0.861444		
27445	O	1.867382	-0.529513	-0.296468		
27446	O	2.991172	-1.267368	0.160978		
27447	H	3.721096	-0.703619	-0.125852		
27448	C	-2.194604	1.050598	-0.798313		
27449	H	-3.097997	0.529782	-1.111185		
27450	H	-1.771226	1.565899	-1.657047		
27451	H	-2.444456	1.780295	-0.030007		
27452	C	-1.916000	-0.844957	0.743193		
27453	O	-1.855719	-0.700981	1.930537		
27454	H	-2.555427	-1.607329	0.266715		
27455	H	-0.411152	1.223510	1.328879		
27456	O	0.420626	1.811884	-0.458319		
27457	O	1.207033	2.646608	0.146378		
27458	H	0.648870	-1.805679	-0.936283		
27459	H	1.853469	0.562900	1.441705		
27460	H	0.851551	-0.914265	1.469114		
27461	Rotational constants (GHz):		1.0892700	0.8165900	0.6390700	
27462	Vibrational harmonic frequencies (cm-1):					
27463		52.0245	58.7595		89.8758	
27464		106.4004	154.7319		161.5726	
27465		190.9983	222.9701		230.6237	
27466		257.8351	260.9485		283.3439	
27467		301.0547	328.9510		354.8671	
27468		357.4621	453.4556		532.0953	
27469		558.9094	612.1214		619.9873	
27470		721.0268	804.4699		919.3986	
27471		935.8089	963.4043		989.4588	
27472		1040.7556	1055.1154		1064.4509	
27473		1090.8112	1131.7185		1178.0062	
27474		1239.5112	1254.4545		1282.1795	
27475		1296.4305	1349.8513		1383.1504	
27476		1399.9980	1405.5135		1415.3753	
27477		1416.4292	1460.4071		1487.1420	
27478		1502.9480	1514.9987		1865.8880	

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27479          3000.4604          3078.5111          3082.7934
27480          3110.2485          3137.1235          3158.1300
27481          3169.7847          3674.2419          3817.4441
27482 Zero-point correction (Hartree): 0.156251
27483
27484 diHPCARP_Ib.pmtpmtmmd
27485 -----
27486 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17934097
27487 Electronic state : 2-A
27488 Cartesian coordinates (Angs):
27489   O      1.435814      -0.781560      -1.705131
27490   O      1.953873      -0.570363      -0.400263
27491   C      1.113503      0.338044      0.274637
27492   C     -0.338703     -0.150471      0.444743
27493   C     -1.259091     -0.149646     -0.767102
27494   O     -2.604230     -0.296588     -0.374667
27495   O     -2.975772      0.938816      0.241974
27496   H     -3.615920      0.625802      0.891565
27497   C      1.786402      0.515291      1.635514
27498   H      2.816024      0.841413      1.498316
27499   H      1.786238     -0.433517      2.168319
27500   H      1.248389      1.263579      2.213630
27501   C      1.157083      1.687377     -0.433074
27502   O      0.352587      2.553541     -0.244639
27503   H      2.031577      1.816360     -1.096511
27504   H     -0.803363      0.481802      1.199911
27505   O     -0.318093     -1.462094      1.062489
27506   O      0.029286     -2.401548      0.236171
27507   H      1.008811     -1.643865     -1.582284
27508   H     -1.133502      0.769364     -1.338502
27509   H     -1.081137     -1.006134     -1.410215
27510 Rotational constants (GHz):      1.1239500      0.8283800      0.6453100
27511 Vibrational harmonic frequencies (cm-1):
27512      34.3750      72.8794      96.8304
27513     135.5393      159.6923      166.1535
27514     168.4903      192.4210      206.6138
27515     227.5889      264.8160      289.6317
27516     297.2667      311.0620      346.6219
27517     392.9300      466.7323      485.7636
27518     550.0086      555.9964      601.4965
27519     720.5078      833.1136      907.8422
27520     941.5821      953.9058      973.9638
27521     984.2290     1047.1419     1062.6897
27522    1102.0981     1126.2490     1179.6661
27523    1233.4714     1253.4654     1258.4906
27524    1313.6143     1344.7651     1387.9721
27525    1394.7992     1406.8613     1418.6276
27526    1428.1785     1437.3883     1460.6113
27527    1490.6275     1504.0555     1868.0519
27528    2980.9020     3078.9522     3113.0583
27529    3133.4611     3159.9371     3168.7352
27530    3183.7739     3748.9845     3846.3616
27531 Zero-point correction (Hartree): 0.155989
27532
27533 diHPCARP_Ib.pmtpmttmd
27534 -----
27535 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17860110
27536 Electronic state : 2-A
27537 Cartesian coordinates (Angs):
27538   O     -1.797938     -1.098554     -1.549807
27539   O     -1.790759      0.279129     -1.160043
27540   C     -1.193470      0.352960      0.123226
27541   C      0.330322      0.247959      0.124372
27542   C      0.928280     -0.949167     -0.600920
27543   O      2.334733     -0.903510     -0.609728
27544   O      2.794999     -0.961499      0.731263
27545   H      2.996782     -0.027737      0.894478
27546   C     -1.655202      1.702934      0.671050
27547   H     -2.734072      1.694475      0.816637
27548   H     -1.399357      2.490110     -0.034263
27549   H     -1.162782      1.899790      1.621565
27550   C     -1.808877     -0.719391      1.018409

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27551	O	-1.230953	-1.229665	1.932457	
27552	H	-2.864080	-0.941400	0.780359	
27553	H	0.660431	0.240121	1.162059	
27554	O	0.846184	1.454966	-0.480253	
27555	O	1.999032	1.792051	0.014091	
27556	H	-1.577907	-1.025272	-2.486389	
27557	H	0.565435	-1.869340	-0.138309	
27558	H	0.666850	-0.935861	-1.656798	
27559	Rotational constants (GHz):		1.2435700	0.7000300	0.6482200
27560	Vibrational harmonic frequencies (cm-1):				
27561		42.8191	87.9576		89.5213
27562		115.2878	150.6979		162.4440
27563		175.4614	199.6656		206.5868
27564		227.1668	270.1352		271.6510
27565		299.3269	324.0274		350.5662
27566		429.2985	443.8454		472.9555
27567		541.8156	560.7692		571.3682
27568		643.3404	880.9807		903.2359
27569		938.6041	961.3883		980.7998
27570		996.9478	1048.8804		1081.4914
27571		1096.4002	1142.2762		1176.4088
27572		1229.9315	1257.5898		1292.4657
27573		1304.1056	1338.5925		1370.9216
27574		1391.7181	1407.3289		1410.3018
27575		1414.9373	1432.7435		1460.7177
27576		1487.3818	1503.3507		1873.6483
27577		2991.8738	3079.5053		3079.9215
27578		3132.1173	3159.4172		3160.7692
27579		3170.2372	3764.3491		3836.2290
27580	Zero-point correction (Hartree): 0.155814				
27581					
27582	diHPCARP_Ib.pmtpptmmd				
27583	-----				
27584	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18051173				
27585	Electronic state : 2-A				
27586	Cartesian coordinates (Angs):				
27587	O	1.445239	-0.657608	-1.731639	
27588	O	1.979151	-0.422461	-0.437078	
27589	C	1.080829	0.399211	0.273516	
27590	C	-0.321834	-0.211127	0.459438	
27591	C	-1.258657	-0.262012	-0.738773	
27592	O	-2.598782	-0.418555	-0.317515	
27593	O	-2.970743	0.751570	0.396406	
27594	H	-3.440074	1.260678	-0.276708	
27595	C	1.765144	0.607005	1.624314	
27596	H	2.759092	1.025362	1.474429	
27597	H	1.859843	-0.349777	2.133975	
27598	H	1.176201	1.290548	2.232314	
27599	C	1.004718	1.759913	-0.408585	
27600	O	0.104174	2.532949	-0.249559	
27601	H	1.889737	1.993419	-1.028436	
27602	H	-0.824107	0.364496	1.235262	
27603	O	-0.180119	-1.528097	1.049182	
27604	O	0.232899	-2.418666	0.199794	
27605	H	1.087375	-1.551276	-1.609029	
27606	H	-1.150227	0.635767	-1.346124	
27607	H	-1.073603	-1.140218	-1.351865	
27608	Rotational constants (GHz):		1.1202000	0.8399800	0.6511600
27609	Vibrational harmonic frequencies (cm-1):				
27610		45.2083	73.2472		100.8006
27611		136.7387	163.0910		173.8698
27612		185.0055	203.8484		224.4234
27613		229.8452	270.4503		289.7534
27614		300.1499	312.3613		352.2902
27615		395.7104	480.5338		504.7323
27616		554.3270	559.0043		601.0670
27617		720.3456	840.9419		907.3479
27618		938.3733	954.4515		973.1134
27619		984.0052	1048.6484		1062.6792
27620		1094.5137	1136.0221		1178.3995
27621		1232.5550	1253.2244		1262.2708
27622		1321.3118	1345.3069		1387.5155

27623	1396.4755	1402.0708	1407.9597			
27624	1428.7047	1435.5004	1463.7866			
27625	1489.4431	1503.9766	1866.9166			
27626	2979.6603	3078.6412	3109.3249			
27627	3135.7436	3159.2012	3169.0503			
27628	3173.6679	3742.9287	3810.6722			
27629	Zero-point correction (Hartree): 0.156171					
27630						
27631	diHPCARP_Ib.ppmmtmmd					
27632	-----					
27633	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18146117					
27634	Electronic state : 2-A					
27635	Cartesian coordinates (Angs):					
27636	O	0.449296	-2.234624	-0.173820		
27637	O	-0.207449	-1.381079	-1.104741		
27638	C	-0.896814	-0.385377	-0.369308		
27639	C	0.107233	0.545585	0.342635		
27640	C	1.338834	0.870865	-0.497312		
27641	O	2.303723	-0.166535	-0.418106		
27642	O	2.803779	-0.192160	0.915808		
27643	H	3.710947	0.112844	0.787956		
27644	C	-1.778187	0.310953	-1.396319		
27645	H	-2.407881	-0.435219	-1.878779		
27646	H	-1.169260	0.797468	-2.156361		
27647	H	-2.405713	1.058337	-0.917746		
27648	C	-1.795995	-1.085242	0.644745		
27649	O	-1.967659	-0.693437	1.760875		
27650	H	-2.300224	-1.983742	0.244021		
27651	H	0.413342	0.093728	1.284549		
27652	O	-0.548789	1.763726	0.750343		
27653	O	-0.573916	2.647128	-0.204545		
27654	H	1.352843	-1.878021	-0.199726		
27655	H	1.109549	0.938933	-1.558753		
27656	H	1.774101	1.810821	-0.158316		
27657	Rotational constants (GHz):			1.0807800	0.8758100	0.6667500
27658	Vibrational harmonic frequencies (cm-1):					
27659	63.3480	88.5944	101.9611			
27660	133.6111	151.8851	177.9831			
27661	195.6862	224.6438	228.6955			
27662	239.0554	248.7769	292.3016			
27663	308.0991	332.2352	374.2132			
27664	408.3243	485.4116	510.0464			
27665	547.2297	564.8969	653.2924			
27666	678.2715	776.2619	922.7195			
27667	934.2642	960.3298	990.8130			
27668	1001.6266	1049.2376	1056.8214			
27669	1100.4051	1134.0395	1180.8467			
27670	1234.8591	1248.0317	1260.2759			
27671	1300.8577	1353.2349	1386.1774			
27672	1398.4855	1400.0440	1411.2572			
27673	1429.6864	1436.5775	1471.8320			
27674	1488.8632	1499.2985	1877.9217			
27675	2975.9933	3080.5977	3094.7186			
27676	3138.5914	3154.5706	3161.7271			
27677	3174.2754	3713.9070	3822.2756			
27678	Zero-point correction (Hartree): 0.156351					
27679						
27680	diHPCARP_Ib.ppmmttmd					
27681	-----					
27682	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18092344					
27683	Electronic state : 2-A					
27684	Cartesian coordinates (Angs):					
27685	O	-0.005491	-2.220858	-0.537404		
27686	O	0.520261	-1.661700	0.661036		
27687	C	1.002840	-0.365753	0.357183		
27688	C	-0.156009	0.574574	-0.007940		
27689	C	-1.406788	0.366934	0.839526		
27690	O	-2.184821	-0.727072	0.382814		
27691	O	-2.706468	-0.383042	-0.896437		
27692	H	-3.639647	-0.236522	-0.695574		
27693	C	1.762698	0.063374	1.606092		
27694	H	2.531729	-0.676159	1.823634		

27695	H	1.088985	0.117706	2.460327	
27696	H	2.223973	1.035444	1.454543	
27697	C	1.993797	-0.485439	-0.796088	
27698	O	2.088889	0.319845	-1.674071	
27699	H	2.641401	-1.379254	-0.732791	
27700	H	-0.405989	0.494147	-1.064231	
27701	O	0.316907	1.923231	0.212409	
27702	O	-0.466745	2.799381	-0.336815	
27703	H	-0.956207	-2.063451	-0.414767	
27704	H	-1.162074	0.107034	1.869295	
27705	H	-2.001661	1.280628	0.814667	
27706	Rotational constants (GHz):		1.0525900	0.8803700	0.6534600
27707	Vibrational harmonic frequencies (cm-1):				
27708		58.3451	79.2816		94.0960
27709		110.8973	132.2702		166.6781
27710		192.4081	205.8157		208.7194
27711		236.7871	245.9374		269.7415
27712		320.0001	340.2922		378.7286
27713		411.4640	441.9842		521.9956
27714		545.4084	576.9887		596.8213
27715		659.7497	784.0993		926.2958
27716		936.3750	961.5251		986.8256
27717		1039.3414	1054.8904		1057.8870
27718		1093.1633	1126.0901		1191.8692
27719		1237.2690	1268.0211		1285.0050
27720		1299.3919	1332.4213		1388.4208
27721		1396.9759	1401.8257		1409.7151
27722		1424.3133	1435.0981		1471.1792
27723		1493.4964	1501.4434		1878.8406
27724		2976.3752	3078.7878		3084.5662
27725		3136.5799	3148.0689		3151.4478
27726		3177.5110	3718.1537		3818.3012
27727	Zero-point correction (Hartree): 0.155977				
27728					
27729	diHPCARP_Ib.ppmppmpd				
27730	-----				
27731	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18259468				
27732	Electronic state : 2-A				
27733	Cartesian coordinates (Angs):				
27734	O	0.550529	-2.068859	-0.861088	
27735	O	0.335929	-1.508505	0.428450	
27736	C	0.605407	-0.112248	0.409900	
27737	C	-0.367885	0.564292	-0.580050	
27738	C	-1.768609	0.828465	-0.035207	
27739	O	-2.324679	-0.307266	0.575358	
27740	O	-2.459223	-1.311418	-0.420545	
27741	H	-1.713484	-1.893561	-0.206979	
27742	C	0.454972	0.323851	1.864234	
27743	H	1.198870	-0.189427	2.471711	
27744	H	-0.536062	0.057158	2.223125	
27745	H	0.595922	1.399196	1.947647	
27746	C	2.061629	0.133104	0.022844	
27747	O	2.828620	-0.757491	-0.221110	
27748	H	2.389373	1.185001	0.033491	
27749	H	-0.419505	-0.065725	-1.464816	
27750	O	0.167617	1.805511	-1.095600	
27751	O	0.300846	2.713529	-0.174223	
27752	H	1.511213	-2.208242	-0.845828	
27753	H	-1.731954	1.582998	0.750273	
27754	H	-2.404560	1.183797	-0.848887	
27755	Rotational constants (GHz):		1.1163300	0.9204000	0.6466300
27756	Vibrational harmonic frequencies (cm-1):				
27757		69.3178	94.6598		116.4405
27758		126.3681	161.6659		192.5168
27759		216.8372	243.2422		252.1782
27760		276.8785	293.6833		319.0529
27761		327.2495	368.7653		399.6955
27762		442.2769	474.7257		492.1872
27763		530.8540	550.6485		629.3692
27764		721.7252	820.0568		916.2393
27765		931.6691	963.1935		988.2591
27766		1013.6557	1033.9982		1048.0022

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27767      1108.7981      1137.1011      1184.5308
27768      1236.4843      1242.8030      1263.9229
27769      1290.7826      1365.3484      1384.0734
27770      1401.2217      1419.3009      1420.7029
27771      1430.0890      1434.4703      1486.7326
27772      1494.2191      1515.7187      1852.7090
27773      3013.9289      3071.4687      3083.6435
27774      3136.1469      3154.9328      3162.2121
27775      3179.3560      3737.8033      3760.1562
27776      Zero-point correction (Hartree): 0.157157
27777
27778      diHPCARP_Ib.ppmpppppd
27779      -----
27780      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18253103
27781      Electronic state : 2-A
27782      Cartesian coordinates (Angs):
27783      O      0.215284      -1.822316      -1.179078
27784      O      -0.004401      -1.551984      0.200571
27785      C      0.487067      -0.260361      0.525565
27786      C      -0.269232      0.799275      -0.300505
27787      C      -1.684845      1.107132      0.184595
27788      O      -2.441118      -0.043296      0.451050
27789      O      -2.612423      -0.733432      -0.778095
27790      H      -1.966147      -1.451076      -0.689141
27791      C      0.276231      -0.116446      2.028391
27792      H      0.904297      -0.828232      2.561620
27793      H      -0.764898      -0.313394      2.272480
27794      H      0.539617      0.893672      2.342429
27795      C      1.997957      -0.212733      0.290122
27796      O      2.613626      -1.143867      -0.150741
27797      H      2.508978      0.703963      0.623521
27798      H      -0.261994      0.496592      -1.344431
27799      O      0.413390      2.071151      -0.212958
27800      O      1.426007      2.139603      -1.023976
27801      H      1.143262      -2.109051      -1.167322
27802      H      -1.645931      1.643995      1.133780
27803      H      -2.183179      1.735456      -0.556128
27804      Rotational constants (GHz):      1.1665400      0.8580400      0.6659200
27805      Vibrational harmonic frequencies (cm-1):
27806      65.1901      86.1571      92.1871
27807      140.1934      164.2927      188.4967
27808      219.3903      243.1462      255.5698
27809      265.0795      291.7759      334.9470
27810      351.8690      393.1376      396.8076
27811      470.8729      478.8277      484.4433
27812      515.4736      531.7901      627.3353
27813      690.0380      821.9293      913.6573
27814      925.7622      963.1528      991.9345
27815      1019.5988      1045.1984      1048.1066
27816      1123.2578      1140.4092      1187.6759
27817      1238.3971      1257.1338      1282.9527
27818      1294.7518      1343.4976      1376.0123
27819      1402.8408      1414.6118      1420.9051
27820      1427.1160      1435.9534      1483.7537
27821      1493.4101      1515.7660      1851.8827
27822      3017.6078      3071.2937      3075.4607
27823      3124.3314      3150.4470      3154.0498
27824      3172.3773      3727.7331      3763.8337
27825      Zero-point correction (Hartree): 0.157111
27826
27827      diHPCARP_Ib.ppmmpptpd
27828      -----
27829      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18134265
27830      Electronic state : 2-A
27831      Cartesian coordinates (Angs):
27832      O      0.918864      -1.603391      -1.257316
27833      O      0.745014      -1.442215      0.145628
27834      C      0.715578      -0.063163      0.473191
27835      C      -0.468745      0.618444      -0.236430
27836      C      -1.845084      0.315182      0.360058
27837      O      -2.062044      -1.049563      0.596118
27838      O      -2.052496      -1.705039      -0.663745

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27839	H	-1.176818	-2.121106	-0.660539	
27840	C	0.616661	-0.018063	1.993947	
27841	H	1.519934	-0.434320	2.436520	
27842	H	-0.238282	-0.606987	2.318311	
27843	H	0.496801	1.012364	2.327835	
27844	C	2.041562	0.590188	0.088001	
27845	O	2.946028	-0.020962	-0.410824	
27846	H	2.140600	1.658015	0.339859	
27847	H	-0.438921	0.377075	-1.296488	
27848	O	-0.264525	2.044196	-0.105488	
27849	O	-0.981611	2.713423	-0.959275	
27850	H	1.884601	-1.546002	-1.334140	
27851	H	-1.934103	0.787804	1.339564	
27852	H	-2.607484	0.726041	-0.304307	
27853	Rotational constants (GHz):		1.0593700	0.8841000	0.6427900
27854	Vibrational harmonic frequencies (cm-1):				
27855		60.0563	74.0256		102.9142
27856		105.1977	165.1799		179.8873
27857		214.4062	240.9699		246.0251
27858		266.4525	296.0762		316.4260
27859		334.6984	361.2116		433.5868
27860		446.2040	461.1257		477.9609
27861		500.6002	529.9823		593.0129
27862		721.9905	829.6964		916.7974
27863		925.4621	962.9398		988.9994
27864		1016.0415	1047.7435		1066.6420
27865		1101.8668	1141.4402		1183.0192
27866		1243.6669	1261.5002		1287.1466
27867		1293.7456	1334.6166		1380.9325
27868		1400.5459	1410.3817		1418.2972
27869		1422.2473	1429.8367		1484.1541
27870		1493.7127	1515.2186		1854.5350
27871		3017.1982	3073.5849		3076.7143
27872		3126.3104	3147.4743		3154.1435
27873		3169.4561	3742.3770		3773.0503
27874	Zero-point correction (Hartree):		0.156782		
27875	diHPCARP_Ib.pmpmpmpd				
27876	-----				
27877	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17980839				
27878	Electronic state : 2-A				
27879	Cartesian coordinates (Angs):				
27880	O	0.805265	-1.923176	-1.078776	
27881	O	0.469027	-1.507072	0.236567	
27882	C	0.622972	-0.100021	0.365445	
27883	C	-0.318874	0.607987	-0.634317	
27884	C	-1.813372	0.617030	-0.309020	
27885	O	-2.406569	-0.638616	-0.532540	
27886	O	-2.308811	-1.411506	0.653955	
27887	H	-1.486075	-1.903819	0.503533	
27888	C	0.338863	0.192534	1.834524	
27889	H	1.083202	-0.308651	2.451729	
27890	H	-0.648383	-0.177947	2.100243	
27891	H	0.376907	1.264593	2.016721	
27892	C	2.079173	0.285538	0.114619	
27893	O	2.930067	-0.519246	-0.146703	
27894	H	2.318818	1.353693	0.240416	
27895	H	-0.176232	0.134921	-1.604780	
27896	O	0.127710	1.966542	-0.852388	
27897	O	-0.163967	2.752816	0.142967	
27898	H	1.770306	-1.998238	-1.003529	
27899	H	-2.021660	0.963402	0.701172	
27900	H	-2.291231	1.295704	-1.017660	
27901	Rotational constants (GHz):		1.1060600	0.8997800	0.6348100
27902	Vibrational harmonic frequencies (cm-1):				
27903		47.6883	88.7020		97.5709
27904		118.8217	152.6779		188.1486
27905		214.2987	241.0893		255.7021
27906		276.7233	291.1294		324.4974
27907		331.6236	366.9459		392.4400
27908		438.7440	489.7435		507.4604
27909		532.6486	537.5403		608.8443


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27911      736.5665      824.2925      916.2849
27912      929.2705      954.7131      983.5566
27913      1002.4046     1039.9862     1056.6121
27914      1103.8373     1136.6189     1179.6828
27915      1230.4552     1244.2186     1265.6139
27916      1295.6893     1358.5992     1381.8616
27917      1406.1369     1415.7479     1422.1178
27918      1447.0690     1461.5499     1480.7852
27919      1487.5760     1517.0846     1854.7493
27920      3012.4291     3080.7882     3088.1736
27921      3131.2607     3151.3885     3160.3015
27922      3174.6328     3734.4357     3741.3702
27923      Zero-point correction (Hartree): 0.156991
27924
27925      diHPCARP_Ib.pppmpptmd
27926      -----
27927      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17971552
27928      Electronic state : 2-A
27929      Cartesian coordinates (Angs):
27930      O      -0.903746     -1.675067     -1.224996
27931      O      -0.772995     -1.469222      0.176074
27932      C       0.410231     -0.714727      0.419395
27933      C       0.329971      0.666208     -0.242152
27934      C      -0.968439      1.441187     -0.016839
27935      O      -2.081233      0.793458     -0.615401
27936      O      -2.917149      0.249058      0.393634
27937      H      -2.485833     -0.603338      0.572351
27938      C       0.525887     -0.665867      1.935273
27939      H       0.593139     -1.680306      2.325696
27940      H      -0.354126     -0.188439      2.365333
27941      H       1.412034     -0.107406      2.226115
27942      C       1.577221     -1.521380     -0.149205
27943      O       2.475495     -1.044848     -0.774715
27944      H       1.518315     -2.600906      0.083963
27945      H       0.544244      0.580145     -1.306435
27946      O       1.389243      1.458476      0.335571
27947      O       1.687762      2.473985     -0.416554
27948      H      -1.471470     -0.925155     -1.478601
27949      H      -1.167902      1.593218      1.042582
27950      H      -0.856647      2.412945     -0.498745
27951      Rotational constants (GHz): 1.1343100 0.8672200 0.6357300
27952      Vibrational harmonic frequencies (cm-1):
27953      52.2745      84.8033      85.8758
27954      119.2104     165.0992     194.4908
27955      209.9236     219.9172     230.0127
27956      252.9877     266.5927     322.6361
27957      341.7232     384.7935     417.6761
27958      450.8991     500.9348     525.2482
27959      570.9146     577.5418     625.8950
27960      657.6654     766.4590     925.5645
27961      946.1609     968.3916     989.6677
27962      1041.8010     1048.5759     1062.2342
27963      1105.4685     1125.7037     1182.9078
27964      1233.6028     1273.2633     1281.4112
27965      1291.7904     1331.6385     1391.1126
27966      1398.6274     1407.6098     1418.9128
27967      1455.8373     1475.3366     1487.1855
27968      1495.0817     1507.3492     1883.1728
27969      2972.1042     3076.8083     3090.5175
27970      3124.4373     3147.8723     3151.9744
27971      3174.0839     3669.3116     3746.7813
27972      Zero-point correction (Hartree): 0.156979
27973
27974      diHPCARP_Ib.ppppppppd
27975      -----
27976      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17872730
27977      Electronic state : 2-A
27978      Cartesian coordinates (Angs):
27979      O       1.529903     -1.661465     -1.063957
27980      O       0.973111     -1.499699      0.235775
27981      C       0.648239     -0.138972      0.436027
27982      C      -0.291378      0.329336     -0.701135

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27983	C	-1.407253	-0.642582	-1.044332	
27984	O	-2.128433	-1.172309	0.040847	
27985	O	-2.847658	-0.102400	0.645722	
27986	H	-3.760391	-0.351648	0.455608	
27987	C	0.036740	-0.060450	1.830059	
27988	H	0.800907	-0.299535	2.568863	
27989	H	-0.782372	-0.766257	1.917504	
27990	H	-0.340827	0.943130	2.016804	
27991	C	1.922112	0.704571	0.451436	
27992	O	3.004471	0.252979	0.190236	
27993	H	1.800353	1.755523	0.757839	
27994	H	0.288307	0.480667	-1.611148	
27995	O	-0.858933	1.619603	-0.374342	
27996	O	-0.031520	2.583434	-0.645831	
27997	H	2.451018	-1.401438	-0.901816	
27998	H	-2.085405	-0.158733	-1.752061	
27999	H	-0.949893	-1.514277	-1.511517	
28000	Rotational constants (GHz):		1.2731800	0.7915100	0.6402300
28001	Vibrational harmonic frequencies (cm-1):				
28002		41.4624	63.6399		88.2253
28003		111.7097	130.7199		177.0697
28004		184.5520	204.8827		239.6769
28005		253.9148	273.4823		280.1270
28006		326.0834	340.7960		374.7752
28007		407.2020	453.9229		482.7200
28008		519.9549	546.7230		626.0449
28009		783.1631	845.9566		866.9053
28010		911.9756	931.7953		972.1039
28011		995.9978	1043.8099		1050.1375
28012		1124.8129	1155.9161		1160.8138
28013		1237.9795	1266.3085		1289.6044
28014		1326.0955	1354.4831		1377.3315
28015		1390.1755	1406.3232		1422.6396
28016		1429.8205	1435.6139		1463.6087
28017		1485.2366	1509.1120		1848.2722
28018		3016.3982	3064.8020		3083.2732
28019		3116.4820	3144.6182		3156.5548
28020		3197.7205	3741.0486		3826.2799
28021	Zero-point correction (Hartree):		0.156193		
28022					
28023	diHPCARP_Ib.pppppptpd				
28024	-----				
28025	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17938399		
28026	Electronic state : 2-A				
28027	Cartesian coordinates (Angs):				
28028	O	1.813849	-1.184870	-1.334765	
28029	O	1.312133	-1.316224	-0.009943	
28030	C	0.797010	-0.072292	0.409758	
28031	C	-0.286657	0.406685	-0.577159	
28032	C	-1.274866	-0.658343	-1.022268	
28033	O	-1.831478	-1.443145	0.004066	
28034	O	-2.662211	-0.596107	0.792439	
28035	H	-3.537964	-0.954604	0.602789	
28036	C	0.301702	-0.293366	1.835876	
28037	H	1.151207	-0.552294	2.466386	
28038	H	-0.422536	-1.101272	1.853357	
28039	H	-0.169492	0.610491	2.215814	
28040	C	1.901959	0.974542	0.462631	
28041	O	3.049831	0.736736	0.205739	
28042	H	1.578605	1.984809	0.771848	
28043	H	0.180438	0.794914	-1.483406	
28044	O	-0.938288	1.536484	0.052679	
28045	O	-1.660248	2.202507	-0.793519	
28046	H	2.712686	-0.864517	-1.160848	
28047	H	-2.060021	-0.172457	-1.606305	
28048	H	-0.736519	-1.371482	-1.646232	
28049	Rotational constants (GHz):		1.3364000	0.7313300	0.6327800
28050	Vibrational harmonic frequencies (cm-1):				
28051		51.9728	75.9099		84.6556
28052		107.9356	151.1693		167.6551
28053		180.0500	196.7739		211.5026
28054		240.4457	251.9515		282.9588

28055	319.4168	328.5485	349.0191			
28056	416.7800	448.5478	457.5286			
28057	491.4229	562.7958	645.2118			
28058	785.0801	834.9697	868.8030			
28059	916.5407	932.1442	970.7229			
28060	993.7166	1046.9606	1056.2645			
28061	1100.7341	1147.7473	1167.3954			
28062	1241.3813	1279.8225	1295.2929			
28063	1317.2377	1359.2236	1371.2729			
28064	1390.1232	1402.0095	1416.6485			
28065	1425.4723	1428.1203	1461.2499			
28066	1487.9432	1506.9324	1857.5412			
28067	2981.8372	3070.8582	3085.2598			
28068	3098.5467	3143.4106	3161.9635			
28069	3192.6407	3749.5023	3823.6881			
28070	Zero-point correction (Hartree): 0.155807					
28071						
28072	diHPCARP_Ib.pptpmpd					
28073	-----					
28074	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18197668					
28075	Electronic state : 2-A					
28076	Cartesian coordinates (Angs):					
28077	O	1.352744	-1.932164	-0.501262		
28078	O	1.546910	-1.130536	0.656242		
28079	C	1.101507	0.177717	0.380473		
28080	C	-0.373912	0.155366	-0.069062		
28081	C	-1.232175	-0.778642	0.778102		
28082	O	-2.603463	-0.589146	0.539030		
28083	O	-2.870354	-0.984139	-0.798729		
28084	H	-2.917102	-0.121932	-1.238103		
28085	C	1.329811	0.956600	1.670886		
28086	H	2.377120	0.864964	1.953201		
28087	H	0.716019	0.553395	2.473130		
28088	H	1.082810	2.006775	1.533929		
28089	C	1.942951	0.813333	-0.717816		
28090	O	2.880297	0.266875	-1.227722		
28091	H	1.632910	1.830899	-1.018746		
28092	H	-0.462012	-0.118041	-1.119030		
28093	O	-0.854586	1.513171	0.049647		
28094	O	-1.848436	1.754231	-0.751475		
28095	H	2.182596	-1.774388	-0.977578		
28096	H	-0.933773	-1.806792	0.571392		
28097	H	-1.112553	-0.567452	1.840462		
28098	Rotational constants (GHz):			1.4088100	0.6632600	0.5848500
28099	Vibrational harmonic frequencies (cm-1):					
28100		55.9976		73.3909		105.7331
28101		136.0156		146.7838		182.4468
28102		197.3286		211.3786		227.6459
28103		266.0616		273.6303		299.1729
28104		317.7069		373.9178		416.1750
28105		443.4672		456.0543		470.2287
28106		480.3619		545.8351		585.6642
28107		762.4109		857.8728		883.2722
28108		922.9107		958.3692		975.1164
28109		1004.8222		1049.3939		1073.4189
28110		1097.3633		1143.6302		1177.0387
28111		1235.7769		1278.9314		1296.6578
28112		1305.7394		1345.8641		1365.9711
28113		1407.0000		1410.6320		1417.3486
28114		1428.2632		1433.7752		1467.8550
28115		1491.7530		1503.6374		1862.5435
28116		2975.1978		3084.3825		3091.5860
28117		3127.8059		3150.3087		3163.8674
28118		3173.5149		3758.4794		3770.6075
28119	Zero-point correction (Hartree): 0.156551					
28120						
28121	diHPCARP_Ib.ptpmpmd					
28122	-----					
28123	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18137020					
28124	Electronic state : 2-A					
28125	Cartesian coordinates (Angs):					
28126	O	2.627244	0.286861	0.470691		

28127	O	2.077216	-0.604397	-0.490462	
28128	C	0.681000	-0.740083	-0.249403	
28129	C	-0.094365	0.454774	-0.835716	
28130	C	-1.549515	0.205030	-1.219975	
28131	O	-2.322012	-0.486126	-0.276696	
28132	O	-2.687276	0.429473	0.743998	
28133	H	-1.993029	0.252977	1.403749	
28134	C	0.313497	-2.037766	-0.967208	
28135	H	0.951058	-2.838271	-0.596792	
28136	H	0.492123	-1.927999	-2.036809	
28137	H	-0.729413	-2.289262	-0.791319	
28138	C	0.511926	-0.970247	1.247521	
28139	O	-0.407633	-0.590014	1.914027	
28140	H	1.324283	-1.580249	1.675583	
28141	H	0.441145	0.760087	-1.736766	
28142	O	-0.060665	1.608735	0.048177	
28143	O	0.946401	2.388421	-0.189851	
28144	H	2.529854	1.151414	0.042083	
28145	H	-2.017369	1.161650	-1.459175	
28146	H	-1.560115	-0.424216	-2.110937	
28147	Rotational constants (GHz):				1.2673700 0.8275700 0.7182400
28148	Vibrational harmonic frequencies (cm-1):				
28149		68.8656	77.9975	108.1714	
28150		137.3845	159.5632	194.1442	
28151		219.1215	240.3980	256.9985	
28152		272.1305	293.2410	330.1174	
28153		349.6459	367.9153	420.7967	
28154		453.7282	484.2778	502.3131	
28155		562.1418	589.3566	621.1517	
28156		673.5529	859.5647	875.0543	
28157		930.5082	956.7298	979.5271	
28158		1001.6361	1035.2915	1057.4572	
28159		1111.8795	1152.3885	1181.4091	
28160		1204.7006	1282.2299	1303.7299	
28161		1316.0272	1348.5200	1364.8815	
28162		1401.1523	1408.6317	1429.3701	
28163		1439.7540	1465.0681	1478.6574	
28164		1501.4599	1505.4522	1872.2869	
28165		3014.4277	3075.3076	3078.3851	
28166		3096.9688	3130.5518	3151.0178	
28167		3176.7873	3672.9696	3744.4001	
28168	Zero-point correction (Hartree):				0.157164
28169	diHPCARP_Ib.ptppmttmd				
28171	-----				
28172	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.18020668
28173	Electronic state :				2-A
28174	Cartesian coordinates (Angs):				
28175	O	2.537621	0.875437	0.563494	
28176	O	2.238156	-0.003772	-0.512703	
28177	C	0.926050	-0.530088	-0.322297	
28178	C	-0.121064	0.499457	-0.760801	
28179	C	-1.494567	-0.021523	-1.169180	
28180	O	-2.060872	-0.976206	-0.314503	
28181	O	-2.582986	-0.291797	0.814178	
28182	H	-1.852660	-0.406231	1.447598	
28183	C	0.886496	-1.769636	-1.211349	
28184	H	1.705219	-2.432466	-0.937862	
28185	H	1.014750	-1.478643	-2.253788	
28186	H	-0.061007	-2.289404	-1.089229	
28187	C	0.854155	-0.994128	1.129438	
28188	O	-0.112176	-0.956226	1.834579	
28189	H	1.806783	-1.428160	1.476459	
28190	H	0.294401	1.020368	-1.627025	
28191	O	-0.227300	1.498221	0.288346	
28192	O	-0.775879	2.587837	-0.154376	
28193	H	2.212422	1.731674	0.253132	
28194	H	-2.162552	0.834062	-1.283414	
28195	H	-1.396279	-0.523653	-2.132866	
28196	Rotational constants (GHz):				1.2102000 0.8408600 0.7124200
28197	Vibrational harmonic frequencies (cm-1):				
28198		51.3256	79.4859	98.8972	

28199	133.2404	161.3064	177.0328		
28200	194.8935	220.3049	246.3707		
28201	265.2848	291.3375	313.9937		
28202	330.4723	351.7894	367.7154		
28203	381.6963	472.5442	536.4120		
28204	563.0143	582.3980	603.2362		
28205	700.3628	857.4634	865.8984		
28206	928.8132	956.7750	986.6801		
28207	994.2717	1043.0173	1059.1799		
28208	1098.2171	1150.1973	1181.2549		
28209	1207.0170	1286.4108	1297.2571		
28210	1309.1576	1349.1541	1365.4901		
28211	1402.4634	1405.0105	1410.5040		
28212	1431.7211	1464.1709	1473.4303		
28213	1501.0766	1504.7842	1876.1123		
28214	3006.0106	3073.0709	3074.9756		
28215	3083.3592	3129.7147	3151.5162		
28216	3172.7496	3664.2035	3793.5659		
28217	Zero-point correction (Hartree): 0.156460				
28218					
28219	diHPCARP_Ib.tmmptmmd				
28220	-----				
28221	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18069710				
28222	Electronic state : 2-A				
28223	Cartesian coordinates (Angs):				
28224	O	-2.155909	-1.333874	-1.230787	
28225	O	-1.294954	-0.212479	-1.008835	
28226	C	-0.664599	-0.433972	0.240349	
28227	C	0.225110	0.791611	0.495859	
28228	C	1.130320	1.140964	-0.679635	
28229	O	1.950544	0.037938	-0.998700	
28230	O	2.929899	-0.084939	0.022533	
28231	H	2.641294	-0.888299	0.487381	
28232	C	-1.667545	-0.638059	1.370219	
28233	H	-2.239785	-1.547660	1.209050	
28234	H	-2.348013	0.209433	1.409099	
28235	H	-1.132162	-0.720768	2.314386	
28236	C	0.256944	-1.646502	0.130556	
28237	O	1.005475	-1.968144	1.016821	
28238	H	0.185346	-2.212133	-0.810376	
28239	H	0.827807	0.560784	1.373982	
28240	O	-0.548121	1.932697	0.906314	
28241	O	-1.106842	2.545884	-0.097302	
28242	H	-2.142387	-1.368029	-2.194591	
28243	H	0.547461	1.333013	-1.576256	
28244	H	1.738329	2.012740	-0.437106	
28245	Rotational constants (GHz): 1.0733800			0.9006000	0.6674200
28246	Vibrational harmonic frequencies (cm-1):				
28247	52.6150	95.2340	112.6364		
28248	125.6269	149.7235	174.2340		
28249	183.8863	186.5344	221.8221		
28250	233.0783	255.8243	283.6858		
28251	307.0545	336.8182	350.3595		
28252	413.7063	446.2250	483.2387		
28253	510.6142	579.6156	613.1442		
28254	703.0840	756.9147	910.2692		
28255	950.9593	965.9063	988.2384		
28256	1024.1334	1033.1139	1061.1784		
28257	1121.2782	1139.8642	1198.3360		
28258	1213.9817	1242.2621	1245.8591		
28259	1286.3144	1349.1252	1377.9453		
28260	1400.8769	1413.0980	1421.1198		
28261	1431.4711	1462.8891	1486.4565		
28262	1489.6701	1506.3957	1834.4744		
28263	3036.2906	3086.7615	3096.2164		
28264	3126.5229	3168.1323	3175.6559		
28265	3176.7189	3711.4180	3844.5101		
28266	Zero-point correction (Hartree): 0.156175				
28267					
28268	diHPCARP_Ib.tmmptmpd				
28269	-----				
28270	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18172930				

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28271 Electronic state : 2-A
28272 Cartesian coordinates (Angs):
28273 O -2.062740 -1.372952 -1.326128
28274 O -1.285349 -0.221548 -1.020990
28275 C -0.656023 -0.439686 0.233781
28276 C 0.223987 0.791399 0.493336
28277 C 1.123800 1.153807 -0.682390
28278 O 1.959778 0.062004 -0.997572
28279 O 2.932663 -0.049868 0.031542
28280 H 2.659499 -0.866331 0.482302
28281 C -1.652262 -0.658150 1.365515
28282 H -2.208272 -1.579414 1.209923
28283 H -2.342751 0.181792 1.414317
28284 H -1.115309 -0.735444 2.309180
28285 C 0.275352 -1.645628 0.116153
28286 O 1.021035 -1.966708 1.005136
28287 H 0.208605 -2.204257 -0.829031
28288 H 0.831642 0.563541 1.368772
28289 O -0.558478 1.923886 0.911876
28290 O -1.159440 2.510694 -0.083074
28291 H -2.960136 -1.023152 -1.261197
28292 H 0.538948 1.334485 -1.580132
28293 H 1.718897 2.034276 -0.438818
28294 Rotational constants (GHz): 1.0762800 0.8998600 0.6689600
28295 Vibrational harmonic frequencies (cm-1):
28296 52.6018 96.8201 110.9981
28297 123.0866 172.6121 182.6666
28298 186.1878 216.6228 227.3099
28299 247.9322 257.8561 283.7853
28300 306.7548 335.7208 350.4281
28301 416.8522 443.4979 483.2453
28302 510.6610 579.1183 617.1599
28303 704.7636 760.8396 910.2903
28304 951.2002 966.4037 989.9098
28305 1023.4486 1034.2287 1056.6294
28306 1121.1050 1137.3173 1201.4573
28307 1217.3202 1241.1885 1246.5045
28308 1286.5216 1351.1710 1379.9614
28309 1397.5094 1405.2471 1416.8274
28310 1426.0031 1462.2266 1487.2425
28311 1489.8755 1508.9818 1834.0165
28312 3042.4471 3082.4508 3095.1693
28313 3127.2226 3163.5988 3168.2131
28314 3176.2662 3714.4746 3822.2670
28315 Zero-point correction (Hartree): 0.156287
28316
28317 diHPCARP_Ib.tmmmpmpd
28318 -----
28319 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18166884
28320 Electronic state : 2-A
28321 Cartesian coordinates (Angs):
28322 O -2.016654 -1.815063 -0.981334
28323 O -1.142672 -0.694344 -1.126237
28324 C -0.694577 -0.349020 0.175535
28325 C 0.174160 0.902672 -0.015327
28326 C 1.229333 0.737950 -1.103082
28327 O 2.029444 -0.395781 -0.851127
28328 O 2.908673 -0.069981 0.215002
28329 H 2.530160 -0.571913 0.956770
28330 C -1.846139 -0.095546 1.139977
28331 H -2.403682 -1.012857 1.310274
28332 H -2.514329 0.654493 0.722544
28333 H -1.448486 0.262135 2.087683
28334 C 0.200709 -1.460140 0.712725
28335 O 0.840431 -1.341072 1.725413
28336 H 0.213891 -2.386405 0.118295
28337 H 0.629156 1.144202 0.943978
28338 O -0.637374 2.021351 -0.409664
28339 O -1.007281 2.747995 0.603670
28340 H -1.791213 -2.313241 -1.775920
28341 H 0.758480 0.550806 -2.066751
28342 H 1.848577 1.632446 -1.161613

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28343	Rotational constants (GHz):	1.0187500	0.8804800	0.6702300
28344	Vibrational harmonic frequencies (cm-1):			
28345	61.2921	79.7703		105.6881
28346	128.0073	172.7584		183.0544
28347	188.0477	209.3006		214.7895
28348	245.2260	253.5585		278.2319
28349	323.6748	348.1002		384.8842
28350	402.4586	435.0032		443.7053
28351	519.7583	577.1017		624.1912
28352	650.9240	759.1436		911.4185
28353	953.5886	966.5883		989.1997
28354	1024.9760	1059.1325		1064.1180
28355	1118.0823	1146.5862		1198.4803
28356	1214.6855	1243.1613		1280.2723
28357	1289.4324	1339.0549		1368.2704
28358	1401.3264	1411.3618		1416.3345
28359	1425.5947	1466.6509		1484.3269
28360	1487.8098	1507.1115		1834.4083
28361	3025.5536	3087.4165		3096.2268
28362	3132.5851	3158.4661		3170.8064
28363	3173.9617	3702.3876		3840.8201
28364	Zero-point correction (Hartree):	0.156234		
28365				
28366	diHPCARP_Ib.tmmmpptppd			
28367	-----			
28368	E(UM062X/Aug-CC-pVTZ) (Hartree):	-722.18271869		
28369	Electronic state : 2-A			
28370	Cartesian coordinates (Angs):			
28371	O	-1.948335	-1.842067	-1.058131
28372	O	-1.163796	-0.660717	-1.135270
28373	C	-0.689020	-0.353429	0.169992
28374	C	0.182611	0.898188	-0.005423
28375	C	1.232365	0.750418	-1.100968
28376	O	2.043586	-0.376852	-0.859537
28377	O	2.907193	-0.057436	0.221704
28378	H	2.542424	-0.598103	0.942677
28379	C	-1.814159	-0.122358	1.169323
28380	H	-2.367665	-1.043854	1.335001
28381	H	-2.488666	0.646929	0.797113
28382	H	-1.393473	0.205702	2.117665
28383	C	0.211129	-1.487577	0.653402
28384	O	0.844904	-1.409607	1.674042
28385	H	0.227505	-2.383371	0.014993
28386	H	0.644465	1.125533	0.954061
28387	O	-0.633109	2.022960	-0.377223
28388	O	-1.008428	2.725887	0.650778
28389	H	-2.839920	-1.496231	-1.191511
28390	H	0.759497	0.562664	-2.063366
28391	H	1.842151	1.651934	-1.155486
28392	Rotational constants (GHz):	1.0207500	0.8811200	0.6698800
28393	Vibrational harmonic frequencies (cm-1):			
28394	62.8397	81.9891		107.3588
28395	127.4655	172.7136		183.2286
28396	190.3907	214.9754		246.2978
28397	254.4634	277.4176		286.4481
28398	324.4393	348.2291		385.2344
28399	404.2564	436.6587		443.2610
28400	518.3207	580.4129		624.5742
28401	652.6722	760.6963		911.5217
28402	955.1852	966.4953		992.1520
28403	1025.4647	1058.1069		1060.4806
28404	1118.9041	1144.9138		1200.1370
28405	1218.7107	1242.1156		1280.8855
28406	1291.1497	1338.3729		1373.7145
28407	1398.6513	1408.7405		1410.9041
28408	1416.6339	1464.7604		1485.5020
28409	1487.9365	1509.2876		1833.1721
28410	3039.5212	3082.0514		3094.8982
28411	3133.0994	3159.3918		3163.5525
28412	3167.2454	3705.5657		3816.1765
28413	Zero-point correction (Hartree):	0.156373		
28414				

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28415 diHPCARP_Ib.tmmmpptmd
28416 -----
28417 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18164034
28418 Electronic state : 2-A
28419 Cartesian coordinates (Angs):
28420 O -2.731129 -0.275719 -1.050522
28421 O -1.396610 0.233397 -1.081047
28422 C -0.858423 0.048636 0.218964
28423 C 0.542871 0.659528 0.171749
28424 C 1.390240 0.150349 -0.989159
28425 O 1.477316 -1.257064 -0.963262
28426 O 2.356571 -1.613792 0.092916
28427 H 1.745123 -1.972221 0.758181
28428 C -1.712416 0.695865 1.303391
28429 H -2.686338 0.216520 1.355457
28430 H -1.844198 1.752262 1.082403
28431 H -1.211918 0.581960 2.263412
28432 C -0.705133 -1.444375 0.496000
28433 O -0.146545 -1.862707 1.476372
28434 H -1.150664 -2.114200 -0.254882
28435 H 1.033519 0.459427 1.123852
28436 O 0.403811 2.087350 0.040719
28437 O 1.494830 2.698485 0.395170
28438 H -2.791968 -0.653206 -1.936109
28439 H 0.915034 0.392041 -1.938680
28440 H 2.382624 0.597787 -0.942072
28441 Rotational constants (GHz): 1.0041400 0.8945700 0.6463600
28442 Vibrational harmonic frequencies (cm-1):
28443 57.9799 77.8970 107.4325
28444 115.3874 163.4098 168.4582
28445 186.3054 191.2958 215.2735
28446 229.9789 254.0865 276.6433
28447 318.6766 331.3518 371.0573
28448 413.7781 434.6200 461.7375
28449 496.1069 571.9789 625.5604
28450 649.2678 781.2953 911.8552
28451 954.0306 966.6526 987.8644
28452 1023.2483 1058.7468 1081.2221
28453 1108.2252 1135.1974 1195.8006
28454 1220.0137 1252.6258 1281.9079
28455 1288.6780 1333.8533 1374.6573
28456 1398.7986 1405.7487 1415.1255
28457 1426.4883 1465.0705 1484.6517
28458 1490.6148 1505.8289 1836.9824
28459 3027.6789 3088.1877 3096.4613
28460 3123.5688 3158.8513 3169.3407
28461 3178.5314 3713.7836 3841.7243
28462 Zero-point correction (Hartree): 0.156058
28463
28464 diHPCARP_Ib.tmmmpptpd
28465 -----
28466 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18260026
28467 Electronic state : 2-A
28468 Cartesian coordinates (Angs):
28469 O -2.675274 -0.425334 -1.129408
28470 O -1.408230 0.215031 -1.081611
28471 C -0.857007 0.010784 0.213402
28472 C 0.522945 0.668853 0.174729
28473 C 1.390331 0.204379 -0.990129
28474 O 1.543092 -1.196868 -0.967828
28475 O 2.417708 -1.515965 0.104640
28476 H 1.814375 -1.931487 0.743435
28477 C -1.719395 0.594148 1.325632
28478 H -2.675320 0.078233 1.376730
28479 H -1.883375 1.655210 1.148685
28480 H -1.208903 0.463353 2.278068
28481 C -0.655404 -1.486559 0.440585
28482 O -0.106116 -1.913425 1.422783
28483 H -1.058767 -2.143340 -0.344151
28484 H 1.021320 0.476496 1.124358
28485 O 0.328032 2.092414 0.060744
28486 O 1.390222 2.744136 0.430036

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28487      H      -3.276975      0.329566      -1.147472
28488      H      0.902851      0.423937      -1.938611
28489      H      2.360505      0.698484      -0.941198
28490      Rotational constants (GHz):      1.0044000      0.8963500      0.6455000
28491      Vibrational harmonic frequencies (cm-1):
28492      59.6297      79.5452      107.7675
28493      114.6196      167.5297      184.5223
28494      186.7252      217.9830      227.5748
28495      253.4779      275.5120      290.7374
28496      319.7679      333.9135      370.9863
28497      418.1481      439.1689      464.2237
28498      496.2251      573.5266      626.7076
28499      652.3180      781.7316      912.1589
28500      955.2485      967.7977      991.1779
28501      1022.9211      1055.6936      1079.2211
28502      1108.3586      1134.2270      1199.5856
28503      1224.0363      1249.4935      1282.7056
28504      1290.2281      1332.8073      1380.4747
28505      1396.9644      1405.4279      1410.0714
28506      1415.2916      1464.7285      1484.6986
28507      1491.6161      1508.4337      1835.7050
28508      3038.3123      3083.2650      3095.7578
28509      3123.7651      3159.8116      3164.6100
28510      3168.3871      3714.1250      3815.8974
28511      Zero-point correction (Hartree): 0.156294
28512
28513
28514
28515      (2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)
28516      =====
28517
28518      diHPCARP_Ic.mmppttpd
28519      -----
28520      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18275343
28521      Electronic state : 2-A
28522      Cartesian coordinates (Angs):
28523      O      -0.135038      2.254815      0.279563
28524      O      -0.934837      1.391580      -0.507499
28525      C      -1.160039      0.169507      0.182288
28526      C      0.065989      -0.747393      0.201788
28527      C      0.824769      -0.769056      -1.123633
28528      O      1.569312      0.452812      -1.306283
28529      O      2.712680      0.424237      -0.687077
28530      H      0.751615      2.078151      -0.068289
28531      C      -1.747251      0.392108      1.571400
28532      H      -2.683557      0.943397      1.488414
28533      H      -1.050493      0.962967      2.176598
28534      H      -1.932415      -0.567778      2.051613
28535      C      -2.260514      -0.460758      -0.672098
28536      O      -2.300453      -1.618333      -0.973817
28537      H      -3.048879      0.253487      -0.966905
28538      H      -0.285591      -1.765372      0.389542
28539      O      0.898531      -0.331399      1.261948
28540      O      1.889325      -1.330252      1.448893
28541      H      2.635656      -0.943635      0.965048
28542      H      1.537657      -1.588711      -1.152480
28543      H      0.142114      -0.826636      -1.967836
28544      Rotational constants (GHz):      1.2433200      0.7616100      0.7187500
28545      Vibrational harmonic frequencies (cm-1):
28546      62.0167      87.0430      94.1277
28547      156.8662      163.6158      168.0209
28548      184.1233      210.1903      236.7075
28549      257.2048      281.0102      296.9756
28550      332.1345      361.5065      395.0782
28551      414.3537      451.1888      466.9739
28552      517.2926      549.4391      667.6400
28553      714.9717      821.0616      893.1118
28554      914.4578      967.0284      974.4590
28555      1016.6720      1040.2579      1059.1200
28556      1066.8653      1149.5323      1178.5447
28557      1222.9120      1246.7494      1272.1039
28558      1321.1668      1356.0909      1380.8957

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28559      1389.6109          1399.7948          1412.8757
28560      1434.5931          1440.9968          1482.4831
28561      1483.5072          1501.5233          1868.2185
28562      2994.1527          3076.8950          3080.9467
28563      3121.6259          3151.2518          3184.6038
28564      3188.5782          3751.6631          3778.4007
28565      Zero-point correction (Hartree): 0.156490
28566
28567      diHPCARP_Ic.mmtmptmmd
28568      -----
28569      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18525353
28570      Electronic state : 2-A
28571      Cartesian coordinates (Angs):
28572      O      1.302217      -2.046932      -0.948643
28573      O      1.250569      -0.647288      -1.154206
28574      C      1.190118      0.071590      0.072510
28575      C      -0.254525      0.365628      0.514055
28576      C      -1.093104      0.877268      -0.648318
28577      O      -2.424806      1.193832      -0.202955
28578      O      -3.179112      0.141211      -0.123097
28579      H      0.380160      -2.251704      -0.715611
28580      C      1.997726      -0.579338      1.189621
28581      H      3.007508      -0.788815      0.840678
28582      H      1.532836      -1.509865      1.499514
28583      H      2.038125      0.098094      2.041915
28584      C      1.908517      1.376936      -0.265986
28585      O      1.562685      2.453639      0.127665
28586      H      2.811027      1.232879      -0.885348
28587      H      -0.211535      1.135387      1.287221
28588      O      -0.874767      -0.712540      1.186806
28589      O      -1.154549      -1.760546      0.268877
28590      H      -2.058463      -1.527719      -0.005724
28591      H      -0.685043      1.815942      -1.014946
28592      H      -1.164903      0.152287      -1.454572
28593      Rotational constants (GHz):      1.2482200      0.7972900      0.6022200
28594      Vibrational harmonic frequencies (cm-1):
28595      57.4672          88.2672          96.2046
28596      128.4790          159.6176          188.5892
28597      212.2966          231.3710          261.5478
28598      280.8320          295.8026          308.1187
28599      321.8138          343.4764          449.8849
28600      454.5912          500.2913          533.7619
28601      577.8369          618.4898          628.5433
28602      710.8744          822.0193          897.2932
28603      926.9966          969.2241          983.6727
28604      986.2939          1013.3188          1063.6422
28605      1114.2217          1140.4116          1179.4891
28606      1222.9632          1255.0342          1260.9799
28607      1302.5763          1338.8816          1381.1718
28608      1394.6296          1402.3693          1410.6338
28609      1441.0876          1480.3317          1486.0513
28610      1486.6547          1495.4125          1863.8550
28611      2993.0562          3080.3216          3104.3710
28612      3125.3889          3156.0753          3184.5751
28613      3188.3813          3671.4734          3699.6121
28614      Zero-point correction (Hartree): 0.157127
28615
28616      diHPCARP_Ic.mmtpptmmd
28617      -----
28618      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18042893
28619      Electronic state : 2-A
28620      Cartesian coordinates (Angs):
28621      O      1.866882      -1.806493      -0.669317
28622      O      1.501262      -0.488505      -1.035453
28623      C      1.137954      0.289145      0.099362
28624      C      -0.358957      0.183053      0.430808
28625      C      -1.228553      0.469306      -0.785349
28626      O      -2.584308      0.053818      -0.537110
28627      O      -3.140267      0.765709      0.397695
28628      H      1.004567      -2.249885      -0.619605
28629      C      2.005475      -0.003810      1.319581
28630      H      3.057752      0.034953      1.042453

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28631	H	1.781668	-0.991487	1.710125	
28632	H	1.803799	0.740775	2.088720	
28633	C	1.487000	1.710951	-0.333158	
28634	O	0.844338	2.675441	-0.032029	
28635	H	2.421343	1.778632	-0.917724	
28636	H	-0.585975	0.908799	1.213179	
28637	O	-0.702634	-1.050117	1.044946	
28638	O	-0.769997	-2.073995	0.061479	
28639	H	-1.723339	-2.144732	-0.088443	
28640	H	-1.226409	1.533473	-1.008489	
28641	H	-0.913121	-0.109262	-1.649365	
28642	Rotational constants (GHz):		1.2065200	0.8158900	0.5967300
28643	Vibrational harmonic frequencies (cm-1):				
28644		49.7819	67.1736		91.3791
28645		106.7040	125.3148		171.6574
28646		215.0610	229.4993		245.3563
28647		259.1653	277.6580		301.3268
28648		328.6923	340.1427		359.7847
28649		440.5113	451.2310		488.7111
28650		544.8139	591.0081		623.6971
28651		739.3734	804.0243		903.2861
28652		927.8912	961.3898		982.2442
28653		991.2331	1005.3487		1062.6807
28654		1117.9520	1132.6434		1187.4182
28655		1221.5784	1242.7707		1262.8184
28656		1311.6119	1320.2720		1376.7737
28657		1394.7352	1399.5194		1405.0255
28658		1410.8287	1468.6454		1486.6198
28659		1496.3542	1498.0338		1864.5399
28660		2992.1413	3080.5106		3112.3596
28661		3122.1965	3156.0159		3184.5613
28662		3186.6216	3722.8641		3788.7631
28663	Zero-point correction (Hartree): 0.156351				
28664					
28665	diHPCARP_Ic.mttmptmmd				
28666	-----				
28667	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18429244				
28668	Electronic state : 2-A				
28669	Cartesian coordinates (Angs):				
28670	O	-2.005575	-1.897952	-0.483653	
28671	O	-1.975595	-0.797031	0.407025	
28672	C	-1.174564	0.235216	-0.145479	
28673	C	0.223489	-0.324230	-0.503942	
28674	C	1.278058	0.755710	-0.711300	
28675	O	2.525895	0.128538	-1.059005	
28676	O	3.164688	-0.276816	-0.003136	
28677	H	-1.356366	-2.483721	-0.067523	
28678	C	-1.834537	0.868628	-1.361452	
28679	H	-2.842259	1.186877	-1.101406	
28680	H	-1.893544	0.142597	-2.170294	
28681	H	-1.273737	1.742702	-1.687191	
28682	C	-1.097658	1.244992	0.997452	
28683	O	-0.653102	2.347714	0.840272	
28684	H	-1.490984	0.894603	1.964333	
28685	H	0.125691	-0.904433	-1.423505	
28686	O	0.641162	-1.292557	0.431399	
28687	O	0.817569	-0.653134	1.685208	
28688	H	1.774679	-0.486574	1.670227	
28689	H	1.023914	1.393338	-1.554234	
28690	H	1.443543	1.362622	0.173037	
28691	Rotational constants (GHz):		1.2920800	0.7478400	0.6541700
28692	Vibrational harmonic frequencies (cm-1):				
28693		66.3322	91.4148		120.8985
28694		132.3998	159.3177		171.1986
28695		190.0103	208.7913		219.1788
28696		246.7120	300.3474		306.2639
28697		333.8419	383.9061		400.5010
28698		436.9431	462.7755		511.0717
28699		513.8791	580.7874		659.8850
28700		671.5491	831.4140		914.7669
28701		924.7482	962.4100		999.6125
28702		1002.8045	1017.8752		1055.0093

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28703      1111.3070      1146.4837      1186.1048
28704      1202.6673      1252.1169      1254.0401
28705      1318.4312      1334.0149      1388.2976
28706      1399.6374      1408.0590      1418.7097
28707      1426.4040      1434.3596      1477.2899
28708      1488.5469      1503.8543      1857.9874
28709      3024.3769      3079.9995      3103.1827
28710      3130.2226      3159.9951      3164.8898
28711      3196.1290      3720.5926      3777.1321
28712 Zero-point correction (Hartree): 0.156832
28713
28714 diHPCARP_Ic.mtptptmmd
28715 -----
28716 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18108150
28717 Electronic state : 2-A
28718 Cartesian coordinates (Angs):
28719 O      -1.731347      -2.013625      -0.567002
28720 O      -1.999972      -0.752795      0.019466
28721 C      -1.018519      0.180227      -0.404614
28722 C      0.392064      -0.348920      -0.062451
28723 C      1.473237      0.714773      -0.064330
28724 O      2.767513      0.083568      0.020027
28725 O      3.052999      -0.560250      -1.069946
28726 H      -1.286481      -2.463874      0.165650
28727 C      -1.140846      0.484037      -1.891568
28728 H      -2.159606      0.796514      -2.113605
28729 H      -0.912510      -0.409080      -2.469706
28730 H      -0.464947      1.288232      -2.174477
28731 C      -1.361779      1.424890      0.409079
28732 O      -0.798127      2.469596      0.239162
28733 H      -2.171219      1.299555      1.145891
28734 H      0.657794      -1.105655      -0.802911
28735 O      0.380753      -1.085647      1.146849
28736 O      -0.081959      -0.221302      2.178846
28737 H      0.691905      -0.170779      2.754212
28738 H      1.446723      1.317941      -0.967961
28739 H      1.414529      1.360740      0.806999
28740 Rotational constants (GHz):      1.1450500      0.7362900      0.6845200
28741 Vibrational harmonic frequencies (cm-1):
28742      51.4133      71.2301      115.5145
28743      121.0371      148.5357      158.4193
28744      189.6480      203.7982      215.2221
28745      251.7788      271.7080      296.3990
28746      301.3570      332.7648      382.3034
28747      391.4568      442.5030      462.3205
28748      497.6893      585.4233      658.9685
28749      672.2821      835.2411      915.9107
28750      926.3640      965.3893      984.9052
28751      1003.2919      1015.7174      1056.7091
28752      1123.2015      1133.0804      1182.3024
28753      1201.8559      1246.3438      1262.1806
28754      1310.4192      1321.6242      1376.6839
28755      1398.6197      1403.4547      1414.0059
28756      1418.7708      1430.9544      1473.2492
28757      1489.0176      1503.5950      1859.8742
28758      3014.7980      3081.7454      3108.3054
28759      3130.0085      3160.4676      3169.2843
28760      3192.1356      3780.6329      3818.8759
28761 Zero-point correction (Hartree): 0.156125
28762
28763 diHPCARP_Ic.mtptptmpd
28764 -----
28765 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18209198
28766 Electronic state : 2-A
28767 Cartesian coordinates (Angs):
28768 O      -1.807544      -1.791919      -0.931514
28769 O      -1.992130      -0.640774      -0.128207
28770 C      -0.951380      0.295994      -0.397066
28771 C      0.411567      -0.359552      -0.078448
28772 C      1.527532      0.621096      0.226616
28773 O      2.797769      -0.055601      0.133368
28774 O      3.069045      -0.377081      -1.093943

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28775	H	-1.282780	-2.356440	-0.343906			
28776	C	-0.997728	0.803065	-1.829860			
28777	H	-1.967431	1.254468	-2.031937			
28778	H	-0.840328	-0.024540	-2.517571			
28779	H	-0.226963	1.556198	-1.982311			
28780	C	-1.274686	1.439891	0.559833			
28781	O	-0.652069	2.462405	0.570917			
28782	H	-2.143112	1.273998	1.221537			
28783	H	0.712685	-0.958594	-0.940660			
28784	O	0.273519	-1.321547	0.952878			
28785	O	-0.236569	-0.658754	2.102962			
28786	H	-1.167883	-0.922835	2.073749			
28787	H	1.539051	1.457957	-0.466592			
28788	H	1.468770	0.982993	1.249538			
28789	Rotational constants (GHz):				1.1441600	0.7393500	0.6843300
28790	Vibrational harmonic frequencies (cm-1):						
28791		61.4041	69.4622			115.2976	
28792		123.4532	152.0772			162.0309	
28793		199.2704	206.1261			210.0233	
28794		253.1852	282.6376			303.0555	
28795		337.6007	374.1338			391.4475	
28796		405.6699	455.9261			463.3058	
28797		501.3411	588.3320			657.9722	
28798		675.1613	845.9860			910.1960	
28799		930.4817	965.0270			986.1896	
28800		1001.1452	1013.1692			1057.0460	
28801		1122.8907	1132.9650			1181.4389	
28802		1197.0535	1248.0168			1261.0574	
28803		1313.9968	1326.3740			1385.0229	
28804		1400.5033	1411.7400			1418.7138	
28805		1419.6476	1436.9684			1470.6597	
28806		1485.3125	1504.1011			1868.3576	
28807		2985.3731	3081.8842			3097.9003	
28808		3127.9405	3160.5648			3171.0955	
28809		3191.9742	3757.7064			3774.3664	
28810	Zero-point correction (Hartree):				0.156355		
28811	diHPCARP_Ic.pmmmpmmpd						
28812	-----						
28813	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18224011						
28814	Electronic state : 2-A						
28815	Cartesian coordinates (Angs):						
28816	O	0.585633	0.835843	-1.833310			
28817	O	1.214515	1.098840	-0.585320			
28818	C	0.363542	0.709687	0.480662			
28819	C	0.195611	-0.824288	0.585974			
28820	C	-0.631632	-1.510477	-0.496551			
28821	O	-1.957275	-0.945606	-0.508744			
28822	O	-2.610875	-1.232625	0.578133			
28823	H	0.031084	1.627297	-1.928225			
28824	C	1.079761	1.224779	1.730238			
28825	H	1.261765	2.292814	1.632392			
28826	H	2.025900	0.700736	1.845320			
28827	H	0.470270	1.043871	2.614765			
28828	C	-0.961880	1.452269	0.411428			
28829	O	-1.180691	2.323504	-0.384075			
28830	H	-1.698167	1.180961	1.188011			
28831	H	-0.294510	-1.024787	1.542663			
28832	O	1.452896	-1.451656	0.715956			
28833	O	2.059929	-1.571654	-0.565512			
28834	H	2.369795	-0.669035	-0.737534			
28835	H	-0.241462	-1.344289	-1.491636			
28836	H	-0.710154	-2.572552	-0.273292			
28837	Rotational constants (GHz):				1.0321500	0.9608900	0.7165900
28838	Vibrational harmonic frequencies (cm-1):						
28839		35.8699	76.3932			124.7225	
28840		134.0937	159.4926			190.6279	
28841		216.3729	220.3445			231.9252	
28842		271.6498	298.0233			320.7625	
28843		358.6886	362.8271			387.7320	
28844		435.3683	468.7911			500.8965	
28845		519.3076	599.4238			605.8516	

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28847      734.1990      833.9197      899.0398
28848      935.6538      958.4227      986.7676
28849      997.6162      1046.3798      1052.9694
28850     1119.4476      1127.2469      1191.4875
28851     1202.4398      1236.8736      1277.3043
28852     1302.2790      1333.5516      1384.9063
28853     1400.8820      1406.4287      1423.1608
28854     1437.1436      1446.0676      1489.9352
28855     1492.2040      1502.4996      1853.7636
28856     2991.5021      3077.9801      3082.7545
28857     3123.2255      3158.4724      3170.9487
28858     3229.0661      3736.5602      3757.3862
28859 Zero-point correction (Hartree): 0.157011
28860
28861 diHPCARP_Ic.pmpmtttd
28862 -----
28863 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18436804
28864 Electronic state : 2-A
28865 Cartesian coordinates (Angs):
28866 O      -1.001876      -1.940505      -0.733947
28867 O      -0.994195      -0.651885      -1.342296
28868 C      -1.096847      0.328858      -0.322565
28869 C       0.207460      0.627028      0.425762
28870 C       0.895220      -0.558141      1.097819
28871 O       1.525864      -1.426824      0.131928
28872 O       2.683537      -0.984673      -0.255413
28873 H      -0.084549      -2.221653      -0.859184
28874 C      -1.606870      1.573392      -1.045091
28875 H      -2.615244      1.396436      -1.415907
28876 H      -0.952412      1.795923      -1.883908
28877 H      -1.611033      2.422987      -0.364894
28878 C      -2.182676      -0.115258      0.650695
28879 O      -2.141548      0.071432      1.833029
28880 H      -3.044259      -0.596792      0.155986
28881 H      -0.050310      1.319803      1.232523
28882 O       1.061446      1.263288      -0.497559
28883 O       2.163564      1.797612      0.217317
28884 H       2.829797      1.107724      0.070699
28885 H       1.676839      -0.210860      1.768077
28886 H       0.179105      -1.176397      1.632425
28887 Rotational constants (GHz): 1.2645000 0.7885400 0.6763600
28888 Vibrational harmonic frequencies (cm-1):
28889      60.4919      96.4777      116.4268
28890     158.5622     163.4335     184.3607
28891     209.6677     224.8395     234.8563
28892     259.5383     280.3371     308.6813
28893     319.5078     351.0496     394.9812
28894     454.1147     487.9563     517.2157
28895     538.7360     562.2017     625.7883
28896     711.2216     814.0684     891.6137
28897     935.2048     963.8468     978.1692
28898    1017.7867    1041.1848    1052.2381
28899    1072.4899    1149.7524    1178.9413
28900    1239.7832    1250.5236    1266.9594
28901    1325.3555    1359.3665    1380.8721
28902    1395.6553    1403.2091    1415.8163
28903    1422.3267    1444.8883    1481.8200
28904    1487.1831    1500.8222    1866.6009
28905    2993.6529    3068.8371    3080.1251
28906    3124.9859    3159.7020    3172.9712
28907    3188.5880    3748.4196    3787.9504
28908 Zero-point correction (Hartree): 0.157016
28909
28910 diHPCARP_Ic.pmtmmtmmd
28911 -----
28912 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18481813
28913 Electronic state : 2-A
28914 Cartesian coordinates (Angs):
28915 O       0.792610      -1.100212      -1.768563
28916 O       1.408891      -1.295120      -0.503878
28917 C       1.253948      -0.120830      0.260304
28918 C      -0.221380      0.225117      0.584799

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28919	C	-1.006087	0.957536	-0.497109		
28920	O	-2.285597	1.353745	0.039717		
28921	O	-3.153142	0.389280	0.010897		
28922	H	-0.040079	-1.576186	-1.617252		
28923	C	2.000096	-0.435639	1.556632		
28924	H	3.017975	-0.749965	1.332649		
28925	H	1.483498	-1.243001	2.072221		
28926	H	2.028321	0.448675	2.190134		
28927	C	1.994461	1.017495	-0.422623		
28928	O	1.779939	2.176375	-0.200367		
28929	H	2.793752	0.682974	-1.108304		
28930	H	-0.203712	0.883419	1.456594		
28931	O	-0.907072	-0.914280	1.068811		
28932	O	-1.298283	-1.749671	-0.013366		
28933	H	-2.210442	-1.441417	-0.145807		
28934	H	-0.507716	1.887629	-0.751721		
28935	H	-1.186589	0.364867	-1.386536		
28936	Rotational constants (GHz):			1.3101400	0.7610800	0.6420500
28937	Vibrational harmonic frequencies (cm-1):					
28938		76.0225	95.8343			113.5586
28939		141.5155	175.3831			192.3206
28940		202.9681	214.8259			230.9488
28941		267.4294	278.4073			302.1831
28942		315.8492	342.9187			378.4958
28943		501.9520	523.6224			549.8253
28944		567.3294	573.3247			603.9204
28945		712.8825	838.3753			908.1784
28946		938.1859	967.7331			975.6244
28947		978.8265	1011.8006			1059.3849
28948		1109.0448	1135.4586			1181.6216
28949		1248.2310	1255.2444			1261.1124
28950		1312.2623	1342.7521			1375.0471
28951		1394.8198	1403.6395			1409.4297
28952		1439.3140	1458.5982			1486.8148
28953		1490.5138	1502.3223			1861.3533
28954		2983.2434	3077.5847			3092.1067
28955		3148.6643	3160.5153			3167.0783
28956		3213.4838	3713.2936			3731.4429
28957	Zero-point correction (Hartree):			0.157181		
28958						
28959	diHPCARP_Ic.pmtmptmmd					
28960	-----					
28961	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.18193222		
28962	Electronic state : 2-A					
28963	Cartesian coordinates (Angs):					
28964	O	1.195877	-0.838005	1.881763		
28965	O	1.255234	0.479291	1.320720		
28966	C	1.137784	0.350496	-0.090215		
28967	C	-0.278406	0.021839	-0.596034		
28968	C	-0.994406	-1.021599	0.249129		
28969	O	-2.281640	-1.302501	-0.331744		
28970	O	-3.174215	-0.429543	0.023766		
28971	H	1.924028	-0.798344	2.513090		
28972	C	1.603857	1.696748	-0.632305		
28973	H	2.656348	1.848654	-0.397391		
28974	H	1.011664	2.486828	-0.176253		
28975	H	1.459765	1.728259	-1.710298		
28976	C	2.139826	-0.705047	-0.544549		
28977	O	1.960969	-1.466601	-1.449476		
28978	H	3.093133	-0.673676	0.015743		
28979	H	-0.162792	-0.370039	-1.609129		
28980	O	-1.072758	1.168421	-0.795490		
28981	O	-1.358554	1.763869	0.462466		
28982	H	-2.230261	1.378264	0.647744		
28983	H	-0.453896	-1.964575	0.233066		
28984	H	-1.149210	-0.689443	1.271236		
28985	Rotational constants (GHz):			1.3068200	0.7150300	0.6543400
28986	Vibrational harmonic frequencies (cm-1):					
28987		49.4704	92.3640			102.8438
28988		140.6819	172.1356			183.3150
28989		190.6870	200.9976			205.2196
28990		251.4025	265.0823			289.5952

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28991      318.7579      335.3480      346.5003
28992      399.3338      493.3925      509.7858
28993      575.3407      580.3290      590.5119
28994      700.7822      826.9130      909.8993
28995      932.8415      969.3530      987.5882
28996      990.0669      1009.7450     1041.7835
28997      1114.8820     1143.9866     1182.0535
28998      1229.2344     1249.7906     1259.5575
28999      1316.1868     1340.3556     1390.4031
29000      1391.7300     1405.0296     1406.7831
29001      1411.0720     1441.6318     1478.8392
29002      1484.8855     1499.2165     1873.1185
29003      2964.7918     3078.6090     3099.8798
29004      3128.2785     3160.5083     3171.5292
29005      3195.3768     3733.3378     3839.2889
29006      Zero-point correction (Hartree): 0.156402
29007
29008      diHPCARP_Ic.pmtpmtmmd
29009      -----
29010      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18065063
29011      Electronic state : 2-A
29012      Cartesian coordinates (Angs):
29013      O      1.191439      -1.237797      -1.567976
29014      O      1.647867      -1.151314      -0.224834
29015      C      1.207422      0.069120      0.332160
29016      C      -0.329581      0.151752      0.499677
29017      C      -1.117602      0.607840      -0.724599
29018      O      -2.523228      0.384162      -0.494614
29019      O      -2.982674      1.150737      0.448596
29020      H      0.429149      -1.826139      -1.449557
29021      C      1.875377      0.095754      1.705930
29022      H      2.951559      -0.030303      1.601227
29023      H      1.478511      -0.721645      2.305701
29024      H      1.669311      1.044988      2.196527
29025      C      1.782571      1.218470      -0.478929
29026      O      1.321248      2.325157      -0.480579
29027      H      2.703957      0.959222      -1.030767
29028      H      -0.538161      0.865569      1.298398
29029      O      -0.831388      -1.060736      1.036316
29030      O      -0.997875      -2.017023      -0.003684
29031      H      -1.958770      -2.002846      -0.116593
29032      H      -0.958719      1.668256      -0.896856
29033      H      -0.889058      0.039802      -1.619310
29034      Rotational constants (GHz):      1.2260100      0.7847500      0.6465000
29035      Vibrational harmonic frequencies (cm-1):
29036      54.5735      77.9803      104.1073
29037      114.1322      152.7533      178.7190
29038      194.5686      208.8672      235.3594
29039      255.9937      293.2469      304.2986
29040      315.8991      332.6821      374.9826
29041      385.4593      494.5468      507.3084
29042      552.6209      574.3456      612.9806
29043      735.9273      810.0824      917.6167
29044      939.1727      960.2709      977.4170
29045      986.3712      1013.5339     1057.6955
29046      1113.2969     1132.4899     1186.4850
29047      1238.5812     1252.2088     1258.4568
29048      1309.2919     1334.3844     1371.6863
29049      1396.1065     1402.4941     1407.9971
29050      1413.5449     1447.4125     1490.0963
29051      1498.7129     1504.5734     1862.8776
29052      2987.6985     3076.1300     3103.7784
29053      3140.7590     3159.2246     3165.2863
29054      3208.6388     3739.5175     3788.3707
29055      Zero-point correction (Hartree): 0.156541
29056
29057      diHPCARP_Ic.pmtppmpd
29058      -----
29059      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18193829
29060      Electronic state : 2-A
29061      Cartesian coordinates (Angs):
29062      O      -1.259535      0.334422      -1.751194

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29063	O	-1.682956	0.697221	-0.443766			
29064	C	-0.955948	-0.055711	0.510239			
29065	C	0.561103	0.230540	0.478352			
29066	C	1.308716	-0.304440	-0.732591			
29067	O	2.692351	-0.528454	-0.385443			
29068	O	2.809860	-1.500475	0.465340			
29069	H	-1.845587	-0.417747	-1.930538			
29070	C	-1.544143	0.366521	1.853612			
29071	H	-2.623835	0.232863	1.840492			
29072	H	-1.305873	1.411603	2.039136			
29073	H	-1.117820	-0.234274	2.656117			
29074	C	-1.213888	-1.541785	0.335784			
29075	O	-1.989105	-1.990753	-0.462076			
29076	H	-0.643877	-2.199984	1.018211			
29077	H	0.985527	-0.264727	1.356598			
29078	O	0.822377	1.598695	0.717807			
29079	O	0.579218	2.356813	-0.458716			
29080	H	-0.388148	2.403709	-0.489233			
29081	H	0.904741	-1.255973	-1.074737			
29082	H	1.322148	0.414020	-1.544054			
29083	Rotational constants (GHz):				1.1415700	0.7842700	0.6466900
29084	Vibrational harmonic frequencies (cm-1):						
29085		48.2675		70.4852		116.6495	
29086		131.3362		163.1805		177.9077	
29087		217.8658		220.1739		224.3580	
29088		275.7636		300.1171		318.1655	
29089		325.9586		371.9201		383.0789	
29090		412.7953		441.1284		495.2802	
29091		525.4047		573.6978		650.6243	
29092		772.7501		872.1381		889.0621	
29093		926.6830		952.5583		965.1144	
29094		995.2507		999.4967		1051.2872	
29095		1117.5058		1143.1222		1177.3419	
29096		1205.3210		1246.6834		1286.7282	
29097		1314.0460		1331.8294		1384.7291	
29098		1402.6002		1410.0725		1421.8374	
29099		1431.6789		1445.0445		1473.8533	
29100		1491.3355		1501.7883		1858.6993	
29101		2966.1868		3076.1640		3079.9161	
29102		3112.6302		3156.5863		3169.9785	
29103		3207.5869		3749.7394		3765.6590	
29104	Zero-point correction (Hartree):				0.156731		
29105	diHPCARP_Ic.ppmmtmpd						
29106	-----						
29107	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18262307						
29108	Electronic state : 2-A						
29109	Cartesian coordinates (Angs):						
29110	O	0.921407	2.067817	-0.928867			
29111	O	0.644353	1.613970	0.387850			
29112	C	-0.364742	0.608606	0.350685			
29113	C	0.083044	-0.576038	-0.546105			
29114	C	1.075195	-1.523573	0.115516			
29115	O	2.240223	-0.814235	0.586130			
29116	O	2.841246	-0.185378	-0.374444			
29117	H	1.808980	1.703388	-1.067891			
29118	C	-0.555900	0.273551	1.827504			
29119	H	-0.894595	1.160591	2.360201			
29120	H	0.394238	-0.038292	2.257258			
29121	H	-1.289662	-0.518273	1.942187			
29122	C	-1.650531	1.241418	-0.173567			
29123	O	-2.710529	0.675585	-0.187051			
29124	H	-1.550953	2.291178	-0.494502			
29125	H	0.554451	-0.146067	-1.428375			
29126	O	-0.971641	-1.321003	-1.101351			
29127	O	-1.733714	-1.918201	-0.059134			
29128	H	-2.454887	-1.267887	0.014870			
29129	H	0.661381	-2.007604	0.995705			
29130	H	1.397890	-2.269254	-0.608722			
29131	Rotational constants (GHz):				1.2619800	0.8590200	0.6553200
29132	Vibrational harmonic frequencies (cm-1):						
29133		72.7441		108.9680		112.3133	
29134							

29135	166.0499	167.3950	176.8722			
29136	202.4703	213.5305	237.3323			
29137	269.9449	276.5511	299.6384			
29138	331.5348	358.6598	409.1962			
29139	426.8616	448.8421	522.0675			
29140	588.9923	596.3064	632.0026			
29141	653.9571	786.9875	925.1438			
29142	950.3243	968.6501	983.5089			
29143	989.8194	1036.8454	1054.3101			
29144	1120.9475	1147.2287	1182.1916			
29145	1227.3298	1238.6771	1258.9049			
29146	1300.5386	1349.9386	1382.5101			
29147	1400.0583	1407.8686	1422.5048			
29148	1426.4108	1470.1508	1485.2469			
29149	1496.9643	1517.4606	1849.7430			
29150	3017.8323	3086.4975	3111.0889			
29151	3134.1226	3156.3659	3182.5056			
29152	3194.8167	3666.4782	3757.7295			
29153	Zero-point correction (Hartree): 0.157102					
29154						
29155	diHPCARP_Ic.ppmmtpm					
29156	-----					
29157	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18348033					
29158	Electronic state : 2-A					
29159	Cartesian coordinates (Angs):					
29160	O	-0.858324	-1.776643	-1.151178		
29161	O	-0.688570	-1.629408	0.253045		
29162	C	0.379713	-0.722990	0.469849		
29163	C	0.041118	0.702756	0.003683		
29164	C	-1.215581	1.301228	0.628337		
29165	O	-2.404110	0.545401	0.326236		
29166	O	-2.620431	0.486678	-0.951095		
29167	H	-1.670087	-1.268676	-1.313831		
29168	C	0.661092	-0.813695	1.963474		
29169	H	1.060513	-1.796092	2.211799		
29170	H	-0.267384	-0.680747	2.517405		
29171	H	1.375308	-0.045921	2.252047		
29172	C	1.586711	-1.274778	-0.281908		
29173	O	2.401843	-0.618661	-0.868926		
29174	H	1.661991	-2.375335	-0.226800		
29175	H	-0.057436	0.718690	-1.080293		
29176	O	1.094296	1.568990	0.391097		
29177	O	1.746880	2.089472	-0.752954		
29178	H	2.317507	1.337634	-0.990376		
29179	H	-1.164342	1.317313	1.714649		
29180	H	-1.347063	2.311373	0.244989		
29181	Rotational constants (GHz):			1.1566400	0.8507000	0.6725300
29182	Vibrational harmonic frequencies (cm-1):					
29183		41.0943	80.1468			104.3207
29184		137.2265	146.8010			178.8458
29185		198.5431	220.4695			228.2590
29186		258.9609	281.4440			318.8804
29187		338.2250	345.6939			389.6120
29188		426.1874	441.7570			520.9360
29189		558.7299	580.6058			598.8991
29190		676.6224	762.2890			926.0180
29191		954.1142	969.5735			980.4526
29192		1029.7634	1042.7394			1054.7135
29193		1123.0047	1138.0771			1186.9041
29194		1225.2727	1256.8852			1273.2789
29195		1302.1226	1338.9551			1379.2603
29196		1401.1484	1405.2700			1415.3707
29197		1440.6758	1476.2641			1485.8384
29198		1491.2527	1511.6214			1861.0903
29199		2990.5248	3075.2933			3108.6897
29200		3130.9034	3146.9571			3170.1017
29201		3174.0127	3684.1745			3718.1791
29202	Zero-point correction (Hartree): 0.156517					
29203						
29204	diHPCARP_Ic.ppmptpm					
29205	-----					
29206	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18186222					

```

29207 Electronic state : 2-A
29208 Cartesian coordinates (Angs):
29209 O -0.581980 -1.891101 -1.160807
29210 O -0.408099 -1.722729 0.242350
29211 C 0.554552 -0.703006 0.438451
29212 C 0.043416 0.664338 -0.049835
29213 C -1.368023 0.992816 0.415291
29214 O -2.286917 0.263343 -0.427448
29215 O -3.521383 0.459928 -0.080103
29216 H -1.433566 -1.450451 -1.303124
29217 C 0.851064 -0.736319 1.932628
29218 H 1.299011 -1.692906 2.198338
29219 H -0.074312 -0.631177 2.496774
29220 H 1.529818 0.071515 2.192705
29221 C 1.822819 -1.103083 -0.301878
29222 O 2.573392 -0.329107 -0.830326
29223 H 2.020999 -2.189176 -0.292507
29224 H 0.059598 0.689962 -1.139750
29225 O 0.908351 1.673798 0.440518
29226 O 1.571899 2.308380 -0.638805
29227 H 2.257869 1.649535 -0.844071
29228 H -1.569233 0.708904 1.446434
29229 H -1.555245 2.055214 0.274225
29230 Rotational constants (GHz): 1.1987700 0.7632500 0.5965800
29231 Vibrational harmonic frequencies (cm-1):
29232 47.7099 71.8135 76.8656
29233 112.0963 139.4455 166.7202
29234 187.7744 198.0627 212.8526
29235 248.9292 283.9820 297.6800
29236 326.3374 347.0919 388.4708
29237 442.4513 466.6071 491.8440
29238 545.0876 566.9281 605.6824
29239 682.3476 770.9593 925.4096
29240 952.2680 977.0462 997.0325
29241 1030.8177 1052.0834 1054.2716
29242 1134.1523 1140.0192 1179.9282
29243 1220.2046 1255.9810 1272.7846
29244 1292.3356 1340.0196 1369.3278
29245 1399.6267 1408.5863 1421.3254
29246 1430.7252 1478.1848 1488.2859
29247 1495.4242 1507.2758 1857.1876
29248 2996.7417 3079.3180 3103.1895
29249 3108.8596 3149.7666 3167.1904
29250 3178.4653 3695.2117 3760.5147
29251 Zero-point correction (Hartree): 0.156276
29252
29253 diHPCARP_Ic.ppmmpmpmd
29254 -----
29255 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18186226
29256 Electronic state : 2-A
29257 Cartesian coordinates (Angs):
29258 O -0.582089 -1.890964 -1.160955
29259 O -0.408329 -1.722597 0.242179
29260 C 0.554418 -0.702966 0.438520
29261 C 0.043478 0.664474 -0.049774
29262 C -1.367941 0.992875 0.415452
29263 O -2.286798 0.263568 -0.427585
29264 O -3.521259 0.460083 -0.080161
29265 H -1.433552 -1.450136 -1.303478
29266 C 0.850691 -0.736432 1.932727
29267 H 1.298249 -1.693199 2.198428
29268 H -0.074728 -0.631018 2.496732
29269 H 1.529707 0.071117 2.192977
29270 C 1.822707 -1.103186 -0.301718
29271 O 2.573389 -0.329329 -0.830161
29272 H 2.020759 -2.189299 -0.292262
29273 H 0.059563 0.689985 -1.139693
29274 O 0.908519 1.673831 0.440456
29275 O 1.572350 2.308069 -0.638915
29276 H 2.258149 1.648988 -0.844015
29277 H -1.569147 0.708422 1.446440
29278 H -1.555384 2.055261 0.274783

```

29279	Rotational constants (GHz):	1.1988100	0.7632500	0.5966000
29280	Vibrational harmonic frequencies (cm-1):			
29281		47.7238	71.8705	76.7950
29282		112.1789	139.4018	166.7596
29283		187.6357	198.0473	212.8421
29284		248.9969	283.8897	297.6826
29285		326.3242	347.0621	388.4602
29286		442.5774	466.6013	491.8595
29287		545.1043	566.9826	605.6806
29288		682.3576	770.9447	925.3624
29289		952.2456	977.0237	996.9276
29290		1030.8060	1052.1380	1054.2047
29291		1134.1905	1140.0878	1179.9062
29292		1220.1682	1255.9621	1272.7698
29293		1292.2930	1340.0236	1369.2765
29294		1399.6132	1408.5785	1421.3265
29295		1430.7268	1478.2186	1488.2529
29296		1495.4059	1507.2710	1857.2473
29297		2996.7629	3079.3733	3103.2792
29298		3108.9025	3149.8252	3167.3520
29299		3178.5278	3695.0189	3760.4736
29300	Zero-point correction (Hartree):	0.156276		
29301				
29302	diHPCARP_Ic.ppppppmmmd			
29303	-----			
29304	E(UM062X/Aug-CC-pVTZ) (Hartree):	-722.18118512		
29305	Electronic state : 2-A			
29306	Cartesian coordinates (Angs):			
29307	O	2.272071	-1.348838	-0.913133
29308	O	1.596627	-1.265073	0.333401
29309	C	0.793342	-0.095736	0.383620
29310	C	-0.253320	-0.174550	-0.748880
29311	C	-1.357877	-1.195433	-0.529445
29312	O	-2.289108	-0.853421	0.520767
29313	O	-3.249327	-0.094456	0.094665
29314	H	3.020526	-0.750978	-0.756120
29315	C	0.251095	-0.101914	1.810203
29316	H	1.087646	-0.037971	2.504712
29317	H	-0.282421	-1.031064	1.999821
29318	H	-0.425815	0.732703	1.966037
29319	C	1.648208	1.159190	0.227960
29320	O	2.840408	1.115427	0.085657
29321	H	1.107920	2.115126	0.301568
29322	H	0.297467	-0.538433	-1.619770
29323	O	-0.712694	1.085503	-1.195011
29324	O	-1.238869	1.829342	-0.101811
29325	H	-2.190400	1.674130	-0.192415
29326	H	-1.940392	-1.318369	-1.439737
29327	H	-0.916089	-2.142354	-0.221118
29328	Rotational constants (GHz):	1.5644900	0.6856100	0.6074600
29329	Vibrational harmonic frequencies (cm-1):			
29330		65.5450	66.7680	97.6887
29331		137.5724	182.1185	196.2874
29332		210.7535	234.0013	250.2984
29333		267.9179	286.0434	311.1984
29334		328.1206	354.7104	382.7548
29335		432.8407	495.9039	512.0285
29336		542.1236	555.7870	611.7679
29337		806.6330	818.3366	867.0057
29338		929.6967	950.7670	957.0182
29339		997.8725	1021.2422	1052.6837
29340		1075.2338	1144.5030	1167.1623
29341		1238.3292	1262.4590	1277.1396
29342		1331.5857	1361.9446	1388.5466
29343		1394.7248	1403.5835	1415.9407
29344		1422.8238	1441.8029	1469.4108
29345		1490.7587	1504.8409	1849.1219
29346		3038.0301	3083.2585	3091.2365
29347		3103.4994	3156.6602	3168.1860
29348		3186.5548	3735.8298	3770.0079
29349	Zero-point correction (Hartree):	0.156958		
29350				

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29351 diHPCARP_Ic.pppppptpd
29352 -----
29353 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.21164044
29354 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09635753
29355 T1 diagnostic: 0.020031
29356 E(MP2/Aug-CC-pVTZ) (Hartree): -721.05077172
29357 E(MP3/Aug-CC-pVTZ) (Hartree): -721.07357021
29358 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05394254
29359 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07543930
29360 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.54290918
29361 E(UHF/Aug-CC-pVTZ) (Hartree): -718.53772682
29362 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18602223
29363 Electronic state : 2-A
29364 Cartesian coordinates (Angs):
29365 O 1.901724 -1.236812 -1.272631
29366 O 1.504093 -1.263142 0.092400
29367 C 0.897311 -0.033348 0.423073
29368 C -0.283275 0.266062 -0.530827
29369 C -1.185703 -0.932258 -0.801332
29370 O -1.965967 -1.285390 0.354334
29371 O -2.987547 -0.497828 0.507833
29372 H 2.770291 -0.810579 -1.202853
29373 C 0.494381 -0.171760 1.886635
29374 H 1.386978 -0.344964 2.485776
29375 H -0.183441 -1.012797 2.008231
29376 H -0.004172 0.732889 2.226903
29377 C 1.901117 1.106826 0.308466
29378 O 3.044098 0.941613 -0.019046
29379 H 1.507462 2.107705 0.555093
29380 H 0.112179 0.574280 -1.502681
29381 O -0.971216 1.345812 0.060636
29382 O -1.942547 1.811454 -0.860098
29383 H -2.727469 1.332150 -0.548248
29384 H -1.878884 -0.709341 -1.608950
29385 H -0.587025 -1.808126 -1.036783
29386 Rotational constants (GHz): 1.4884200 0.6793500 0.6054400
29387 Vibrational harmonic frequencies (cm-1):
29388 34.9619 75.3424 99.2385
29389 149.5395 174.1478 176.5562
29390 206.3859 218.8385 242.8983
29391 250.9283 295.2067 308.1161
29392 313.0974 346.0364 408.5670
29393 447.2392 483.3846 515.6812
29394 521.2268 559.3409 659.4319
29395 769.1411 831.6278 875.1743
29396 923.0011 934.0307 991.8552
29397 1000.1645 1044.1280 1055.1054
29398 1074.2578 1158.2361 1176.8835
29399 1236.9282 1260.5532 1287.2137
29400 1319.6289 1360.3818 1377.0899
29401 1399.7821 1415.0905 1416.9621
29402 1427.0692 1451.0365 1480.1303
29403 1490.5870 1503.9038 1855.9502
29404 2999.5532 3067.8601 3084.5770
29405 3119.3768 3163.6461 3177.3477
29406 3185.5029 3734.5769 3749.1929
29407 Zero-point correction (Hartree): 0.156929
29408
29409 diHPCARP_Ic.ppppttpd
29410 -----
29411 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18028634
29412 Electronic state : 2-A
29413 Cartesian coordinates (Angs):
29414 O 1.857664 -1.414085 -1.214231
29415 O 1.405844 -1.430654 0.143453
29416 C 0.949278 -0.118511 0.444648
29417 C -0.190119 0.302096 -0.501632
29418 C -1.113715 -0.838796 -0.909101
29419 O -1.861149 -1.340006 0.213771
29420 O -2.879132 -0.581678 0.492829
29421 H 2.735684 -1.803769 -1.125213
29422 C 0.556300 -0.188327 1.914051

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29423	H	1.427845	-0.466833	2.505707	
29424	H	-0.222703	-0.933564	2.056907	
29425	H	0.185988	0.778729	2.243383	
29426	C	2.148263	0.818716	0.307455	
29427	O	2.148094	1.851787	-0.289302	
29428	H	3.048393	0.444632	0.836201	
29429	H	0.242586	0.711586	-1.418092	
29430	O	-0.882402	1.322775	0.184440	
29431	O	-1.852047	1.868700	-0.691696	
29432	H	-2.641942	1.381605	-0.407510	
29433	H	-1.828436	-0.495896	-1.652936	
29434	H	-0.542434	-1.682271	-1.285083	
29435	Rotational constants (GHz):		1.2995900	0.7730900	0.6336900
29436	Vibrational harmonic frequencies (cm-1):				
29437		52.0892	78.6452		90.9222
29438		131.1388	139.5588		157.3706
29439		180.6049	206.4963		212.0623
29440		236.3332	245.0966		273.1641
29441		321.7172	333.0144		372.6890
29442		395.5444	505.2372		508.5566
29443		535.6317	560.3148		615.3415
29444		727.1830	799.1606		897.5745
29445		927.8690	956.4523		990.3874
29446		1005.9294	1037.4930		1050.8259
29447		1072.1858	1151.3895		1203.2182
29448		1225.2727	1246.6958		1275.7122
29449		1321.9995	1353.4803		1383.1733
29450		1389.4304	1397.8562		1410.8320
29451		1415.8719	1446.5844		1485.0572
29452		1490.7441	1502.7318		1887.8536
29453		2935.8870	3080.5592		3081.4214
29454		3124.5822	3159.3313		3180.3835
29455		3191.5589	3742.5161		3838.1614
29456	Zero-point correction (Hartree): 0.156143				
29457					
29458	diHPCARP_Ic.pptmppmmd				
29459	-----				
29460	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18549850				
29461	Electronic state : 2-A				
29462	Cartesian coordinates (Angs):				
29463	O	-1.666967	1.934239	-0.057485	
29464	O	-1.545919	0.905798	0.917091	
29465	C	-1.012014	-0.252235	0.305171	
29466	C	0.334890	0.073634	-0.388002	
29467	C	1.227423	0.926783	0.497959	
29468	O	2.403781	1.323239	-0.232732	
29469	O	3.300052	0.386168	-0.280600	
29470	H	-2.535478	1.726652	-0.436428	
29471	C	-0.927549	-1.279639	1.426285	
29472	H	-1.911353	-1.368179	1.885268	
29473	H	-0.210452	-0.968322	2.182066	
29474	H	-0.615932	-2.244544	1.035304	
29475	C	-1.969758	-0.785766	-0.750978	
29476	O	-3.033316	-0.280772	-0.985605	
29477	H	-1.620778	-1.681192	-1.293498	
29478	H	0.128862	0.642673	-1.296897	
29479	O	0.970831	-1.084976	-0.889486	
29480	O	1.583891	-1.811126	0.166953	
29481	H	2.483058	-1.445027	0.132063	
29482	H	0.718609	1.853483	0.746504	
29483	H	1.546696	0.407233	1.397921	
29484	Rotational constants (GHz):		1.5277900	0.6655900	0.5635600
29485	Vibrational harmonic frequencies (cm-1):				
29486		55.9927	80.3486		113.5244
29487		134.8332	175.8005		198.0797
29488		218.6916	242.4701		257.1780
29489		279.0553	294.3402		302.3048
29490		322.7345	330.1908		385.0842
29491		461.9964	500.2947		528.5662
29492		543.4721	562.1491		643.1933
29493		751.2171	839.1823		877.9834
29494		927.3048	959.8300		980.1612

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29495          996.9577              1012.9272              1048.9464
29496          1111.1151             1149.8560              1177.9713
29497          1233.4880             1257.0803              1274.6648
29498          1319.1392             1345.1925              1377.8311
29499          1403.9945             1411.6452              1418.1901
29500          1426.0588             1455.0392              1480.0701
29501          1486.7731             1500.9435              1854.6851
29502          2996.1294             3083.4201              3093.7133
29503          3125.8689             3161.1747              3177.9259
29504          3194.0318             3727.4379              3754.0313
29505          Zero-point correction (Hartree): 0.157244
29506
29507          diHPCARP_Ic.pptmppppd
29508          -----
29509          E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18082102
29510          Electronic state : 2-A
29511          Cartesian coordinates (Angs):
29512          O          1.500674          -1.453671          -1.412726
29513          O          1.404597          -1.484245          0.005176
29514          C          0.933450          -0.237179          0.475562
29515          C          -0.451431          0.074434          -0.133061
29516          C          -1.491688          -0.939783          0.296436
29517          O          -2.637991          -0.827292          -0.563592
29518          O          -3.561705          -0.069074          -0.052757
29519          H          2.358692          -1.014685          -1.527620
29520          C          0.881100          -0.377118          1.993041
29521          H          1.888048          -0.475598          2.395040
29522          H          0.317755          -1.268094          2.264585
29523          H          0.402297          0.498424          2.428571
29524          C          1.933088          0.869849          0.156135
29525          O          2.933320          0.675836          -0.480147
29526          H          1.707349          1.856981          0.588132
29527          H          -0.375216          0.061332          -1.219934
29528          O          -0.923404          1.340560          0.293415
29529          O          -0.350603          2.332706          -0.547469
29530          H          -1.115605          2.606247          -1.070442
29531          H          -1.101832          -1.946662          0.159406
29532          H          -1.827701          -0.777716          1.318370
29533          Rotational constants (GHz):          1.3813200          0.6565800          0.5675400
29534          Vibrational harmonic frequencies (cm-1):
29535          37.1151              58.4786              72.8933
29536          88.9026              123.0039             167.3128
29537          201.1923             234.5301             239.5372
29538          257.9527             278.6494             292.8626
29539          308.7797             337.6209             360.8927
29540          391.0400             476.8285             509.7227
29541          537.1894             559.4069             564.3672
29542          732.1408             842.1519             888.5583
29543          930.3912             956.6025             993.4674
29544          999.2160             1048.9716            1051.6972
29545          1114.9060            1143.2248            1179.2805
29546          1238.9176            1256.2211            1269.9902
29547          1320.3497            1332.3738            1374.5217
29548          1401.7981            1409.7248            1412.6168
29549          1421.3417            1442.0429            1471.4062
29550          1491.8208            1509.8623            1849.8404
29551          3025.0926            3077.0476            3106.8176
29552          3117.6239            3155.6176            3161.9061
29553          3176.7261            3738.0510            3811.8173
29554          Zero-point correction (Hartree): 0.156174
29555
29556          diHPCARP_Ic.pptmpptpd
29557          -----
29558          E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18291850
29559          Electronic state : 2-A
29560          Cartesian coordinates (Angs):
29561          O          1.617483          -1.703510          -0.912169
29562          O          1.619216          -1.221598          0.424945
29563          C          1.069434          0.077027          0.445583
29564          C          -0.349240          0.094012          -0.171722
29565          C          -1.173696          -1.081472          0.327124
29566          O          -2.429824          -1.150481          -0.378526

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29567	O	-3.326804	-0.369346	0.136954	
29568	H	2.453875	-1.338163	-1.240908	
29569	C	1.088000	0.490025	1.912455	
29570	H	2.112256	0.453830	2.279565	
29571	H	0.483382	-0.193863	2.504690	
29572	H	0.695107	1.497562	2.025378	
29573	C	1.942136	1.042596	-0.345047	
29574	O	2.969629	0.709927	-0.868688	
29575	H	1.566574	2.077955	-0.406226	
29576	H	-0.282086	0.048003	-1.259466	
29577	O	-0.901371	1.347024	0.193697	
29578	O	-1.771484	1.792911	-0.833318	
29579	H	-2.633983	1.496563	-0.506675	
29580	H	-0.670244	-2.017917	0.102129	
29581	H	-1.399443	-0.996516	1.387995	
29582	Rotational constants (GHz):		1.4808700	0.6422700	0.5601300
29583	Vibrational harmonic frequencies (cm-1):				
29584		38.7520	58.0242		93.3507
29585		122.7498	150.9027		170.9353
29586		196.8673	206.3389		218.0166
29587		271.4462	286.0121		288.9075
29588		321.6434	364.6573		409.9130
29589		440.2096	459.9788		486.0004
29590		487.3685	537.5193		569.5035
29591		753.3012	857.9431		897.1113
29592		923.6354	966.5326		990.0481
29593		995.5514	1047.5817		1056.2891
29594		1104.5643	1139.8872		1176.5126
29595		1236.3793	1260.3854		1283.1661
29596		1322.5190	1332.9697		1377.9362
29597		1399.8546	1412.3266		1418.0692
29598		1425.9389	1430.2354		1468.8904
29599		1490.9391	1504.5011		1855.7536
29600		3004.3956	3083.5170		3099.1998
29601		3115.3021	3159.8867		3174.1946
29602		3187.4900	3750.6034		3772.1382
29603	Zero-point correction (Hartree): 0.156407				
29604	diHPCARP_Ic.pptpmtmpd				
29605	-----				
29607	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18175617				
29608	Electronic state : 2-A				
29609	Cartesian coordinates (Angs):				
29610	O	0.647491	2.244916	-0.630450	
29611	O	0.091613	1.769979	0.588031	
29612	C	-0.680249	0.595402	0.349406	
29613	C	0.249388	-0.470286	-0.284633	
29614	C	1.351553	-0.893130	0.678283	
29615	O	2.620173	-0.954068	-0.013051	
29616	O	2.981204	0.220293	-0.425756	
29617	H	1.562476	1.924915	-0.567160	
29618	C	-1.247244	0.267639	1.728679	
29619	H	-1.632805	1.186424	2.168951	
29620	H	-0.481512	-0.133869	2.387934	
29621	H	-2.052884	-0.453108	1.647530	
29622	C	-1.831002	0.906182	-0.597970	
29623	O	-2.702915	0.110541	-0.822877	
29624	H	-1.827092	1.911567	-1.048163	
29625	H	0.725316	0.008680	-1.140466	
29626	O	-0.401474	-1.554974	-0.891461	
29627	O	-1.226349	-2.210412	0.060656	
29628	H	-2.086158	-1.813902	-0.161011	
29629	H	1.482508	-0.179712	1.488814	
29630	H	1.177523	-1.896038	1.060239	
29631	Rotational constants (GHz):		1.2268600	0.8197700	0.6183600
29632	Vibrational harmonic frequencies (cm-1):				
29633		63.5339	84.3133		113.4566
29634		146.9652	158.4043		173.4479
29635		190.2733	196.0567		246.2281
29636		270.2744	289.0156		299.3062
29637		310.9879	341.8770		424.7347
29638		475.3137	511.8753		519.2765

29639	570.8102	581.9267	645.9108			
29640	676.0247	840.5553	911.8188			
29641	938.4360	956.1343	978.9433			
29642	996.3296	1007.4828	1050.5084			
29643	1117.1853	1165.6130	1171.6421			
29644	1227.7505	1249.3592	1257.9937			
29645	1328.4172	1336.4130	1393.4314			
29646	1405.4636	1417.9803	1429.7337			
29647	1445.3380	1457.8724	1481.3939			
29648	1488.2613	1502.3857	1848.5681			
29649	3024.5173	3090.0483	3112.6464			
29650	3121.2795	3161.0436	3182.7429			
29651	3200.7965	3714.6608	3722.8252			
29652	Zero-point correction (Hartree): 0.157252					
29653						
29654	diHPCARP_Ic.pptpmpmd					
29655	-----					
29656	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18440380					
29657	Electronic state : 2-A					
29658	Cartesian coordinates (Angs):					
29659	O	-0.435076	-1.984195	-1.080953		
29660	O	-0.082080	-1.850407	0.291524		
29661	C	0.687000	-0.668171	0.424885		
29662	C	-0.171935	0.577132	0.121787		
29663	C	-1.482095	0.545519	0.909584		
29664	O	-2.617209	0.759709	0.041622		
29665	O	-2.759847	-0.211568	-0.802630		
29666	H	-1.324926	-1.589748	-1.097500		
29667	C	1.205208	-0.684740	1.857399		
29668	H	1.844208	-1.552481	2.015129		
29669	H	0.369982	-0.748833	2.554344		
29670	H	1.767710	0.225257	2.051285		
29671	C	1.882902	-0.796068	-0.507950		
29672	O	2.437109	0.121071	-1.049083		
29673	H	2.238830	-1.834481	-0.622436		
29674	H	-0.403632	0.605315	-0.942809		
29675	O	0.533703	1.757657	0.459025		
29676	O	0.950565	2.431529	-0.715319		
29677	H	1.727456	1.903688	-0.970247		
29678	H	-1.648922	-0.408531	1.404586		
29679	H	-1.514503	1.367407	1.619927		
29680	Rotational constants (GHz):			1.1178100	0.8398800	0.6514700
29681	Vibrational harmonic frequencies (cm-1):					
29682		54.4086	75.4121	90.9455		
29683		132.6174	147.6555	185.4117		
29684		200.8242	215.6480	236.9020		
29685		262.6543	284.5037	299.2830		
29686		325.5333	356.7832	437.7981		
29687		463.6147	526.4415	557.0942		
29688		571.0733	585.1704	596.3219		
29689		664.8365	827.1411	916.4524		
29690		930.5966	962.2255	981.6842		
29691		1014.0501	1050.9046	1054.5198		
29692		1104.0524	1153.6570	1175.3109		
29693		1232.8508	1259.3388	1269.9458		
29694		1322.4369	1340.4139	1365.7086		
29695		1402.6898	1410.3708	1419.4441		
29696		1467.1176	1482.5464	1486.5467		
29697		1492.0366	1502.6901	1859.3673		
29698		3001.2601	3075.2228	3112.0676		
29699		3116.4571	3146.6913	3173.0814		
29700		3180.5472	3677.4897	3684.0943		
29701	Zero-point correction (Hartree): 0.157016					
29702						
29703	diHPCARP_Ic.pptppmmd					
29704	-----					
29705	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18205996					
29706	Electronic state : 2-A					
29707	Cartesian coordinates (Angs):					
29708	O	1.405074	-1.987874	0.277713		
29709	O	1.446804	-0.794969	1.050778		
29710	C	1.020750	0.286417	0.246104		

29711	C	-0.390611	0.012241	-0.324973		
29712	C	-1.292940	-0.624818	0.719541		
29713	O	-2.653563	-0.622290	0.246576		
29714	O	-2.804162	-1.406569	-0.778574		
29715	H	2.274931	-1.960821	-0.150459		
29716	C	1.103846	1.509269	1.149915		
29717	H	2.119586	1.588248	1.534553		
29718	H	0.414705	1.417805	1.985831		
29719	H	0.852129	2.408846	0.593345		
29720	C	1.974810	0.496820	-0.919285		
29721	O	2.969323	-0.154892	-1.083143		
29722	H	1.688813	1.302904	-1.618041		
29723	H	-0.316654	-0.673028	-1.170921		
29724	O	-0.952222	1.170460	-0.917506		
29725	O	-1.507442	2.009390	0.088884		
29726	H	-2.452094	1.838284	-0.030689		
29727	H	-0.985525	-1.650255	0.905467		
29728	H	-1.321503	-0.057602	1.645262		
29729	Rotational constants (GHz):			1.3775400	0.6982300	0.5807800
29730	Vibrational harmonic frequencies (cm-1):					
29731		61.5681	66.2240			90.9980
29732		126.5646	148.0138			169.2519
29733		200.5924	242.7002			254.6028
29734		280.5349	288.8220			299.0872
29735		314.3516	343.3227			372.0013
29736		383.8627	462.2386			491.5937
29737		530.9327	542.0022			691.7423
29738		735.6408	835.9126			881.1332
29739		925.4159	966.5360			973.4197
29740		987.2166	1018.6282			1049.6605
29741		1112.6011	1150.2888			1181.8413
29742		1231.5432	1244.2451			1284.1181
29743		1311.7824	1343.5078			1374.4218
29744		1403.5039	1411.3621			1418.4939
29745		1421.5318	1425.4754			1479.5928
29746		1491.8342	1502.1200			1856.5316
29747		2985.6933	3084.4255			3102.4143
29748		3130.2263	3163.0072			3175.5801
29749		3194.1745	3752.6743			3792.6417
29750	Zero-point correction (Hartree):			0.156647		
29751	diHPCARP_Ic.pptpppppd					
29752	-----					
29753	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18122456					
29754	Electronic state : 2-A					
29755	Cartesian coordinates (Angs):					
29756	O	0.894125	-2.127992	-0.382506		
29757	O	1.211552	-1.318189	0.743345		
29758	C	0.974768	0.037051	0.412708		
29759	C	-0.495381	0.238273	-0.055617		
29760	C	-1.446054	-0.653395	0.722537		
29761	O	-2.794485	-0.459948	0.250791		
29762	O	-2.934430	-0.881785	-0.968161		
29763	H	1.717386	-2.062756	-0.892163		
29764	C	1.282190	0.820067	1.681176		
29765	H	2.286261	0.571408	2.020658		
29766	H	0.572372	0.567087	2.465985		
29767	H	1.216621	1.888187	1.486229		
29768	C	1.957796	0.479601	-0.668335		
29769	O	2.714451	-0.279494	-1.211129		
29770	H	1.947492	1.553429	-0.910858		
29771	H	-0.602912	0.012302	-1.117828		
29772	O	-0.945321	1.556807	0.194802		
29773	O	-0.283310	2.425183	-0.714353		
29774	H	-1.014383	2.706312	-1.279379		
29775	H	-1.181941	-1.697992	0.594216		
29776	H	-1.481477	-0.384218	1.776029		
29777	Rotational constants (GHz):			1.2161400	0.7390000	0.5984300
29778	Vibrational harmonic frequencies (cm-1):					
29779		33.0307	48.7569			79.6960
29780		93.4703	146.1623			187.5634
29781		213.1509	222.2999			230.2454
29782						

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29783      247.8516      256.8138      300.1984
29784      306.4686      317.2461      361.0181
29785      387.8990      466.0223      502.5674
29786      532.0320      569.0645      595.0857
29787      740.6591      839.2478      889.2491
29788      921.0814      957.1576      975.8400
29789      1004.3976      1049.1226      1049.3158
29790      1126.0675      1141.5436      1185.8734
29791      1222.4015      1249.4655      1271.9122
29792      1325.4362      1340.4183      1372.4745
29793      1399.3793      1411.5447      1419.7213
29794      1421.2122      1432.9350      1474.6868
29795      1488.5277      1500.2366      1848.7754
29796      3027.6242      3082.4275      3096.7708
29797      3125.2291      3161.3372      3169.4311
29798      3197.7136      3743.5129      3816.9725
29799      Zero-point correction (Hartree): 0.156228
29800
29801      diHPCARP_Ic.pptppptpd
29802      -----
29803      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18178891
29804      Electronic state : 2-A
29805      Cartesian coordinates (Angs):
29806      O      1.319888      -1.924420      -0.567035
29807      O      1.528971      -1.166276      0.616689
29808      C      1.093581      0.156819      0.394053
29809      C      -0.386464      0.182078      -0.046229
29810      C      -1.218366      -0.806024      0.753648
29811      O      -2.609877      -0.635438      0.410734
29812      O      -2.876577      -1.136017      -0.759983
29813      H      2.136879      -1.735564      -1.054609
29814      C      1.339775      0.880751      1.712405
29815      H      2.393906      0.795448      1.970532
29816      H      0.750081      0.431059      2.508610
29817      H      1.069458      1.930137      1.623573
29818      C      1.925101      0.825890      -0.690390
29819      O      2.855888      0.289076      -1.224595
29820      H      1.611841      1.849982      -0.958125
29821      H      -0.475041      -0.057540      -1.106616
29822      O      -0.832380      1.515068      0.152965
29823      O      -1.795877      1.836272      -0.836381
29824      H      -2.624392      1.553636      -0.424221
29825      H      -0.931384      -1.832183      0.540172
29826      H      -1.173388      -0.598177      1.820599
29827      Rotational constants (GHz):      1.3605900      0.6721500      0.5828100
29828      Vibrational harmonic frequencies (cm-1):
29829      57.6652      62.3981      81.8415
29830      117.3698      130.6411      150.3263
29831      198.1335      205.9111      221.2592
29832      264.1777      271.2036      294.6066
29833      316.6169      362.5853      371.0664
29834      408.0716      443.6998      484.1518
29835      488.5944      543.0294      582.2772
29836      758.5169      858.8736      897.5981
29837      923.0668      966.5993      975.1957
29838      1002.7591      1045.6722      1055.4415
29839      1112.0578      1142.1428      1178.7280
29840      1236.4512      1240.1556      1287.7472
29841      1314.2089      1336.1890      1367.0615
29842      1403.0497      1413.0863      1417.8186
29843      1426.8001      1427.0843      1471.9128
29844      1492.6448      1503.5238      1857.4078
29845      2994.8384      3083.2634      3103.4630
29846      3116.6866      3159.8968      3173.2711
29847      3185.5970      3753.3231      3789.9234
29848      Zero-point correction (Hartree): 0.156118
29849
29850      diHPCARP_Ic.pptppppd
29851      -----
29852      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18106023
29853      Electronic state : 2-A
29854      Cartesian coordinates (Angs):

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29855	O	1.198092	-1.597469	-1.427949		
29856	O	1.099988	-1.623131	-0.010186		
29857	C	0.892409	-0.311797	0.474548		
29858	C	-0.408863	0.271561	-0.115581		
29859	C	-1.625609	-0.484815	0.359060		
29860	O	-2.703585	-0.135809	-0.530197		
29861	O	-3.834645	-0.609443	-0.108816		
29862	H	2.127570	-1.341721	-1.541269		
29863	C	0.827958	-0.452592	1.991633		
29864	H	1.796306	-0.763758	2.379863		
29865	H	0.092904	-1.207880	2.264173		
29866	H	0.549256	0.499927	2.439785		
29867	C	2.093231	0.574731	0.157073		
29868	O	3.031132	0.188456	-0.486113		
29869	H	2.075719	1.581242	0.602384		
29870	H	-0.359290	0.222622	-1.203275		
29871	O	-0.599289	1.619067	0.289693		
29872	O	0.174489	2.452163	-0.560591		
29873	H	-0.504445	2.833976	-1.132410		
29874	H	-1.461284	-1.559623	0.296468		
29875	H	-1.920959	-0.197986	1.367155		
29876	Rotational constants (GHz):			1.3285900	0.6363500	0.5451900
29877	Vibrational harmonic frequencies (cm-1):					
29878		39.3514	58.0552			87.5461
29879		104.3391	122.3204			179.9383
29880		190.5049	235.4211			246.8781
29881		258.1972	283.9184			297.3508
29882		304.7492	346.7092			359.3548
29883		396.0968	426.7662			488.5037
29884		522.2380	555.4515			633.8307
29885		725.7566	840.0008			882.8179
29886		930.1005	960.1017			1005.8053
29887		1027.8775	1051.4235			1054.6569
29888		1122.7191	1143.2073			1176.1686
29889		1239.0589	1268.3303			1277.9271
29890		1295.4334	1328.6975			1371.7118
29891		1401.8005	1411.6957			1422.1397
29892		1428.0642	1444.9520			1486.5585
29893		1491.1754	1511.1496			1850.1635
29894		3028.4049	3076.0345			3096.7935
29895		3114.5519	3154.3997			3160.7858
29896		3162.2725	3743.3617			3808.6416
29897	Zero-point correction (Hartree):			0.156356		
29898						
29899	diHPCARP_Ic.ppttpptpd					
29900	-----					
29901	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.18113588		
29902	Electronic state : 2-A					
29903	Cartesian coordinates (Angs):					
29904	O	1.349778	-1.808220	-0.957483		
29905	O	1.409511	-1.369712	0.393322		
29906	C	1.088377	0.002801	0.441700		
29907	C	-0.299551	0.262826	-0.184086		
29908	C	-1.300320	-0.792201	0.245263		
29909	O	-2.576750	-0.381951	-0.292773		
29910	O	-3.531888	-1.176509	0.082700		
29911	H	2.245125	-1.592425	-1.261720		
29912	C	1.161570	0.376611	1.917160		
29913	H	2.159707	0.152542	2.289508		
29914	H	0.439616	-0.200228	2.491229		
29915	H	0.952180	1.435517	2.048626		
29916	C	2.116249	0.827597	-0.319177		
29917	O	3.088824	0.346940	-0.831916		
29918	H	1.906663	1.910153	-0.369359		
29919	H	-0.223517	0.274760	-1.272069		
29920	O	-0.693920	1.556527	0.247292		
29921	O	-1.455055	2.175950	-0.775893		
29922	H	-2.342966	1.822352	-0.620363		
29923	H	-1.052259	-1.770150	-0.160414		
29924	H	-1.406497	-0.842517	1.327401		
29925	Rotational constants (GHz):			1.3755100	0.6318600	0.5338200
29926	Vibrational harmonic frequencies (cm-1):					

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29927      44.4925      71.7314      82.3796
29928      112.4107      126.9727      146.1118
29929      175.0402      198.3919      216.5598
29930      259.9135      280.0551      291.1085
29931      318.9970      367.1933      386.8742
29932      392.7483      424.6518      448.4001
29933      501.3486      564.6384      583.1057
29934      750.9824      856.8581      902.3319
29935      924.8746      967.6797      998.4404
29936      1023.0088      1047.3252      1055.1949
29937      1096.1503      1151.3595      1174.9086
29938      1238.3751      1256.7144      1284.9659
29939      1295.8490      1335.5429      1368.5131
29940      1403.2158      1413.8496      1427.1722
29941      1429.4058      1441.8532      1484.1207
29942      1491.9290      1503.9134      1858.1867
29943      2995.9650      3083.6205      3098.4888
29944      3108.3024      3160.3986      3172.6656
29945      3175.8435      3755.7723      3777.3132
29946 Zero-point correction (Hartree): 0.156064
29947
29948 diHPCARP_Ic.ptmmtmpd
29949 -----
29950 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17992089
29951 Electronic state : 2-A
29952 Cartesian coordinates (Angs):
29953 O      2.582143      0.160997      -0.851907
29954 O      1.551207      -0.756708      -1.210604
29955 C      0.479398      -0.717272      -0.267876
29956 C      -0.319198      0.595375      -0.414310
29957 C      -1.472035      0.788423      0.568669
29958 O      -2.581953      -0.071109      0.244194
29959 O      -3.095038      0.224515      -0.911155
29960 H      2.389118      0.903462      -1.440695
29961 C      -0.384946      -1.912615      -0.659352
29962 H      0.238219      -2.803588      -0.706700
29963 H      -0.843640      -1.744799      -1.632326
29964 H      -1.161932      -2.060815      0.085394
29965 C      1.026898      -0.968609      1.135065
29966 O      0.318690      -1.187474      2.076513
29967 H      2.127037      -0.993895      1.214647
29968 H      -0.728596      0.614337      -1.427539
29969 O      0.506401      1.743670      -0.386205
29970 O      1.098045      1.830393      0.903677
29971 H      1.980355      1.465065      0.730973
29972 H      -1.206800      0.533848      1.589668
29973 H      -1.810419      1.820296      0.497293
29974 Rotational constants (GHz):      1.2483700      0.7552300      0.6943000
29975 Vibrational harmonic frequencies (cm-1):
29976      33.1405      77.1951      119.6233
29977      126.4076      167.7429      189.6724
29978      196.1062      218.6416      249.4244
29979      255.6528      280.8736      312.9492
29980      327.6837      341.3960      410.0082
29981      431.5570      462.3986      505.0050
29982      511.0058      564.5744      632.6482
29983      689.2619      802.2431      916.0922
29984      940.1147      963.3723      990.7048
29985      995.1365      1036.7357      1057.8199
29986      1099.6416      1139.0844      1179.9135
29987      1210.1739      1235.9918      1263.9603
29988      1307.7614      1330.8032      1380.8632
29989      1405.4736      1410.9419      1415.2130
29990      1423.1722      1433.7379      1487.2500
29991      1490.7225      1505.0376      1860.3657
29992      2997.4707      3082.4532      3093.7182
29993      3115.5995      3159.9594      3182.5684
29994      3196.1719      3733.3587      3794.7548
29995 Zero-point correction (Hartree): 0.156604
29996
29997 diHPCARP_Ic.pttmtmmd
29998 -----

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29999 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18433740
30000 Electronic state : 2-A
30001 Cartesian coordinates (Angs):
30002 O 2.001428 1.779151 -0.099810
30003 O 2.018780 0.584792 -0.868819
30004 C 1.152801 -0.388511 -0.302712
30005 C -0.305364 -0.061030 -0.694430
30006 C -1.340647 -1.017415 -0.115257
30007 O -2.644286 -0.650092 -0.605274
30008 O -3.168718 0.310055 0.094079
30009 H 1.187354 2.208900 -0.400865
30010 C 1.585590 -1.701242 -0.950000
30011 H 2.649909 -1.850974 -0.780417
30012 H 1.406158 -1.666948 -2.023743
30013 H 1.043541 -2.534109 -0.508687
30014 C 1.371162 -0.508213 1.203141
30015 O 0.812183 -1.351880 1.849188
30016 H 2.105013 0.182937 1.639446
30017 H -0.351780 -0.096141 -1.786137
30018 O -0.648072 1.286165 -0.427464
30019 O -0.700032 1.478180 0.979609
30020 H -1.650830 1.357070 1.142948
30021 H -1.175605 -2.031755 -0.468374
30022 H -1.365279 -1.001486 0.969299
30023 Rotational constants (GHz): 1.3601900 0.7434300 0.6541200
30024 Vibrational harmonic frequencies (cm-1):
30025 64.2884 91.5256 109.3858
30026 141.7359 165.6709 186.9530
30027 196.2948 209.7329 235.1733
30028 279.7322 292.9895 302.0843
30029 325.2695 351.0658 393.0612
30030 469.9354 489.7308 517.6206
30031 531.1947 578.5809 649.6372
30032 656.8530 834.9128 905.0888
30033 932.1428 967.9344 979.4032
30034 999.6628 1010.0815 1056.1948
30035 1120.8784 1132.9334 1186.6458
30036 1209.4572 1244.6553 1253.7251
30037 1307.3597 1334.3418 1385.2308
30038 1399.9852 1404.2464 1416.2328
30039 1432.7587 1440.3419 1480.2287
30040 1489.1402 1506.3373 1849.3845
30041 3052.5855 3078.4471 3084.3045
30042 3135.2628 3156.6548 3171.2976
30043 3201.9216 3707.6479 3772.8082
30044 Zero-point correction (Hartree): 0.156917
30045
30046 diHPCARP_Ic.pttpmtmmd
30047 -----
30048 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18066657
30049 Electronic state : 2-A
30050 Cartesian coordinates (Angs):
30051 O 2.304349 1.260405 -0.687636
30052 O 1.822610 0.042223 -1.236832
30053 C 0.933952 -0.588736 -0.326788
30054 C -0.455484 0.075562 -0.413634
30055 C -1.491949 -0.467040 0.553321
30056 O -2.780376 0.100327 0.236206
30057 O -3.229921 -0.341884 -0.898097
30058 H 1.583367 1.875524 -0.885155
30059 C 0.856780 -2.032262 -0.822063
30060 H 1.860147 -2.452081 -0.860589
30061 H 0.428849 -2.058540 -1.823170
30062 H 0.252636 -2.633407 -0.147441
30063 C 1.529842 -0.618297 1.075825
30064 O 0.928550 -1.079105 2.006384
30065 H 2.564946 -0.255965 1.159896
30066 H -0.816216 -0.084022 -1.432852
30067 O -0.387105 1.493085 -0.349648
30068 O 0.030670 1.873241 0.958937
30069 H -0.755971 2.327683 1.287788
30070 H -1.574926 -1.548546 0.489202

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30071      H      -1.291886      -0.172354      1.577839
30072 Rotational constants (GHz):      1.2756900      0.7141900      0.6581000
30073 Vibrational harmonic frequencies (cm-1):
30074      33.9412      63.2489      83.1995
30075      119.8894      140.7023      177.0282
30076      190.4076      211.9096      234.3091
30077      274.6321      277.5024      290.4023
30078      317.5021      324.6119      350.7728
30079      375.9386      474.6498      492.3214
30080      518.1226      575.7091      650.0348
30081      661.9497      834.2424      910.0228
30082      936.7519      956.8511      980.2943
30083      988.9518      1006.8824      1057.3104
30084      1119.2708      1137.7344      1183.8911
30085      1202.6142      1245.5444      1259.0560
30086      1310.4173      1316.4257      1380.1316
30087      1399.3027      1402.3630      1409.1462
30088      1420.0411      1432.0754      1472.4495
30089      1489.2070      1506.3776      1854.7537
30090      3037.9822      3079.4621      3094.9853
30091      3135.1624      3156.6535      3174.4277
30092      3204.2154      3784.5203      3813.1890
30093 Zero-point correction (Hartree): 0.156126
30094
30095 diHPCARP_Ic.pttpmtmpd
30096 -----
30097 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18116379
30098 Electronic state : 2-A
30099 Cartesian coordinates (Angs):
30100      O      -2.328758      -1.143434      -0.739146
30101      O      -1.795955      0.079366      -1.240745
30102      C      -0.826308      0.621306      -0.347265
30103      C      0.469741      -0.214676      -0.363401
30104      C      1.536463      0.263565      0.607813
30105      O      2.811214      -0.290322      0.219908
30106      O      3.228962      0.229141      -0.892962
30107      H      -1.825069      -1.792712      -1.250017
30108      C      -0.564880      2.012730      -0.920294
30109      H      -1.512099      2.532832      -1.049321
30110      H      -0.070425      1.932990      -1.886791
30111      H      0.055447      2.585775      -0.236888
30112      C      -1.426977      0.786961      1.044414
30113      O      -0.833043      1.332672      1.930537
30114      H      -2.460652      0.420457      1.166495
30115      H      0.874167      -0.155225      -1.376921
30116      O      0.234231      -1.602037      -0.200470
30117      O      -0.306788      -1.818719      1.095104
30118      H      -1.255209      -1.872941      0.897993
30119      H      1.635904      1.344808      0.619374
30120      H      1.350786      -0.108630      1.610656
30121 Rotational constants (GHz):      1.2518500      0.7208200      0.6608700
30122 Vibrational harmonic frequencies (cm-1):
30123      54.6685      74.4712      101.4021
30124      126.7470      150.4695      173.9076
30125      191.0340      215.6776      238.9018
30126      271.1342      285.3048      305.1329
30127      325.6519      351.5947      382.5515
30128      434.9526      484.1616      511.8402
30129      524.2137      578.3786      653.3278
30130      665.4007      848.2133      911.0518
30131      938.1531      961.9623      984.1582
30132      990.0994      1012.1143      1044.0228
30133      1124.8831      1133.3287      1177.8060
30134      1206.1852      1248.8691      1253.2512
30135      1314.6062      1316.8607      1386.0953
30136      1402.6266      1414.0089      1414.7183
30137      1420.4611      1439.6205      1471.1433
30138      1490.2995      1506.5963      1861.5999
30139      2996.9819      3083.9265      3093.0338
30140      3137.2891      3160.5754      3181.2811
30141      3202.8671      3736.3340      3789.3885
30142 Zero-point correction (Hartree): 0.156636

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30143
30144 diHPCARP_Ic.tmmmmmmmpd
30145 -----
30146 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18158921
30147 Electronic state : 2-A
30148 Cartesian coordinates (Angs):
30149 O -2.659587 -0.325476 -0.774192
30150 O -1.384022 0.289806 -0.706339
30151 C -0.691052 -0.145453 0.454403
30152 C 0.633010 0.652404 0.450212
30153 C 1.546149 0.344722 -0.731051
30154 O 2.140061 -0.957775 -0.542570
30155 O 2.952118 -0.973301 0.471455
30156 H -2.427269 -1.182474 -1.166543
30157 C -1.470958 0.133668 1.734877
30158 H -2.445396 -0.345067 1.692993
30159 H -1.598799 1.207942 1.848602
30160 H -0.923839 -0.246247 2.597796
30161 C -0.402077 -1.636926 0.362888
30162 O -0.814060 -2.330321 -0.525921
30163 H 0.191826 -2.058887 1.193364
30164 H 1.175063 0.398878 1.364547
30165 O 0.396260 2.036774 0.565224
30166 O 0.095286 2.571999 -0.717630
30167 H -0.820372 2.283662 -0.857178
30168 H 1.010439 0.272162 -1.672475
30169 H 2.339465 1.085890 -0.789302
30170 Rotational constants (GHz): 1.1002500 0.8783500 0.6269800
30171 Vibrational harmonic frequencies (cm-1):
30172 44.3416 70.6219 105.4942
30173 136.2279 164.3817 182.6398
30174 195.0905 200.8384 230.3792
30175 255.1393 285.4479 318.3638
30176 340.1104 373.3155 405.1345
30177 436.8522 460.0218 498.3222
30178 521.8472 583.4801 611.3948
30179 737.7541 834.7323 887.2132
30180 932.0411 947.5815 984.1946
30181 1007.1112 1028.4287 1065.7113
30182 1112.2951 1138.0002 1192.5947
30183 1217.9775 1232.1557 1256.8474
30184 1298.1545 1328.6295 1386.3736
30185 1400.3222 1408.1517 1421.9545
30186 1446.6963 1458.2810 1484.6791
30187 1489.8264 1504.1513 1852.8501
30188 2983.8646 3079.7758 3091.6790
30189 3124.0530 3155.1918 3179.4737
30190 3195.9690 3737.6241 3749.8004
30191 Zero-point correction (Hartree): 0.156673
30192
30193 diHPCARP_Ic.tmtmmpmmd
30194 -----
30195 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18186870
30196 Electronic state : 2-A
30197 Cartesian coordinates (Angs):
30198 O 2.467908 0.346704 1.450948
30199 O 1.107492 0.161078 1.096344
30200 C 0.984651 0.238667 -0.310542
30201 C -0.504832 -0.040745 -0.636253
30202 C -1.101180 -1.032768 0.353673
30203 O -2.437272 -1.371458 -0.055900
30204 O -3.296356 -0.474437 0.325076
30205 H 2.795575 -0.564364 1.416158
30206 C 1.430750 1.580640 -0.871840
30207 H 2.491698 1.727076 -0.684823
30208 H 0.862369 2.370702 -0.388445
30209 H 1.241288 1.623442 -1.944171
30210 C 1.782765 -0.884018 -0.961827
30211 O 2.323233 -1.763414 -0.351464
30212 H 1.829536 -0.840851 -2.066971
30213 H -0.558268 -0.468476 -1.642704
30214 O -1.288370 1.116998 -0.776586

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30215	O	-1.409717	1.754747	0.484626	
30216	H	-2.268653	1.411228	0.778583	
30217	H	-0.539860	-1.965295	0.349980	
30218	H	-1.141957	-0.625867	1.358776	
30219	Rotational constants (GHz):			1.4849700	0.6624000 0.5768100
30220	Vibrational harmonic frequencies (cm-1):				
30221		62.7271	75.3255		99.3109
30222		145.3721	163.4262		176.5004
30223		188.1796	229.1305		241.6021
30224		262.6360	301.3829		309.3020
30225		333.3368	371.3543		399.1287
30226		428.7718	471.6093		495.9054
30227		534.8020	580.7924		626.0971
30228		773.6174	845.9034		877.0327
30229		927.9196	949.3394		988.9730
30230		999.4935	1019.1020		1046.0588
30231		1121.6816	1144.8046		1193.8505
30232		1214.8694	1237.0587		1253.4130
30233		1311.6648	1335.6725		1395.2330
30234		1401.9177	1404.9154		1418.3391
30235		1432.8911	1440.0294		1480.9187
30236		1481.6895	1505.2151		1858.3002
30237		2957.3147	3063.5090		3082.6557
30238		3121.4818	3159.5331		3181.7238
30239		3193.3465	3743.6757		3766.6225
30240	Zero-point correction (Hartree): 0.156798				
30241	diHPCARP_Ic.tmtmptmmd				
30242	-----				
30243	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18090079				
30244	Electronic state : 2-A				
30245	Cartesian coordinates (Angs):				
30246	O	2.400386	-1.081345	-1.382117	
30247	O	1.055096	-0.758816	-1.057892	
30248	C	1.053247	-0.004121	0.152566	
30249	C	-0.421058	0.342923	0.447982	
30250	C	-1.179444	0.680076	-0.828556	
30251	O	-2.513705	1.104780	-0.501551	
30252	O	-3.305017	0.093494	-0.307982	
30253	H	2.434223	-2.020573	-1.160268	
30254	C	1.673302	-0.753776	1.321297	
30255	H	2.737927	-0.904605	1.157547	
30256	H	1.171108	-1.711484	1.443022	
30257	H	1.540873	-0.168834	2.229574	
30258	C	1.810119	1.299985	-0.097180	
30259	O	1.787916	2.215715	0.675712	
30260	H	2.376587	1.343007	-1.042931	
30261	H	-0.404758	1.215393	1.105269	
30262	O	-1.088405	-0.617912	1.226918	
30263	O	-1.254813	-1.808113	0.470478	
30264	H	-2.158844	-1.684745	0.139197	
30265	H	-0.718557	1.527331	-1.334250	
30266	H	-1.247212	-0.168433	-1.502339	
30267	Rotational constants (GHz):			1.3584700	0.6712700 0.5938600
30268	Vibrational harmonic frequencies (cm-1):				
30269		45.8552	67.5296		91.5809
30270		117.6388	158.3236		169.2449
30271		178.4203	214.4536		231.5781
30272		260.1971	288.0394		295.0027
30273		305.7316	332.7697		365.7681
30274		397.0197	466.9300		490.1661
30275		531.4156	580.9130		640.7511
30276		693.8299	805.4695		892.6569
30277		942.9833	971.1244		985.1805
30278		999.5750	1018.1732		1042.4457
30279		1117.9569	1152.8018		1185.0402
30280		1220.9149	1239.4877		1257.2582
30281		1310.5796	1336.0591		1393.3111
30282		1396.8194	1405.4230		1412.2958
30283		1414.0189	1439.8908		1479.8715
30284		1487.3705	1504.7723		1861.5296
30285		3000.9403	3082.4892		3101.1710

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30287          3112.8928          3164.4029          3169.0397
30288          3184.7297          3742.4453          3815.9106
30289 Zero-point correction (Hartree): 0.156214
30290
30291 diHPCARP_Ic.tmtppmmpd
30292 -----
30293 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18019186
30294 Electronic state : 2-A
30295 Cartesian coordinates (Angs):
30296 O      -2.720676      0.219522      -0.940769
30297 O      -1.320894      0.429099      -0.840754
30298 C      -0.856591     -0.028645      0.419608
30299 C       0.659480      0.261166      0.423942
30300 C       1.372348     -0.319285     -0.784981
30301 O       2.776713     -0.472827     -0.499644
30302 O       2.972743     -1.374774      0.411861
30303 H      -2.747956     -0.699413     -1.249830
30304 C      -1.551408      0.662887      1.586605
30305 H      -2.621383      0.476759      1.549353
30306 H      -1.367700      1.733870      1.539085
30307 H      -1.154727      0.293546      2.532247
30308 C      -1.052810     -1.532077      0.543266
30309 O      -1.569603     -2.206019     -0.303888
30310 H      -0.691354     -1.976656      1.489073
30311 H       1.074204     -0.208458      1.320231
30312 O       0.938878      1.630840      0.619306
30313 O       0.681539      2.362133     -0.570215
30314 H      -0.285771      2.359898     -0.633683
30315 H       0.979079     -1.299844     -1.048867
30316 H       1.319892      0.352235     -1.635413
30317 Rotational constants (GHz): 1.2353900      0.7387100      0.5803500
30318 Vibrational harmonic frequencies (cm-1):
30319      27.8781          51.9731          99.0341
30320      125.0356         153.9878         161.8178
30321      176.2935         220.1946         241.9736
30322      267.4251         285.1860         317.8652
30323      322.2657         364.9943         376.7231
30324      401.0298         425.6239         486.5271
30325      518.9961         577.3182         640.8662
30326      781.5761         838.3467         882.1829
30327      929.1113         946.9770         967.7613
30328      997.0293         1014.4914        1049.9798
30329      1125.3574        1143.1132        1178.5746
30330      1216.8133        1243.3125        1252.7096
30331      1313.7282        1326.5104        1394.1796
30332      1404.8077        1411.8026        1421.5891
30333      1440.7888        1455.7793        1478.3218
30334      1491.0576        1499.3033        1857.8891
30335      2969.6455        3080.8997        3085.0278
30336      3113.8133        3155.6210        3178.0778
30337      3195.6848        3754.9579        3759.1674
30338 Zero-point correction (Hartree): 0.156280
30339
30340 diHPCARP_Ic.tpppmmpd
30341 -----
30342 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18329845
30343 Electronic state : 2-A
30344 Cartesian coordinates (Angs):
30345 O       2.778805     -1.292457     -0.305303
30346 O       1.542176     -0.831859     -0.819616
30347 C       0.876434     -0.070655      0.170467
30348 C      -0.412439      0.361301     -0.556369
30349 C      -1.309806     -0.795685     -0.988183
30350 O      -1.988094     -1.398676      0.128628
30351 O      -3.015225     -0.702949      0.511080
30352 H       3.349203     -0.531363     -0.495764
30353 C       0.636064     -0.850715      1.457286
30354 H       1.577022     -1.008452      1.979558
30355 H       0.203393     -1.820701      1.223979
30356 H      -0.050336     -0.305223      2.103085
30357 C       1.676959      1.189655      0.490298
30358 O       2.711071      1.455968     -0.057730

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30359	H	1.255475	1.836231	1.276697	
30360	H	-0.116653	0.888558	-1.469518	
30361	O	-1.063803	1.251369	0.320321	
30362	O	-2.135790	1.854990	-0.381310	
30363	H	-2.873109	1.283767	-0.110232	
30364	H	-2.069774	-0.449624	-1.684676	
30365	H	-0.711609	-1.587686	-1.432680	
30366	Rotational constants (GHz):		1.5655000	0.6635400	0.5510200
30367	Vibrational harmonic frequencies (cm-1):				
30368		45.1440	68.8644		89.8987
30369		165.2928	169.0907		186.4797
30370		193.7682	223.0668		249.6092
30371		256.0192	268.1056		304.5681
30372		333.9849	360.2192		386.8402
30373		438.4906	503.2985		513.1060
30374		517.9787	560.8073		661.6203
30375		768.1150	837.4785		861.7815
30376		924.4796	934.3389		994.0694
30377		1006.2159	1045.3808		1057.6548
30378		1072.2037	1168.5740		1173.7571
30379		1238.4934	1253.5388		1285.8762
30380		1321.4775	1363.0043		1375.4289
30381		1399.8456	1410.1047		1416.5047
30382		1440.2876	1452.6116		1479.5562
30383		1488.5852	1504.8283		1854.4625
30384		3012.2317	3057.4953		3084.2977
30385		3114.7523	3163.5618		3170.5224
30386		3178.4437	3730.1729		3748.5746
30387	Zero-point correction (Hartree): 0.156931				
30388					
30389	diHPCARP_Ic.tptmmmmmd				
30390	-----				
30391	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18281895				
30392	Electronic state : 2-A				
30393	Cartesian coordinates (Angs):				
30394	O	2.805979	-1.337741	0.360574	
30395	O	1.473236	-1.237282	-0.109703	
30396	C	0.948701	0.042370	0.201505	
30397	C	-0.456273	-0.017824	-0.445026	
30398	C	-1.330556	-1.088243	0.186194	
30399	O	-2.547998	-1.227347	-0.569244	
30400	O	-3.414411	-0.306475	-0.275020	
30401	H	3.289937	-0.936273	-0.378046	
30402	C	0.966034	0.333115	1.696224	
30403	H	1.992604	0.298434	2.054211	
30404	H	0.390726	-0.416388	2.236191	
30405	H	0.540280	1.312664	1.898942	
30406	C	1.733673	1.127428	-0.528975	
30407	O	2.658508	0.884961	-1.254770	
30408	H	1.401798	2.161550	-0.340332	
30409	H	-0.312465	-0.268646	-1.499512	
30410	O	-1.081989	1.246704	-0.505923	
30411	O	-1.585161	1.610733	0.771354	
30412	H	-2.504378	1.306170	0.691710	
30413	H	-0.834503	-2.053249	0.126584	
30414	H	-1.598788	-0.853754	1.212572	
30415	Rotational constants (GHz):		1.6374500	0.6033800	0.5407700
30416	Vibrational harmonic frequencies (cm-1):				
30417		20.5415	72.0365		99.6155
30418		136.6697	169.6905		181.6760
30419		196.2933	223.5272		242.3163
30420		272.4114	292.1917		308.4395
30421		336.9964	358.3724		381.8030
30422		421.2028	498.9270		521.6988
30423		535.6884	569.8552		636.3114
30424		753.3897	835.9175		876.7894
30425		933.2807	957.9256		980.8117
30426		999.2604	1010.8325		1050.1344
30427		1111.8370	1149.3875		1178.5476
30428		1235.3632	1254.6207		1272.7106
30429		1314.6608	1336.4105		1381.2833
30430		1405.3801	1409.5358		1417.2378

30431	1441.1593	1451.9589	1485.3476
30432	1490.9256	1508.0241	1854.5009
30433	3007.0238	3081.5986	3087.3597
30434	3126.3512	3163.1382	3175.4379
30435	3192.1127	3723.2589	3750.2351

30436 Zero-point correction (Hartree): 0.156920

30437
30438
30439
30440 1,4-aldehyde-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-HPCARP-Ia)
30441 =====

30442
30443 TS.diHPCARP_I.14aldHshift.mmmmpd
30444 -----

30445 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14160559

30446 Electronic state : 2-A

30447 Cartesian coordinates (Angs):

30448	C	0.790731	1.495885	-0.300244
30449	C	-0.508154	0.615625	-0.210502
30450	O	-0.839482	0.809673	1.142633
30451	O	-0.678632	2.154041	1.407620
30452	H	0.426046	2.232333	0.726958
30453	O	1.637114	1.502687	-1.112789
30454	C	-1.514548	1.214135	-1.180750
30455	H	-1.157535	1.099175	-2.203369
30456	H	-1.666308	2.268063	-0.961893
30457	H	-2.455357	0.679114	-1.068500
30458	C	-0.193029	-0.856302	-0.487139
30459	H	0.410143	-0.885349	-1.398639
30460	O	-1.331338	-1.604142	-0.845616
30461	O	-2.236482	-1.561115	0.258115
30462	H	-2.383321	-2.501129	0.418295
30463	C	0.595578	-1.496206	0.649213
30464	O	1.792400	-0.782683	0.879920
30465	H	0.048643	-1.432812	1.586949
30466	H	0.816244	-2.536693	0.407935
30467	O	2.675879	-1.085979	-0.194081
30468	H	2.782297	-0.221371	-0.617633

30469 Rotational constants (GHz): 1.0560100 0.9357900 0.6778500

30470 Vibrational harmonic frequencies (cm-1):

30471	i2066.0156	70.2036	103.8582
30472	113.2405	152.7801	168.0521
30473	182.4275	205.9644	211.7519
30474	216.7260	242.6532	265.8495
30475	297.5295	319.8005	348.1490
30476	363.5510	460.9331	473.2178
30477	508.3896	571.5470	594.6044
30478	614.2923	716.9597	775.3266
30479	865.7161	938.1747	956.4990
30480	978.4634	1026.8194	1067.6057
30481	1075.0832	1113.5897	1127.1515
30482	1129.3820	1140.7951	1204.0192
30483	1257.8601	1284.8988	1337.5685
30484	1377.2619	1397.3555	1398.4732
30485	1425.5646	1441.5933	1480.5102
30486	1489.1380	1497.4152	1817.9180
30487	1972.5126	3080.8326	3089.1096
30488	3089.6408	3161.7865	3166.2766
30489	3175.0927	3773.9663	3832.7309

30490 Zero-point correction (Hartree): 0.150698

30491
30492 TS.diHPCARP_I.14aldHshift.mmmmtmd
30493 -----

30494 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13918545

30495 Electronic state : 2-A

30496 Cartesian coordinates (Angs):

30497	C	-1.214949	-1.170266	-0.621380
30498	C	0.157359	-0.787775	0.032880
30499	O	-0.273219	-0.251965	1.264370
30500	O	-1.329015	-1.027873	1.722570
30501	H	-1.843536	-1.179332	0.508713
30502	O	-1.456759	-1.494218	-1.716355

30503	C	0.957222	-2.070946	0.172028	
30504	H	1.179873	-2.475449	-0.814369	
30505	H	0.389026	-2.800369	0.745075	
30506	H	1.888261	-1.845949	0.687159	
30507	C	0.846296	0.300956	-0.795640	
30508	H	0.738056	0.012568	-1.844465	
30509	O	2.245996	0.330484	-0.630358	
30510	O	2.516144	0.558418	0.751563	
30511	H	3.051289	1.360423	0.713328	
30512	C	0.209734	1.668603	-0.550954	
30513	O	-1.198976	1.511419	-0.629114	
30514	H	0.479761	2.030056	0.437428	
30515	H	0.543798	2.379743	-1.307752	
30516	O	-1.809254	2.065414	0.523412	
30517	H	-1.719840	1.341446	1.164577	
30518	Rotational constants (GHz):		1.0549200	0.9148800	0.7343700
30519	Vibrational harmonic frequencies (cm-1):				
30520	i1840.8431		86.3148		97.6349
30521	103.1004		125.1755		152.1767
30522	154.0839		192.1971		222.9270
30523	232.4300		246.4247		262.4928
30524	295.6988		320.2935		363.4126
30525	434.8006		452.1557		477.4919
30526	522.6333		558.4857		589.9140
30527	619.9378		716.0332		761.1745
30528	872.7564		932.7250		963.9502
30529	991.2509		1022.4265		1064.0665
30530	1073.4539		1116.9061		1127.6184
30531	1131.5187		1142.6611		1194.6197
30532	1251.0396		1267.1519		1344.2043
30533	1369.4068		1388.4479		1401.5606
30534	1420.9237		1456.6595		1481.6508
30535	1498.6317		1509.1203		1822.3423
30536	2006.5216		3080.4012		3082.2255
30537	3088.5665		3162.4230		3163.1543
30538	3173.4018		3731.6782		3832.1867
30539	Zero-point correction (Hartree):		0.150707		
30540					
30541	TS.diHPCARP_I.14aldHshift.mmmppmd				
30542	-----				
30543	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13915647				
30544	Electronic state : 2-A				
30545	Cartesian coordinates (Angs):				
30546	C	1.737466	-0.731867	-0.358292	
30547	C	0.770891	0.461503	-0.038591	
30548	O	0.400816	0.131478	1.284642	
30549	O	1.545801	-0.287941	1.936965	
30550	H	1.980850	-0.970073	0.897353	
30551	O	2.123113	-1.121378	-1.390462	
30552	C	1.576234	1.750155	-0.103580	
30553	H	2.005449	1.878427	-1.096269	
30554	H	2.370806	1.728086	0.637607	
30555	H	0.902629	2.579123	0.106697	
30556	C	-0.412169	0.452722	-1.013404	
30557	H	0.025436	0.675629	-1.990909	
30558	O	-1.285006	1.547768	-0.839656	
30559	O	-1.808456	1.552579	0.477755	
30560	H	-2.467167	0.840260	0.459753	
30561	C	-1.129956	-0.902058	-1.162441	
30562	O	-1.062323	-1.775734	-0.063891	
30563	H	-2.169884	-0.720036	-1.445273	
30564	H	-0.645324	-1.467281	-1.959283	
30565	O	-1.913204	-1.282247	0.958867	
30566	H	-1.263522	-0.843061	1.534417	
30567	Rotational constants (GHz):		1.1395400	0.8727700	0.7919000
30568	Vibrational harmonic frequencies (cm-1):				
30569	i1964.1068		43.3482		116.1334
30570	128.7894		135.3668		159.0675
30571	198.7064		210.3996		215.6328
30572	243.8556		265.0548		277.3803
30573	299.2280		327.2448		373.7556
30574	428.8099		485.2264		507.9792

30575	555.8227	601.7223	619.0259			
30576	657.9438	730.3278	775.5089			
30577	876.3898	900.9525	958.0330			
30578	982.0984	1032.4170	1057.7095			
30579	1065.3158	1073.7867	1128.1308			
30580	1135.5034	1154.2375	1189.2946			
30581	1254.0295	1310.2269	1362.2835			
30582	1377.8008	1397.9769	1412.7138			
30583	1441.9624	1461.3788	1479.2002			
30584	1485.9114	1496.3261	1822.4026			
30585	1998.9938	3064.1835	3076.0618			
30586	3080.4670	3126.1438	3159.0148			
30587	3176.7132	3692.5900	3742.7777			
30588	Zero-point correction (Hartree): 0.151109					
30589						
30590	TS.diHPCARP_I.14aldHshift.mmmmtmmd					
30591	-----					
30592	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14017248					
30593	Electronic state : 2-A					
30594	Cartesian coordinates (Angs):					
30595	C	2.039312	-1.012999	-0.235045		
30596	C	1.048072	0.210721	-0.133626		
30597	O	1.106459	0.438127	1.254610		
30598	O	2.436574	0.386523	1.619255		
30599	H	2.679833	-0.646256	0.849658		
30600	O	2.129123	-1.836894	-1.058590		
30601	C	1.651499	1.327018	-0.969538		
30602	H	1.619867	1.055580	-2.023636		
30603	H	2.678831	1.511722	-0.666214		
30604	H	1.056329	2.224917	-0.816740		
30605	C	-0.371816	-0.175300	-0.559630		
30606	H	-0.284503	-0.826065	-1.434152		
30607	O	-1.101253	0.915741	-1.067710		
30608	O	-1.321795	1.841966	-0.014904		
30609	H	-2.213761	1.583653	0.263868		
30610	C	-1.111942	-0.926600	0.541293		
30611	O	-2.393090	-1.342302	0.110669		
30612	H	-0.574846	-1.848476	0.773690		
30613	H	-1.193829	-0.334515	1.450338		
30614	O	-3.281888	-0.238137	0.258821		
30615	H	-3.891728	-0.577793	0.925264		
30616	Rotational constants (GHz):			1.4324500	0.6428500	0.5815900
30617	Vibrational harmonic frequencies (cm-1):					
30618	i2008.4590		52.5308			78.2983
30619	116.3820		132.6766			158.5246
30620	181.6552		196.9397			220.8850
30621	247.9031		259.1471			267.3929
30622	313.5472		325.3380			349.3466
30623	417.0789		480.2032			492.1404
30624	517.0068		556.9004			574.1837
30625	646.1562		705.7638			814.1670
30626	857.0083		894.9753			956.4398
30627	988.7424		1004.5072			1055.0371
30628	1071.7319		1104.1608			1123.4507
30629	1132.2854		1154.4361			1194.5036
30630	1260.8598		1308.7765			1321.7002
30631	1391.4657		1396.9845			1400.9475
30632	1425.8040		1440.4566			1468.5768
30633	1477.1759		1498.3844			1816.3452
30634	1999.1521		3081.3014			3083.5654
30635	3084.9173		3151.7159			3164.7112
30636	3176.8392		3753.8138			3825.4149
30637	Zero-point correction (Hartree): 0.150747					
30638						
30639	TS.diHPCARP_I.14aldHshift.mmmtpdp					
30640	-----					
30641	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13885427					
30642	Electronic state : 2-A					
30643	Cartesian coordinates (Angs):					
30644	C	-1.603584	1.364532	-0.182991		
30645	C	-1.009066	-0.096541	-0.184676		
30646	O	-1.322904	-0.476280	1.134304		

30647	O	-2.624211	-0.082424	1.371807			
30648	H	-2.460493	1.068409	0.764564			
30649	O	-1.358715	2.273388	-0.874953			
30650	C	-1.768878	-0.872108	-1.248063			
30651	H	-1.516864	-0.486622	-2.234847			
30652	H	-2.839897	-0.789063	-1.081890			
30653	H	-1.468970	-1.916293	-1.187725			
30654	C	0.506111	-0.087756	-0.395217			
30655	H	0.723964	0.645216	-1.175606			
30656	O	0.981403	-1.285737	-0.964546			
30657	O	0.773550	-2.337619	-0.029159			
30658	H	1.681782	-2.546706	0.224869			
30659	C	1.248177	0.296405	0.877365			
30660	O	2.643177	0.304052	0.686005			
30661	H	0.895823	1.270445	1.230520			
30662	H	1.082644	-0.441718	1.659304			
30663	O	2.936852	1.307862	-0.279574			
30664	H	3.432247	1.943209	0.251242			
30665	Rotational constants (GHz):				1.2296400	0.7099000	0.5868400
30666	Vibrational harmonic frequencies (cm-1):						
30667	i2003.0694		31.0847			53.7608	
30668	100.5262		128.2342			145.5837	
30669	151.6348		202.0316			211.3014	
30670	223.3062		242.0372			267.7840	
30671	289.5198		324.8233			332.1606	
30672	359.6809		416.1115			479.9114	
30673	513.9289		555.2017			579.8164	
30674	673.0979		706.4005			806.9208	
30675	860.5488		901.9464			955.8454	
30676	990.6694		997.3887			1055.6720	
30677	1072.8153		1101.1003			1128.2059	
30678	1140.7649		1156.0210			1195.8739	
30679	1263.0399		1301.3996			1325.4117	
30680	1387.5848		1396.0880			1399.7382	
30681	1411.8749		1427.8354			1471.6863	
30682	1477.9057		1498.8241			1818.3383	
30683	2000.1617		3056.1987			3082.4034	
30684	3097.2885		3155.0128			3163.5099	
30685	3176.2879		3812.3689			3830.1576	
30686	Zero-point correction (Hartree):				0.150142		
30687							
30688	TS.diHPCARP_I.14aldHshift.mmtmmpd						
30689	-----						
30690	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.16978516						
30691	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.04722798						
30692	T1 diagnostic: 0.023190						
30693	E(MP2/Aug-CC-pVTZ) (Hartree): -721.00799454						
30694	E(MP3/Aug-CC-pVTZ) (Hartree): -721.02154034						
30695	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01596912						
30696	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02638124						
30697	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47145410						
30698	E(UHF/Aug-CC-pVTZ) (Hartree): -718.46038391						
30699	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14214706						
30700	Electronic state : 2-A						
30701	Cartesian coordinates (Angs):						
30702	C	-0.751915	1.520446	0.122273			
30703	C	0.506743	0.599272	0.253469			
30704	O	1.048337	0.716324	-1.042003			
30705	O	0.956366	2.048697	-1.400497			
30706	H	-0.254153	2.166466	-0.898597			
30707	O	-1.661390	1.664620	0.848191			
30708	C	1.377692	1.228267	1.333374			
30709	H	0.842251	1.237357	2.281771			
30710	H	1.643513	2.244987	1.055257			
30711	H	2.282091	0.633765	1.451820			
30712	C	0.152031	-0.863812	0.534605			
30713	H	-0.444216	-0.877898	1.450372			
30714	O	1.292912	-1.622808	0.873436			
30715	O	2.056086	-1.862368	-0.301162			
30716	H	2.593636	-1.061706	-0.387497			
30717	C	-0.646871	-1.500150	-0.598181			
30718	O	-1.809446	-0.748103	-0.871248			

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30719      H      -0.083493      -1.485389      -1.526854
30720      H      -0.904561      -2.526183      -0.336142
30721      O      -2.715785      -0.967106      0.204472
30722      H      -2.837777      -0.069589      0.547114
30723      Rotational constants (GHz):      1.0530100      0.9445800      0.6707000
30724      Vibrational harmonic frequencies (cm-1):
30725      i1989.6085      57.2310      104.8505
30726      128.8500      154.3406      177.1738
30727      181.1811      202.3371      217.0907
30728      248.6631      266.5616      283.4700
30729      312.7184      324.0598      351.1731
30730      370.4045      450.6300      487.5059
30731      508.0690      584.5074      595.1405
30732      621.0177      716.1322      771.6264
30733      875.1662      935.4429      954.5329
30734      975.2916      1023.4466      1064.3310
30735      1074.8913      1115.2705      1124.9162
30736      1127.3828      1139.3247      1197.2476
30737      1253.9705      1284.8808      1330.2761
30738      1380.4985      1399.2681      1409.8540
30739      1427.7066      1443.1091      1484.4267
30740      1487.4912      1493.8133      1816.9103
30741      1976.7650      3078.8258      3093.3199
30742      3099.8738      3155.9112      3173.3372
30743      3178.2442      3776.5321      3778.5795
30744      Zero-point correction (Hartree): 0.150919
30745
30746      TS.diHPCARP_I.14aldHshift.mppppmd
30747      -----
30748      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14052230
30749      Electronic state : 2-A
30750      Cartesian coordinates (Angs):
30751      C      1.658490      -0.620273      -0.233806
30752      C      0.604107      0.540036      -0.175338
30753      O      0.301505      0.545192      1.204426
30754      O      1.489423      0.370605      1.895210
30755      H      1.934706      -0.540485      1.025070
30756      O      2.130706      -1.163662      -1.153653
30757      C      1.356000      1.779604      -0.642990
30758      H      1.693383      1.629789      -1.668164
30759      H      2.219836      1.956023      -0.005603
30760      H      0.689794      2.637863      -0.611084
30761      C      -0.710458      0.246523      -0.929601
30762      H      -0.660313      0.705723      -1.920511
30763      O      -1.825400      0.763435      -0.229860
30764      O      -1.685954      2.171601      -0.121980
30765      H      -1.423313      2.266394      0.804697
30766      C      -0.976144      -1.253397      -1.061988
30767      O      -0.531345      -1.986645      0.057434
30768      H      -2.038847      -1.425228      -1.232436
30769      H      -0.398139      -1.650954      -1.895641
30770      O      -1.444644      -1.792180      1.124757
30771      H      -1.083399      -1.000853      1.555341
30772      Rotational constants (GHz):      1.0414300      0.9805600      0.7633500
30773      Vibrational harmonic frequencies (cm-1):
30774      i1824.2514      71.7494      107.9365
30775      126.8582      158.3189      169.0975
30776      190.0747      212.7184      233.1547
30777      253.8600      272.0222      286.2463
30778      339.6350      354.9757      379.1024
30779      425.6473      443.1864      466.9385
30780      499.0776      557.0902      612.4693
30781      668.3569      724.0000      807.0740
30782      870.2919      891.3034      947.7202
30783      978.6305      1029.0452      1060.9211
30784      1070.2517      1081.6246      1115.6221
30785      1144.9938      1162.7151      1175.8848
30786      1248.8275      1307.9010      1344.9563
30787      1377.8607      1396.0649      1404.5148
30788      1421.7651      1464.5696      1469.7898
30789      1487.8857      1499.5554      1823.0663
30790      2000.6288      3068.8074      3079.3505

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30791          3092.4317          3148.7829          3158.0385
30792          3175.1421          3736.2502          3782.7017
30793 Zero-point correction (Hartree): 0.151219
30794
30795 TS.diHPCARP_I.14aldHshift.mppmmpd
30796 -----
30797 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14073786
30798 Electronic state : 2-A
30799 Cartesian coordinates (Angs):
30800 C      -1.050189      1.101086      0.703243
30801 C      0.329647      0.739410      0.055104
30802 O      0.142321      1.257943     -1.239274
30803 O     -0.461081      2.491110     -1.097003
30804 H     -1.264562      2.069935     -0.158229
30805 O     -1.545287      0.709041      1.692617
30806 C      1.390502      1.481509      0.855186
30807 H      1.433454      1.091565      1.870682
30808 H      1.164221      2.544733      0.875707
30809 H      2.353981      1.323406      0.374975
30810 C      0.549299     -0.770998     -0.032246
30811 H      0.410872     -1.192684      0.965392
30812 O      1.844264     -1.087932     -0.500755
30813 O      2.735468     -1.115433      0.610118
30814 H      3.035926     -2.032427      0.583614
30815 C     -0.420809     -1.429212     -1.010393
30816 O     -1.755128     -1.108395     -0.685565
30817 H     -0.272018     -1.040360     -2.015789
30818 H     -0.278952     -2.509161     -1.003314
30819 O     -2.100941     -1.871878      0.464154
30820 H     -2.250546     -1.181415      1.127264
30821 Rotational constants (GHz):      1.0027800      0.9118700      0.6655500
30822 Vibrational harmonic frequencies (cm-1):
30823 i2053.8494          63.9001          83.4830
30824 126.4439          157.1230          172.3251
30825 189.0221          214.3883          221.3998
30826 258.0815          264.1906          274.1486
30827 287.8869          335.9356          350.4015
30828 385.2494          394.0119          489.2565
30829 512.6153          538.3763          599.5008
30830 638.0549          691.5792          761.3270
30831 876.2401          936.8630          958.8297
30832 1018.4220         1023.2535         1069.6517
30833 1079.2858         1107.0416         1119.3452
30834 1134.5147         1146.7169         1197.6519
30835 1262.4763         1289.0632         1331.8475
30836 1392.1776         1401.3163         1408.8039
30837 1413.7849         1447.0880         1480.4535
30838 1484.9413         1506.1461         1814.4742
30839 1970.6946         3083.2541         3091.9385
30840 3099.2932         3163.1591         3166.6034
30841 3174.0157         3766.5526         3823.6914
30842 Zero-point correction (Hartree): 0.150925
30843
30844 TS.diHPCARP_I.14aldHshift.mtmmmd
30845 -----
30846 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13754827
30847 Electronic state : 2-A
30848 Cartesian coordinates (Angs):
30849 C      1.551307      0.555420      0.619159
30850 C      0.666568     -0.643255      0.105494
30851 O      1.094890     -0.733586     -1.228285
30852 O      2.468880     -0.582135     -1.223460
30853 H      2.421997      0.394936     -0.339452
30854 O      1.495400      1.149303      1.622041
30855 C      1.058478     -1.843734      0.955991
30856 H      0.754716     -1.676556      1.988662
30857 H      2.134996     -1.990831      0.914990
30858 H      0.557859     -2.728110      0.569294
30859 C     -0.819659     -0.305019      0.150018
30860 H     -1.040151      0.077229      1.151127
30861 O     -1.529766     -1.512407     -0.066232
30862 O     -2.895571     -1.251850      0.235945

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30863	H	-3.030132	-1.813832	1.008830	
30864	C	-1.201416	0.725636	-0.905756	
30865	O	-0.410717	1.889778	-0.773532	
30866	H	-0.973901	0.340457	-1.897819	
30867	H	-2.260422	0.968182	-0.829814	
30868	O	-0.840665	2.553742	0.412510	
30869	H	-1.156233	3.391474	0.052861	
30870	Rotational constants (GHz):			1.0395000	0.8693200 0.6428100
30871	Vibrational harmonic frequencies (cm-1):				
30872	i1943.7055		54.7349		75.7529
30873	111.6769		134.7143		147.2863
30874	157.9110		183.4346		200.4156
30875	209.9810		220.2632		252.9777
30876	261.5274		276.4562		323.1658
30877	364.2727		437.0888		463.7926
30878	502.0420		545.3528		595.2275
30879	623.2757		695.4041		772.6471
30880	863.3256		936.1725		958.2972
30881	1015.6582		1034.3565		1069.9387
30882	1082.5872		1099.6128		1116.5226
30883	1132.0337		1156.2607		1200.1079
30884	1261.4697		1288.7613		1338.1055
30885	1387.9600		1395.6420		1398.3649
30886	1411.1985		1426.1606		1480.6735
30887	1482.7137		1499.8972		1814.9175
30888	2006.0449		3070.3102		3081.6833
30889	3101.2139		3162.4624		3163.7020
30890	3174.7109		3824.9242		3831.6884
30891	Zero-point correction (Hartree): 0.150079				
30892					
30893	TS.diHPCARP_I.14aldHshift.mtmmmpd				
30894	-----				
30895	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13984602				
30896	Electronic state : 2-A				
30897	Cartesian coordinates (Angs):				
30898	C	1.562586	0.538228	0.535493	
30899	C	0.632586	-0.665288	0.138680	
30900	O	1.054850	-0.888387	-1.182223	
30901	O	2.432519	-0.807323	-1.182287	
30902	H	2.443509	0.227485	-0.389626	
30903	O	1.504132	1.261125	1.457050	
30904	C	0.982081	-1.799660	1.092889	
30905	H	0.695508	-1.528258	2.108181	
30906	H	2.049883	-2.001353	1.059171	
30907	H	0.436945	-2.690133	0.788820	
30908	C	-0.838956	-0.267193	0.153714	
30909	H	-1.057878	0.142166	1.144929	
30910	O	-1.585806	-1.453756	-0.043416	
30911	O	-2.946091	-1.136418	0.227755	
30912	H	-3.124786	-1.701376	0.989454	
30913	C	-1.164398	0.760785	-0.923761	
30914	O	-0.328026	1.893910	-0.809002	
30915	H	-0.949588	0.347898	-1.907594	
30916	H	-2.210871	1.053892	-0.861575	
30917	O	-0.793149	2.648316	0.304840	
30918	H	-0.033556	2.608701	0.904403	
30919	Rotational constants (GHz):			1.0390400	0.8846800 0.6392600
30920	Vibrational harmonic frequencies (cm-1):				
30921	i2061.6827		61.4318		81.6343
30922	115.7802		144.0487		170.9193
30923	179.0278		205.3263		209.2170
30924	223.2711		253.9919		261.1003
30925	275.1116		320.1485		337.2656
30926	363.4884		436.3090		465.1481
30927	501.4338		544.2459		594.3692
30928	626.4301		697.8392		775.2000
30929	862.5135		939.2422		958.7756
30930	1016.2091		1033.5221		1070.3541
30931	1080.4645		1108.0258		1116.7285
30932	1130.6950		1159.3428		1195.9044
30933	1262.0226		1287.9913		1342.0045
30934	1387.6292		1396.8500		1409.3845

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30935      1421.2048          1441.8363          1482.5087
30936      1487.2510          1498.3636          1816.4102
30937      1974.9755          3064.5248          3081.1420
30938      3106.4472          3161.9074          3166.5392
30939      3174.7840          3772.0934          3822.9824
30940      Zero-point correction (Hartree): 0.150526
30941
30942      TS.diHPCARP_I.14aldHshift.mtpmmpd
30943      -----
30944      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14010321
30945      Electronic state : 2-A
30946      Cartesian coordinates (Angs):
30947      C      1.565532      0.547727      0.524710
30948      C      0.637622      -0.661436      0.142111
30949      O      1.057596      -0.895594      -1.178351
30950      O      2.435180      -0.812039      -1.183698
30951      H      2.446726      0.228259      -0.396576
30952      O      1.504656      1.284336      1.435030
30953      C      0.990227      -1.783750      1.108936
30954      H      0.704750      -1.499655      2.120856
30955      H      2.057973      -1.985534      1.074262
30956      H      0.441209      -2.676475      0.819723
30957      C      -0.835570      -0.270852      0.152532
30958      H      -1.060151      0.133122      1.143743
30959      O      -1.576439      -1.461665      -0.037793
30960      O      -2.900667      -1.197883      0.415552
30961      H      -3.416282      -1.390489      -0.377016
30962      C      -1.166512      0.754300      -0.925430
30963      O      -0.345294      1.897771      -0.816653
30964      H      -0.946504      0.343207      -1.909411
30965      H      -2.216069      1.040200      -0.861871
30966      O      -0.812644      2.646954      0.298921
30967      H      -0.058562      2.596384      0.905060
30968      Rotational constants (GHz):      1.0336900      0.8854700      0.6386800
30969      Vibrational harmonic frequencies (cm-1):
30970      i2056.3104          59.6784          75.4442
30971      107.7288          143.4916          170.8857
30972      175.9482          200.0981          204.7900
30973      223.3758          254.2124          260.6451
30974      276.0836          320.5662          346.2966
30975      363.5528          434.6227          463.5955
30976      501.5016          543.2002          594.5984
30977      628.1253          697.6329          774.4645
30978      862.9443          939.5868          959.7870
30979      1017.8754          1033.6131          1071.9747
30980      1081.8111          1109.0512          1116.6041
30981      1133.8032          1154.3433          1197.3014
30982      1264.0374          1291.9686          1342.3358
30983      1383.7930          1398.6861          1415.3239
30984      1417.1331          1443.0714          1482.4169
30985      1485.9445          1496.7716          1816.3365
30986      1975.8193          3075.4485          3083.3264
30987      3094.3772          3156.2621          3164.2499
30988      3176.7568          3768.4632          3831.2990
30989      Zero-point correction (Hartree): 0.150503
30990
30991      TS.diHPCARP_I.14aldHshift.mtpppmd
30992      -----
30993      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14038788
30994      Electronic state : 2-A
30995      Cartesian coordinates (Angs):
30996      C      1.796181      -0.573744      -0.581538
30997      C      0.841801      0.532541      -0.017414
30998      O      0.656495      0.060208      1.301847
30999      O      1.884862      -0.378154      1.755041
31000      H      2.197023      -0.936011      0.604038
31001      O      2.089076      -0.821278      -1.685421
31002      C      1.597181      1.852874      -0.066413
31003      H      1.871877      2.086197      -1.094141
31004      H      2.494116      1.792479      0.545094
31005      H      0.945023      2.634285      0.320352
31006      C      -0.520404      0.579075      -0.719692

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31007	H	-0.421860	1.168134	-1.638118		
31008	O	-1.325513	1.289109	0.213667		
31009	O	-2.670118	1.281489	-0.220390		
31010	H	-3.019277	0.524533	0.275943		
31011	C	-1.057631	-0.793219	-1.111265		
31012	O	-0.915360	-1.775214	-0.113055		
31013	H	-2.097115	-0.709683	-1.426565		
31014	H	-0.471999	-1.170431	-1.950086		
31015	O	-1.758997	-1.408389	0.971913		
31016	H	-1.124118	-0.956829	1.552604		
31017	Rotational constants (GHz):		1.2494700	0.7882800	0.7302500	
31018	Vibrational harmonic frequencies (cm-1):					
31019	i1973.7173		53.9812		77.6036	
31020	108.5155		138.9599		170.4195	
31021	212.4256		218.8330		225.4171	
31022	248.9644		270.2571		289.0124	
31023	340.3993		358.6141		409.3260	
31024	469.4620		479.1486		499.0868	
31025	532.6902		548.2564		627.1475	
31026	668.4512		734.6441		819.9050	
31027	853.3702		896.7453		955.9283	
31028	974.0820		1036.9956		1047.1785	
31029	1073.2925		1078.2172		1125.1846	
31030	1128.5201		1169.3734		1185.8338	
31031	1252.4639		1299.4438		1361.6881	
31032	1384.3158		1398.3624		1411.7356	
31033	1437.3540		1448.4306		1487.2949	
31034	1491.0587		1498.8314		1823.2222	
31035	2000.0828		3048.8729		3077.2441	
31036	3096.8242		3142.2505		3157.4990	
31037	3173.1337		3725.9238		3747.0948	
31038	Zero-point correction (Hartree): 0.151474					
31039						
31040	TS.diHPCARP_I.14aldHshift.mtptpmd					
31041	-----					
31042	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13985991					
31043	Electronic state : 2-A					
31044	Cartesian coordinates (Angs):					
31045	C	1.771440	-1.067795	-0.567847		
31046	C	1.101202	0.284899	-0.106779		
31047	O	1.534072	0.321727	1.230410		
31048	O	2.874004	-0.008631	1.228611		
31049	H	2.707475	-0.966499	0.346391		
31050	O	1.511561	-1.763878	-1.467998		
31051	C	1.701800	1.373953	-0.983336		
31052	H	1.357769	1.249092	-2.009087		
31053	H	2.787221	1.324242	-0.952655		
31054	H	1.371008	2.340983	-0.612511		
31055	C	-0.419173	0.209005	-0.161376		
31056	H	-0.680649	-0.137705	-1.164853		
31057	O	-0.910672	1.529573	0.003377		
31058	O	-2.223790	1.586057	-0.539645		
31059	H	-2.764206	1.477054	0.256202		
31060	C	-0.985528	-0.731797	0.893812		
31061	O	-2.397944	-0.743633	0.884861		
31062	H	-0.599528	-1.745098	0.749911		
31063	H	-0.724516	-0.378581	1.890104		
31064	O	-2.826740	-1.303788	-0.346971		
31065	H	-2.956952	-0.512499	-0.891506		
31066	Rotational constants (GHz):		1.3882300	0.6358100	0.5733900	
31067	Vibrational harmonic frequencies (cm-1):					
31068	i2004.9922		48.4598		80.7538	
31069	118.7443		141.9524		159.5772	
31070	169.7707		208.5388		219.0694	
31071	257.5684		268.3683		283.8410	
31072	343.5057		358.0599		388.8530	
31073	428.5941		469.5608		499.5826	
31074	507.4751		545.6123		557.3738	
31075	625.9406		702.2564		828.2892	
31076	879.9687		902.1136		960.4911	
31077	995.7617		1032.7306		1061.0029	
31078	1075.6024		1094.6810		1122.0672	

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31079      1148.0565          1157.1611          1190.1987
31080      1271.1456          1302.0711          1343.8760
31081      1381.7591          1400.2730          1422.6244
31082      1430.5331          1439.2475          1469.7893
31083      1480.7877          1497.8539          1816.4873
31084      2004.7563          3061.9433          3076.6744
31085      3084.4693          3148.2635          3165.4633
31086      3177.8435          3759.1898          3785.5236
31087      Zero-point correction (Hartree): 0.151161
31088
31089      TS.diHPCARP_I.14aldHshift.mtttmd
31090      -----
31091      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13843487
31092      Electronic state : 2-A
31093      Cartesian coordinates (Angs):
31094      C      -1.956645      -0.744307      0.787845
31095      C      -1.111918      0.301686      -0.036422
31096      O      -1.368592      -0.164726      -1.338951
31097      O      -2.723776      -0.414398      -1.419677
31098      H      -2.763186      -0.959115      -0.224557
31099      O      -1.867599      -1.069128      1.906061
31100      C      -1.712418      1.664961      0.267338
31101      H      -1.500812      1.933364      1.301518
31102      H      -2.787014      1.650359      0.103914
31103      H      -1.251415      2.398307      -0.389502
31104      C      0.381031      0.200216      0.263912
31105      H      0.500262      0.239449      1.349875
31106      O      1.005962      1.338959      -0.296633
31107      O      2.069024      1.742938      0.548848
31108      H      2.807719      1.215909      0.205434
31109      C      0.967229      -1.102215      -0.267970
31110      O      2.253842      -1.380436      0.256540
31111      H      0.361772      -1.947142      0.068068
31112      H      0.997032      -1.094953      -1.357123
31113      O      3.198131      -0.570045      -0.432218
31114      H      3.696039      -1.223540      -0.937599
31115      Rotational constants (GHz): 1.4142300      0.6081400      0.5630800
31116      Vibrational harmonic frequencies (cm-1):
31117      i1992.7901          47.9374          52.5865
31118      105.0096          112.3077          147.2647
31119      150.3573          180.7722          201.8436
31120      226.3574          259.8093          279.9185
31121      306.9095          329.4269          351.8404
31122      403.9364          449.8952          501.4972
31123      517.1139          539.7590          557.5965
31124      617.8611          701.6884          819.3768
31125      872.6954          906.7983          971.6069
31126      983.9337          1041.4850          1061.7576
31127      1074.3809          1101.1930          1120.9636
31128      1127.1494          1160.0751          1182.9101
31129      1265.1172          1311.0794          1330.4158
31130      1376.8745          1385.3595          1399.7354
31131      1432.0071          1454.1478          1460.5149
31132      1480.2114          1495.8039          1814.7143
31133      2001.8333          3075.6606          3081.0699
31134      3084.2875          3138.2372          3164.6651
31135      3178.4071          3734.3589          3830.2092
31136      Zero-point correction (Hartree): 0.150270
31137
31138      TS.diHPCARP_I.14aldHshift.mtttppd
31139      -----
31140      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13912754
31141      Electronic state : 2-A
31142      Cartesian coordinates (Angs):
31143      C      -1.721713      -1.072618      0.625511
31144      C      -1.102387      0.276538      0.092707
31145      O      -1.550613      0.229636      -1.240366
31146      O      -2.879727      -0.140957      -1.207352
31147      H      -2.674642      -1.044328      -0.275878
31148      O      -1.421511      -1.726714      1.545096
31149      C      -1.725762      1.389595      0.920004
31150      H      -1.369483      1.323743      1.947090

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31151	H	-2.809845	1.312400	0.901151	
31152	H	-1.418581	2.344038	0.499529	
31153	C	0.419920	0.257937	0.129799	
31154	H	0.721027	-0.034257	1.138389	
31155	O	0.886422	1.571495	-0.118160	
31156	O	2.097569	1.760310	0.595883	
31157	H	2.740354	1.303519	0.032559	
31158	C	1.005899	-0.701276	-0.896069	
31159	O	2.420961	-0.690528	-0.847285	
31160	H	0.628914	-1.718529	-0.756849	
31161	H	0.771091	-0.357608	-1.902217	
31162	O	2.810560	-1.249124	0.404899	
31163	H	3.246141	-2.062981	0.122790	
31164	Rotational constants (GHz):			1.3461900	0.6425300 0.5740800
31165	Vibrational harmonic frequencies (cm-1):				
31166	i1983.6578		45.8190		67.3809
31167	104.2956		127.3638		143.3990
31168	151.3813		190.0806		204.4186
31169	238.8725		260.1825		272.3100
31170	286.3394		344.3867		360.7680
31171	392.7822		429.2432		483.7118
31172	501.3317		541.9013		556.7208
31173	623.4803		702.3755		828.5640
31174	877.1160		899.7022		957.6644
31175	993.5878		1037.1226		1058.8827
31176	1075.3397		1091.7510		1124.0345
31177	1140.7076		1155.1697		1189.1439
31178	1268.5977		1301.9337		1334.3877
31179	1377.0481		1395.6077		1399.5221
31180	1429.9614		1444.7997		1465.5177
31181	1480.1647		1495.8434		1817.4785
31182	2002.5203		3060.5634		3084.0019
31183	3093.2480		3148.5112		3165.2249
31184	3178.4903		3766.6860		3824.0665
31185	Zero-point correction (Hartree):			0.150340	
31186	-----				
31187	TS.diHPCARP_I.14aldHshift.pmpmmpd				
31188	-----				
31189	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14025176	
31190	Electronic state : 2-A				
31191	Cartesian coordinates (Angs):				
31192	C	-1.879704	0.653764	-0.308640	
31193	C	-0.387116	0.457322	0.140904	
31194	O	0.183274	1.632732	-0.399206	
31195	O	-0.680138	2.675708	-0.128632	
31196	H	-1.739507	1.949241	-0.425194	
31197	O	-2.780043	-0.092622	-0.327645	
31198	C	-0.424078	0.466991	1.665987	
31199	H	-0.893375	-0.442874	2.031144	
31200	H	-0.976898	1.334778	2.018568	
31201	H	0.597203	0.528598	2.035916	
31202	C	0.327659	-0.721675	-0.549089	
31203	H	0.633269	-0.365539	-1.534129	
31204	O	-0.526190	-1.797185	-0.860600	
31205	O	-1.055803	-2.331256	0.348538	
31206	H	-1.984543	-2.069392	0.265536	
31207	C	1.561761	-1.199207	0.209113	
31208	O	2.402642	-0.126813	0.569232	
31209	H	1.279698	-1.664702	1.153056	
31210	H	2.096919	-1.924369	-0.405835	
31211	O	2.883757	0.466875	-0.630906	
31212	H	2.376118	1.291567	-0.654958	
31213	Rotational constants (GHz):			1.1548600	0.8975600 0.6092100
31214	Vibrational harmonic frequencies (cm-1):				
31215	i1993.4013		80.1265		107.3585
31216	144.5191		157.6184		168.7846
31217	176.2489		217.8516		224.7267
31218	239.9538		283.8779		301.6947
31219	336.4885		352.7688		406.7635
31220	418.4597		429.3256		475.2382
31221	503.9221		563.1574		591.6606
31222	646.8450		721.6187		730.7056

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31223      887.5544          936.5085          953.5698
31224      978.9862          1018.9294         1063.9675
31225      1086.1820         1107.5138         1123.4095
31226      1130.3023         1155.0822         1191.1565
31227      1257.8579         1282.0384         1345.2694
31228      1380.7403         1395.4963         1411.0211
31229      1434.1127         1437.5923         1481.2415
31230      1491.2586         1511.2930         1811.1933
31231      1992.7956         3082.0931         3089.8170
31232      3106.9754         3147.0940         3170.2716
31233      3181.6636         3772.1978         3774.3125
31234      Zero-point correction (Hartree): 0.151428
31235
31236      TS.diHPCARP_I.14aldHshift.ppmmpd
31237      -----
31238      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14024573
31239      Electronic state : 2-A
31240      Cartesian coordinates (Angs):
31241      C      -1.762902      0.881425      -0.213142
31242      C      -0.295547      0.517311      0.227449
31243      O      0.416966      1.450524      -0.550873
31244      O      -0.237963      2.662927      -0.453330
31245      H      -1.421539      2.095846      -0.553793
31246      O      -2.774499      0.303776      -0.105726
31247      C      -0.253652      0.797457      1.723674
31248      H      -0.782050      0.003750      2.250215
31249      H      -0.714511      1.755046      1.954120
31250      H      0.788162      0.826475      2.038695
31251      C      0.174331      -0.889253      -0.174136
31252      H      0.246968      -0.942296      -1.259613
31253      O      -0.727104      -1.875286      0.286839
31254      O      -1.637089      -2.206102      -0.750471
31255      H      -2.439249      -1.746653      -0.464745
31256      C      1.511962      -1.268883      0.468815
31257      O      2.463431      -0.237777      0.433051
31258      H      1.361953      -1.476117      1.529260
31259      H      1.889734      -2.168217      -0.018725
31260      O      2.806585      -0.021305      -0.929534
31261      H      2.342752      0.809759      -1.111021
31262      Rotational constants (GHz):      1.1324800      0.8667600      0.6007200
31263      Vibrational harmonic frequencies (cm-1):
31264      i1962.0263      57.0512      95.6140
31265      128.6698      158.3866      162.3191
31266      191.5028      215.6758      220.2902
31267      248.0570      273.0798      285.3239
31268      327.7562      375.2318      405.7349
31269      432.8286      447.3925      477.3042
31270      500.5955      509.5573      577.2633
31271      663.2975      695.6377      732.4075
31272      877.6169      929.7634      963.9198
31273      1017.9562      1022.5318      1066.6294
31274      1077.3603      1109.8348      1122.3644
31275      1143.5148      1154.9610      1191.4972
31276      1264.9575      1288.3232      1330.0025
31277      1381.3039      1394.5147      1405.3970
31278      1435.8255      1440.3457      1477.9751
31279      1487.8213      1509.8090      1814.8269
31280      1992.4658      3078.3056      3081.0554
31281      3116.0001      3137.0118      3163.1260
31282      3167.7891      3769.7366      3790.4853
31283      Zero-point correction (Hartree): 0.151238
31284
31285      TS.diHPCARP_I.14aldHshift.tmpmmd
31286      -----
31287      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14043805
31288      Electronic state : 2-A
31289      Cartesian coordinates (Angs):
31290      C      1.001062      -0.554271      1.170712
31291      C      0.526006      -0.473289      -0.322832
31292      O      1.752673      -0.195096      -0.966314
31293      O      2.716139      -0.996219      -0.378977
31294      H      2.233063      -0.791130      0.841475

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31295	O	0.400760	-0.586174	2.172011	
31296	C	-0.022807	-1.851110	-0.671554	
31297	H	-0.866292	-2.098509	-0.032961	
31298	H	0.766250	-2.590096	-0.552766	
31299	H	-0.353659	-1.842953	-1.709245	
31300	C	-0.427224	0.684152	-0.644547	
31301	H	-0.838029	0.513908	-1.641589	
31302	O	0.263159	1.909896	-0.777939	
31303	O	1.036288	2.111827	0.398669	
31304	H	1.921342	1.902357	0.064391	
31305	C	-1.568672	0.877131	0.354552	
31306	O	-2.327671	-0.289064	0.577879	
31307	H	-1.173737	1.141457	1.334117	
31308	H	-2.202305	1.686749	-0.012385	
31309	O	-2.925673	-0.642590	-0.667512	
31310	H	-3.862222	-0.518099	-0.471553	
31311	Rotational constants (GHz):		1.2598700	0.7821300	0.6860900
31312	Vibrational harmonic frequencies (cm-1):				
31313	i1855.9888		60.6249		85.0943
31314	128.2874		134.0951		159.9624
31315	177.4679		189.6040		199.8242
31316	231.4728		258.2805		269.6532
31317	305.5907		342.7964		368.9340
31318	431.5447		442.9443		480.1002
31319	491.9219		546.1749		614.5910
31320	648.5671		708.5663		760.4149
31321	873.1332		935.2616		950.8487
31322	976.5723		1033.1547		1061.9168
31323	1092.0760		1101.4021		1115.6038
31324	1120.8536		1169.3307		1185.6903
31325	1261.3039		1282.3729		1338.0526
31326	1373.3518		1388.3630		1402.5147
31327	1412.1036		1424.8221		1484.7312
31328	1491.8486		1497.3638		1817.3690
31329	2002.0498		3077.6073		3083.1330
31330	3100.8674		3154.9679		3162.5506
31331	3184.5672		3771.5265		3829.5150
31332	Zero-point correction (Hartree):		0.150800		
31333	TS.diHPCARP_I.14aldHshift.tmptmpd				
31334	-----				
31335	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13959185				
31336	Electronic state : 2-A				
31337	Cartesian coordinates (Angs):				
31338	C	1.357172	-0.319600	1.141387	
31339	C	1.010677	-0.315003	-0.390452	
31340	O	1.731327	0.816829	-0.818521	
31341	O	2.953930	0.793069	-0.170936	
31342	H	2.411540	0.420390	0.980073	
31343	O	0.930491	-0.964433	2.016542	
31344	C	1.559080	-1.622218	-0.949020	
31345	H	1.090435	-2.475554	-0.462127	
31346	H	2.633073	-1.665122	-0.783209	
31347	H	1.363077	-1.661934	-2.019665	
31348	C	-0.463637	-0.083167	-0.723179	
31349	H	-0.609641	-0.262316	-1.791839	
31350	O	-0.819646	1.282974	-0.591243	
31351	O	-0.453100	1.712119	0.714588	
31352	H	0.305455	2.277846	0.506192	
31353	C	-1.427359	-0.976016	0.052502	
31354	O	-2.737872	-0.793056	-0.436065	
31355	H	-1.187400	-2.027259	-0.113594	
31356	H	-1.399683	-0.764778	1.120269	
31357	O	-3.338648	0.277428	0.276826	
31358	H	-2.954309	1.055319	-0.153049	
31359	Rotational constants (GHz):		1.5410700	0.6552300	0.6146000
31360	Vibrational harmonic frequencies (cm-1):				
31361	i1884.1825		61.3560		71.8580
31362	117.6137		126.0424		156.8859
31363	179.1673		195.2701		215.4804
31364	257.9926		276.2333		301.7679
31365	322.1734		346.0034		404.3597

31367	414.1287	422.6537	488.3290			
31368	502.3246	560.9909	612.1130			
31369	637.5762	711.3857	783.7857			
31370	883.2336	919.4112	950.1248			
31371	990.3499	999.7997	1058.7170			
31372	1092.6413	1099.3730	1123.0290			
31373	1134.3091	1150.1282	1197.4362			
31374	1261.1290	1295.6835	1315.2388			
31375	1384.7294	1402.7137	1409.6993			
31376	1414.8251	1440.6933	1465.1924			
31377	1484.6266	1501.6867	1815.7570			
31378	2002.6917	3076.5806	3081.6992			
31379	3089.8623	3151.2348	3158.1847			
31380	3169.5646	3771.7236	3773.9199			
31381	Zero-point correction (Hartree): 0.150886					
31382	-----					
31383	TS.diHPCARP_I.14aldHshift.tmptppd					
31384	-----					
31385	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13927625					
31386	Electronic state : 2-A					
31387	Cartesian coordinates (Angs):					
31388	C	1.426797	-0.254889	1.121708		
31389	C	0.776355	-0.481699	-0.288321		
31390	O	1.727212	0.144627	-1.117221		
31391	O	2.978396	-0.204833	-0.640201		
31392	H	2.610647	-0.056537	0.623904		
31393	O	0.998492	-0.432843	2.194462		
31394	C	0.708885	-1.989562	-0.495151		
31395	H	0.071354	-2.455270	0.253655		
31396	H	1.708265	-2.413044	-0.427048		
31397	H	0.303186	-2.189407	-1.485888		
31398	C	-0.568208	0.221331	-0.485606		
31399	H	-1.029329	-0.162760	-1.398097		
31400	O	-0.403491	1.596474	-0.756309		
31401	O	0.388785	2.151286	0.287129		
31402	H	1.223469	2.293270	-0.182967		
31403	C	-1.531193	0.004155	0.678671		
31404	O	-2.860289	0.241545	0.276535		
31405	H	-1.441839	-0.995893	1.105758		
31406	H	-1.333988	0.743675	1.454453		
31407	O	-3.207247	-0.815797	-0.616030		
31408	H	-3.962443	-1.203728	-0.158489		
31409	Rotational constants (GHz):			1.3889500	0.6609900	0.6200800
31410	Vibrational harmonic frequencies (cm-1):					
31411	i1893.7814		49.4518			68.2291
31412	125.0414		136.4855			146.7238
31413	168.8457		191.5105			196.9406
31414	218.4602		257.2242			277.2890
31415	308.2865		330.5463			347.2176
31416	401.1526		418.9252			488.7398
31417	506.1736		565.6621			615.4701
31418	645.0974		713.9293			795.1143
31419	895.5677		920.2927			951.2217
31420	983.2759		996.8592			1059.5436
31421	1086.0611		1098.7915			1121.8212
31422	1137.6918		1144.4049			1195.5349
31423	1261.4888		1288.4631			1313.7623
31424	1384.6035		1392.5121			1402.4284
31425	1410.6185		1425.5119			1461.8929
31426	1481.4134		1500.8591			1815.6759
31427	1997.9528		3076.9027			3082.7569
31428	3099.1983		3145.3886			3159.5579
31429	3171.0464		3779.5488			3836.0168
31430	Zero-point correction (Hartree): 0.150476					
31431	-----					
31432	TS.diHPCARP_I.14aldHshift.tmptptd					
31433	-----					
31434	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13933950					
31435	Electronic state : 2-A					
31436	Cartesian coordinates (Angs):					
31437	C	1.455926	-0.237914	1.107113		
31438	C	0.793901	-0.474278	-0.296106		

31439	O	1.708756	0.195581	-1.131933			
31440	O	2.979167	-0.110232	-0.676092			
31441	H	2.623626	0.010590	0.595522			
31442	O	1.050757	-0.443988	2.183503			
31443	C	0.780803	-1.981781	-0.515916			
31444	H	0.180025	-2.479346	0.242631			
31445	H	1.797777	-2.364891	-0.473866			
31446	H	0.361921	-2.190262	-1.499382			
31447	C	-0.577479	0.181337	-0.469987			
31448	H	-1.030375	-0.209403	-1.383720			
31449	O	-0.467323	1.565238	-0.725368			
31450	O	0.315711	2.138730	0.314476			
31451	H	1.139983	2.314249	-0.162760			
31452	C	-1.520208	-0.088818	0.697285			
31453	O	-2.855506	0.185498	0.350196			
31454	H	-1.436944	-1.114729	1.060665			
31455	H	-1.299365	0.595983	1.515131			
31456	O	-3.250930	-0.855600	-0.546004			
31457	H	-3.779359	-0.355284	-1.178774			
31458	Rotational constants (GHz):				1.3993500	0.6551100	0.6182700
31459	Vibrational harmonic frequencies (cm-1):						
31460	i1888.3225			45.3369		65.9684	
31461	120.3486			135.6396		145.4479	
31462	156.5391			172.3166		192.3524	
31463	216.3354			256.7161		274.5958	
31464	307.7196			326.9623		345.0372	
31465	377.3455			406.0092		485.0422	
31466	493.0053			568.2806		614.9353	
31467	647.6062			712.9523		792.5077	
31468	891.4310			920.0787		953.7524	
31469	983.0116			996.6902		1059.5744	
31470	1088.2077			1099.0098		1125.5915	
31471	1134.5208			1144.9596		1195.4358	
31472	1261.2589			1282.9314		1311.3511	
31473	1382.5927			1402.2548		1409.0034	
31474	1414.3958			1429.1602		1464.1604	
31475	1482.9719			1501.6542		1816.1970	
31476	1999.4388			3077.4945		3084.3401	
31477	3098.3439			3150.3015		3159.6165	
31478	3171.4496			3778.7020		3843.5699	
31479	Zero-point correction (Hartree):				0.150296		
31480							
31481	TS.diHPCARP_I.14aldHshift.tpmmmmd						
31482	-----						
31483	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13946756						
31484	Electronic state : 2-A						
31485	Cartesian coordinates (Angs):						
31486	C	1.049106	-1.078305	1.016152			
31487	C	0.525420	-0.415173	-0.305739			
31488	O	1.747738	0.091717	-0.815062			
31489	O	2.709929	-0.885545	-0.640055			
31490	H	2.259984	-1.202375	0.569999			
31491	O	0.481598	-1.422426	1.977260			
31492	C	-0.048887	-1.519525	-1.180685			
31493	H	-0.819834	-2.072830	-0.652141			
31494	H	0.755853	-2.187813	-1.477498			
31495	H	-0.493362	-1.068034	-2.066845			
31496	C	-0.383642	0.794029	-0.068047			
31497	H	-0.661094	1.206979	-1.039772			
31498	O	0.299647	1.778966	0.681947			
31499	O	0.994871	2.648596	-0.194854			
31500	H	1.791034	2.133243	-0.396145			
31501	C	-1.640798	0.519378	0.760108			
31502	O	-2.426610	-0.543945	0.278554			
31503	H	-1.368185	0.219796	1.771557			
31504	H	-2.218492	1.444046	0.800526			
31505	O	-2.862162	-0.190061	-1.030649			
31506	H	-3.813195	-0.093852	-0.897556			
31507	Rotational constants (GHz):				1.1384300	0.7764200	0.6456500
31508	Vibrational harmonic frequencies (cm-1):						
31509	i1868.5676			27.4897		76.8057	
31510	123.2229			135.9605		167.6418	

31511	177.0863	181.1688	211.6160			
31512	227.3790	263.7366	277.9598			
31513	304.1933	336.8294	378.8427			
31514	419.4285	457.4217	474.4957			
31515	504.4652	540.6741	609.2551			
31516	616.1709	690.0130	738.2560			
31517	876.6023	935.6327	953.4591			
31518	1017.2035	1018.6535	1062.7068			
31519	1094.8137	1104.3427	1122.8091			
31520	1133.7701	1168.7603	1186.8579			
31521	1265.0648	1288.0051	1329.3309			
31522	1379.5754	1388.0755	1406.2727			
31523	1422.5136	1454.0900	1486.7176			
31524	1487.3922	1495.9720	1823.0580			
31525	2004.5276	3080.5436	3082.8797			
31526	3091.5729	3148.3540	3162.5899			
31527	3183.7851	3758.4328	3826.3197			
31528	Zero-point correction (Hartree): 0.150771					
31529						
31530	TS.diHPCARP_I.14aldHshift.tpmppmd					
31531	-----					
31532	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13931155					
31533	Electronic state : 2-A					
31534	Cartesian coordinates (Angs):					
31535	C	-0.654997	-0.944521	-1.040820		
31536	C	-0.747203	-0.344821	0.413996		
31537	O	-2.002400	0.304501	0.292595		
31538	O	-2.869223	-0.576744	-0.327244		
31539	H	-1.948774	-0.985044	-1.177757		
31540	O	0.243260	-1.270745	-1.711814		
31541	C	-0.771835	-1.506954	1.392364		
31542	H	0.139694	-2.094914	1.303461		
31543	H	-1.635961	-2.135971	1.194026		
31544	H	-0.851318	-1.111646	2.405534		
31545	C	0.273869	0.751906	0.719874		
31546	H	-0.129484	1.344577	1.547232		
31547	O	0.417210	1.606849	-0.400150		
31548	O	-0.529478	2.661496	-0.300517		
31549	H	-1.358221	2.233642	-0.562912		
31550	C	1.636463	0.233934	1.166027		
31551	O	2.166775	-0.817805	0.398032		
31552	H	2.335603	1.069824	1.192105		
31553	H	1.538430	-0.182974	2.169374		
31554	O	2.748468	-0.255529	-0.768005		
31555	H	2.095366	-0.490951	-1.442889		
31556	Rotational constants (GHz):			1.2233000	0.8134500	0.6839500
31557	Vibrational harmonic frequencies (cm-1):					
31558	i1903.1494		74.7830			95.8145
31559	121.8061		140.0186			157.0407
31560	188.8300		194.5895			241.1036
31561	246.3757		287.4541			299.4911
31562	329.5525		372.3555			392.8161
31563	408.5198		424.6887			449.4341
31564	485.3663		544.6472			603.3754
31565	614.1520		715.9946			775.9341
31566	871.0378		911.6343			943.6048
31567	988.2229		1024.1061			1062.1442
31568	1065.4816		1094.3249			1120.6946
31569	1146.3514		1148.7902			1196.1963
31570	1265.4273		1308.5747			1353.6273
31571	1364.0555		1398.9940			1408.6308
31572	1437.8519		1449.6436			1461.6526
31573	1492.5833		1502.1877			1820.0153
31574	2005.8725		3060.4540			3073.6500
31575	3086.1732		3138.0191			3152.6760
31576	3174.6066		3766.5992			3771.0992
31577	Zero-point correction (Hartree): 0.150881					
31578						
31579	TS.diHPCARP_I.14aldHshift.ttpppmd					
31580	-----					
31581	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14216321					
31582	Electronic state : 2-A					

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31583 Cartesian coordinates (Angs):
31584 C 1.071078 -0.525667 1.119420
31585 C 1.011257 -0.022439 -0.376271
31586 O 2.001106 0.980508 -0.327691
31587 O 3.070403 0.460847 0.371122
31588 H 2.308548 -0.109065 1.261730
31589 O 0.308770 -1.136313 1.762719
31590 C 1.410046 -1.201218 -1.252785
31591 H 0.721522 -2.032520 -1.114826
31592 H 2.418493 -1.513354 -0.993821
31593 H 1.399752 -0.886025 -2.296345
31594 C -0.301076 0.664827 -0.747662
31595 H -0.078009 1.405531 -1.525456
31596 O -0.685485 1.334720 0.444144
31597 O -1.905262 2.011322 0.224650
31598 H -2.542411 1.349700 0.538430
31599 C -1.371302 -0.273249 -1.283680
31600 O -1.662342 -1.364847 -0.439810
31601 H -2.279817 0.287955 -1.500496
31602 H -1.023564 -0.726730 -2.211859
31603 O -2.392671 -0.872738 0.678924
31604 H -1.720677 -0.936997 1.376048
31605 Rotational constants (GHz): 1.3863300 0.7525500 0.6874900
31606 Vibrational harmonic frequencies (cm-1):
31607 i2032.8806 88.2383 117.1395
31608 126.4545 137.4884 160.8417
31609 200.8728 226.6396 252.6178
31610 260.5475 283.1848 318.4172
31611 338.4025 378.0509 386.0371
31612 474.6428 486.2873 489.3221
31613 534.0224 544.9453 595.9267
31614 663.4679 719.8255 774.5421
31615 870.0142 906.4473 950.2881
31616 982.4955 1021.6670 1052.4111
31617 1071.7501 1102.8294 1128.4061
31618 1130.9798 1154.4983 1201.0424
31619 1256.7434 1294.2266 1358.4417
31620 1375.9273 1396.1696 1407.6183
31621 1435.9354 1448.7102 1479.6104
31622 1498.8589 1503.7221 1813.6679
31623 1993.8354 3035.3710 3074.7450
31624 3096.3477 3141.2070 3154.6139
31625 3175.8042 3729.8709 3740.6536
31626 Zero-point correction (Hartree): 0.151596
31627
31628
31629
31630 1,5-aldehyde-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-HPCARP-Ib)
31631 =====
31632
31633 TS.diHPCARP_Ib.15aldHshift.dtdppdud
31634 -----
31635 IRC pathway available
31636 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17490389
31637 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05358172
31638 T1 diagnostic: 0.021833
31639 E(MP2/Aug-CC-pVTZ) (Hartree): -721.01092503
31640 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02846002
31641 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01839357
31642 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03324308
31643 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48217422
31644 E(UHF/Aug-CC-pVTZ) (Hartree): -718.47193432
31645 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14830786
31646 Electronic state : 2-A
31647 Cartesian coordinates (Angs):
31648 O -0.426305 2.035649 -0.229600
31649 O -1.583296 1.944097 -0.975531
31650 H -2.170330 0.988930 -0.338632
31651 C -1.933185 -0.179950 0.116524
31652 C -0.437451 -0.247649 0.473465
31653 C 0.305525 0.821335 -0.349470
31654 O -2.694417 -1.080040 0.107447

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31655	C	-0.311104	-0.058033	1.977686	
31656	O	0.034237	-1.559847	0.208499	
31657	H	-0.971790	-0.750325	2.495547	
31658	H	-0.580607	0.963977	2.239976	
31659	H	0.717320	-0.252860	2.274825	
31660	O	-0.223704	-1.882421	-1.152394	
31661	H	-1.019850	-2.427976	-1.075939	
31662	H	0.330645	0.514976	-1.395098	
31663	C	1.704994	1.151529	0.159714	
31664	O	2.460180	0.009309	0.476050	
31665	H	2.219410	1.764028	-0.582084	
31666	H	1.637782	1.709185	1.094979	
31667	O	2.662295	-0.715365	-0.729261	
31668	H	2.032831	-1.444370	-0.622785	
31669	Rotational constants (GHz):		1.2186600	0.8458000	0.6603700
31670	Vibrational harmonic frequencies (cm-1):				
31671	i2017.1992		65.6841		93.8894
31672	139.9752		159.5675		168.9368
31673	196.1744		220.2686		249.9085
31674	258.6779		290.5973		318.4724
31675	342.8098		356.2292		389.4233
31676	418.1540		448.1996		457.2713
31677	480.0584		512.6088		615.5281
31678	645.9252		680.3705		821.5824
31679	892.1178		936.0643		960.4663
31680	1010.3456		1041.8221		1046.6034
31681	1095.5626		1117.9106		1129.9018
31682	1139.0373		1196.1162		1213.0855
31683	1262.6460		1291.8595		1335.1517
31684	1388.5988		1404.3339		1408.5668
31685	1413.1479		1422.6017		1484.3377
31686	1494.6040		1511.9814		1658.6323
31687	1935.2859		3077.2665		3079.2857
31688	3114.8122		3134.4849		3160.6646
31689	3167.0429		3769.4977		3786.5256
31690	Zero-point correction (Hartree): 0.151295				
31691					
31692	TS.diHPCARP_Ib.15aldHshift.umdmudu				
31693	-----				
31694	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14698403				
31695	Electronic state : 2-A				
31696	Cartesian coordinates (Angs):				
31697	O	0.160201	2.146457	0.172998	
31698	O	1.271128	2.405064	-0.600868	
31699	H	1.999880	1.387265	-0.254229	
31700	C	1.919166	0.126591	-0.117672	
31701	C	0.459534	-0.225862	0.243707	
31702	C	-0.437529	0.930125	-0.248866	
31703	O	2.778776	-0.636213	-0.388437	
31704	C	0.372823	-0.458263	1.743470	
31705	O	0.085585	-1.348586	-0.542138	
31706	H	1.139655	-1.154516	2.071248	
31707	H	0.508785	0.492060	2.259186	
31708	H	-0.606223	-0.869787	1.980514	
31709	O	0.710206	-2.521737	-0.057880	
31710	H	1.579282	-2.481269	-0.486327	
31711	H	-0.480267	0.906389	-1.339118	
31712	C	-1.838936	0.949990	0.355259	
31713	O	-2.456275	-0.310863	0.369867	
31714	H	-2.447019	1.675242	-0.187221	
31715	H	-1.782737	1.246419	1.403457	
31716	O	-2.653773	-0.708537	-0.979821	
31717	H	-1.928489	-1.341963	-1.092651	
31718	Rotational constants (GHz):		1.1380100	0.8873300	0.6051000
31719	Vibrational harmonic frequencies (cm-1):				
31720	i1974.8256		64.1866		99.4852
31721	136.2340		165.2921		186.4368
31722	200.8800		224.2246		254.3570
31723	277.3233		295.6688		309.8092
31724	344.8458		360.8710		401.5965
31725	419.0755		450.5973		473.1171
31726	501.1935		538.5863		591.2173

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31727      642.1766      675.0568      811.8038
31728      897.0433      922.7255      962.3623
31729     1022.8077     1034.4758     1057.3849
31730     1096.6589     1126.1235     1135.6965
31731     1143.1125     1195.7529     1204.2750
31732     1260.8578     1292.2822     1333.0562
31733     1386.6501     1406.0038     1414.5605
31734     1439.9690     1451.4573     1483.5794
31735     1496.4989     1509.1440     1658.5748
31736     1924.9167     3079.3872     3081.9568
31737     3096.2301     3135.3661     3161.7066
31738     3177.1031     3755.7601     3758.7759
31739 Zero-point correction (Hartree): 0.151558
31740
31741 TS.diHPCARP_Ib.15aldHshift.umdmuud
31742 -----
31743 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14251690
31744 Electronic state : 2-A
31745 Cartesian coordinates (Angs):
31746 O      0.150085     -1.644987     -0.702437
31747 O      1.037178     -0.963123     -1.517497
31748 H      0.457234      0.231740     -1.594786
31749 C     -0.180285      1.101686     -0.943805
31750 C     -0.892217      0.325984      0.190730
31751 C     -0.066741     -0.929500      0.509649
31752 O     -0.202566      2.252017     -1.167054
31753 C     -1.159103      1.220165      1.384155
31754 O     -2.091986     -0.015756     -0.495843
31755 H     -0.231258      1.638587      1.769659
31756 H     -1.804488      2.036491      1.067801
31757 H     -1.657990      0.649058      2.166642
31758 O     -2.822667     -0.953771      0.281481
31759 H     -2.788183     -1.731834     -0.290996
31760 H     -0.687924     -1.604611      1.097421
31761 C      1.197022     -0.619959      1.298093
31762 O      1.882974      0.514976      0.798377
31763 H      1.863460     -1.481160      1.299233
31764 H      0.916947     -0.390708      2.327604
31765 O      3.034547      0.102990      0.083704
31766 H      2.639629     -0.276594     -0.721360
31767 Rotational constants (GHz): 1.3229400 0.7790700 0.7104000
31768 Vibrational harmonic frequencies (cm-1):
31769 i1670.0971      35.5312      79.4362
31770      101.1826      148.7819      167.6386
31771      200.3649      230.1196      255.8126
31772      263.2943      266.1531      316.9373
31773      332.3317      352.7086      374.3713
31774      436.4887      497.9695      512.3963
31775      528.4716      548.5136      578.7540
31776      652.3641      767.3807      785.9443
31777      863.2019      940.5601      961.3333
31778      971.7418      1025.0073     1045.6987
31779     1048.7868      1084.2181     1126.9275
31780     1145.6711      1157.3733     1219.6045
31781     1233.2976      1292.0134     1339.6225
31782     1380.8353      1395.8223     1406.1501
31783     1407.8967      1471.5105     1477.5648
31784     1489.0396      1498.5594     1667.7107
31785     1969.1781      3075.9643     3081.6280
31786     3125.5514      3141.6387     3157.8953
31787     3167.6698      3661.7456     3804.2815
31788 Zero-point correction (Hartree): 0.150971
31789
31790 TS.diHPCARP_Ib.15aldHshift.umdmppdu
31791 -----
31792 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14509444
31793 Electronic state : 2-A
31794 Cartesian coordinates (Angs):
31795 O      0.403636      2.119031      0.273598
31796 O      1.624765      2.292836     -0.343640
31797 H      2.186726      1.166775     -0.027470
31798 C      1.939847     -0.080515     -0.039710

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31799	C	0.426313	-0.262165	0.189679		
31800	C	-0.274138	1.018799	-0.316267		
31801	O	2.714589	-0.919540	-0.338464		
31802	C	0.201143	-0.529332	1.670576		
31803	O	-0.021805	-1.300887	-0.669233		
31804	H	0.865156	-1.311897	2.027295		
31805	H	0.394508	0.386654	2.228220		
31806	H	-0.829815	-0.839053	1.827186		
31807	O	0.426469	-2.556750	-0.189385		
31808	H	1.310321	-2.619969	-0.582922		
31809	H	-0.177002	1.069593	-1.403405		
31810	C	-1.742072	1.191950	0.064010		
31811	O	-2.592814	0.301772	-0.616337		
31812	H	-2.038547	2.187702	-0.266910		
31813	H	-1.898697	1.120048	1.140292		
31814	O	-2.690621	-0.902867	0.128691		
31815	H	-2.032950	-1.461030	-0.313850		
31816	Rotational constants (GHz):			1.1491200	0.8948000	0.5850400
31817	Vibrational harmonic frequencies (cm-1):					
31818	i1987.3928		67.6778			97.6144
31819	132.6721		166.8607			180.0417
31820	202.2198		223.8901			225.9189
31821	273.9215		303.3059			319.3302
31822	342.2103		353.7077			380.6664
31823	405.4827		447.8340			491.4900
31824	517.2033		537.2415			582.6387
31825	634.6796		666.2806			814.1155
31826	895.1483		919.4727			962.1928
31827	1022.5421		1047.2838			1059.2114
31828	1100.5196		1119.6907			1129.3607
31829	1148.7226		1179.5932			1207.1612
31830	1259.8994		1294.8825			1321.1545
31831	1385.2599		1406.5156			1413.7454
31832	1438.0685		1449.9965			1479.9098
31833	1491.4426		1510.1815			1663.0453
31834	1927.1706		3081.7399			3082.9766
31835	3089.2489		3141.5570			3162.3835
31836	3176.3901		3759.9168			3762.8086
31837	Zero-point correction (Hartree):			0.151398		
31838						
31839	TS.diHPCARP_Ib.15aldHshift.umdppddu					
31840	-----					
31841	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14375046		
31842	Electronic state : 2-A					
31843	Cartesian coordinates (Angs):					
31844	O	-1.101541	1.321269	-0.072878		
31845	O	-0.325800	2.444662	-0.270552		
31846	H	0.790717	2.043525	0.305925		
31847	C	1.576974	1.057302	0.303967		
31848	C	0.739447	-0.210148	0.056335		
31849	C	-0.515260	0.209941	-0.738543		
31850	O	2.753849	1.141098	0.329928		
31851	C	0.443025	-0.851953	1.403539		
31852	O	1.442510	-1.049525	-0.840420		
31853	H	-0.238680	-0.219137	1.968692		
31854	H	1.363790	-0.991157	1.963464		
31855	H	-0.029069	-1.819452	1.247692		
31856	O	2.547464	-1.645212	-0.187850		
31857	H	3.234499	-0.969906	-0.293289		
31858	H	-0.199407	0.518492	-1.738427		
31859	C	-1.572328	-0.879877	-0.860119		
31860	O	-2.279500	-1.102855	0.340537		
31861	H	-2.279269	-0.628800	-1.650094		
31862	H	-1.076688	-1.820963	-1.103718		
31863	O	-3.368070	-0.194460	0.399410		
31864	H	-2.948334	0.615996	0.723284		
31865	Rotational constants (GHz):			1.4515600	0.7014200	0.5519300
31866	Vibrational harmonic frequencies (cm-1):					
31867	i1884.6184		54.9178			70.2865
31868	129.1964		163.4942			174.8686
31869	194.8153		205.2722			237.9442
31870	260.0398		264.6024			301.5263

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31871      333.6324      353.6954      385.0284
31872      400.5218      405.3453      490.4458
31873      508.1666      545.5508      585.0754
31874      638.6543      751.9351      816.9452
31875      887.1878      914.7778      934.8304
31876      1003.0776      1021.0720      1052.1744
31877      1077.3550      1129.5436      1136.6737
31878      1145.1979      1167.2234      1210.9180
31879      1261.7611      1317.4912      1353.2390
31880      1380.4282      1402.9595      1408.0719
31881      1442.1690      1443.8605      1468.0359
31882      1473.5063      1498.0370      1664.7336
31883      1928.2388      3077.7218      3086.9705
31884      3087.6317      3139.7741      3167.8075
31885      3175.6871      3764.9211      3774.7936
31886      Zero-point correction (Hartree): 0.150974
31887
31888      TS.diHPCARP_Ib.15aldHshift.umdtmudu
31889      -----
31890      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14423056
31891      Electronic state : 2-A
31892      Cartesian coordinates (Angs):
31893      O      -1.064829      1.207647      0.294458
31894      O      -0.454075      2.315921      -0.259063
31895      H      0.794901      2.059228      0.063758
31896      C      1.635057      1.117575      0.012044
31897      C      0.863814      -0.207607      0.162851
31898      C      -0.572144      0.033551      -0.343840
31899      O      2.774624      1.249245      -0.264194
31900      C      0.921166      -0.635144      1.623069
31901      O      1.404651      -1.156032      -0.734561
31902      H      0.294755      0.025962      2.220643
31903      H      1.941174      -0.600406      1.995399
31904      H      0.558056      -1.657845      1.709313
31905      O      2.672393      -1.585385      -0.274046
31906      H      3.263480      -0.918018      -0.653982
31907      H      -0.552804      0.203160      -1.422825
31908      C      -1.524428      -1.104871      -0.028411
31909      O      -2.777121      -0.896011      -0.639184
31910      H      -1.121502      -2.023281      -0.457501
31911      H      -1.662672      -1.231441      1.045368
31912      O      -3.578789      -0.118044      0.236867
31913      H      -3.271010      0.782909      0.063328
31914      Rotational constants (GHz):      1.5406600      0.6301000      0.5101500
31915      Vibrational harmonic frequencies (cm-1):
31916      i1893.0040      54.7657      69.8441
31917      115.7085      154.7184      168.7378
31918      192.7720      204.6615      237.4829
31919      273.3640      293.8615      308.6198
31920      320.7996      349.7062      367.5010
31921      374.8414      399.6287      475.1164
31922      509.4272      541.7563      561.2358
31923      629.7901      752.4530      813.3095
31924      880.4634      909.1460      961.4642
31925      982.5990      1041.8856      1059.7980
31926      1101.1203      1131.9032      1137.4204
31927      1142.1615      1182.6537      1214.2663
31928      1265.7493      1312.2264      1332.7199
31929      1364.6788      1404.9366      1420.6870
31930      1441.0014      1443.3713      1468.2690
31931      1488.2825      1507.1832      1665.5704
31932      1929.2954      3079.9133      3084.1086
31933      3088.3701      3142.1517      3160.5069
31934      3174.6603      3765.7468      3785.0725
31935      Zero-point correction (Hartree): 0.150905
31936
31937      TS.diHPCARP_Ib.15aldHshift.umdtppdu
31938      -----
31939      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14367818
31940      Electronic state : 2-A
31941      Cartesian coordinates (Angs):
31942      O      -0.809642      1.536279      0.525130

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31943	O	-0.184977	2.452348	-0.294869		
31944	H	1.039037	2.031204	-0.196884		
31945	C	1.719265	0.955303	-0.258720		
31946	C	0.812461	-0.193052	0.226985		
31947	C	-0.647255	0.236445	-0.023072		
31948	O	2.784641	0.854299	-0.756997		
31949	C	1.111069	-0.456006	1.696508		
31950	O	1.010168	-1.315639	-0.608427		
31951	H	0.749075	0.379114	2.294879		
31952	H	2.178325	-0.579163	1.857541		
31953	H	0.608826	-1.371879	2.004635		
31954	O	2.271933	-1.899407	-0.340189		
31955	H	2.860614	-1.381044	-0.909256		
31956	H	-0.833083	0.268439	-1.098136		
31957	C	-1.652683	-0.674874	0.649058		
31958	O	-2.975673	-0.383426	0.270004		
31959	H	-1.410725	-1.716230	0.425625		
31960	H	-1.646877	-0.519204	1.728208		
31961	O	-3.113847	-0.786707	-1.090073		
31962	H	-3.463154	0.019897	-1.487800		
31963	Rotational constants (GHz):			1.3331100	0.6620800	0.5408300
31964	Vibrational harmonic frequencies (cm-1):					
31965	i1993.6550		46.2652			54.9618
31966	122.5308		139.4026			172.8969
31967	187.7749		211.7444			228.8779
31968	252.5392		263.4158			290.7600
31969	304.1966		322.2493			360.1443
31970	383.6248		406.5257			465.4356
31971	511.6695		539.9839			564.0889
31972	625.8768		755.1104			813.2428
31973	885.4045		906.1949			965.0008
31974	981.3350		1040.5411			1065.3035
31975	1097.4158		1124.6421			1134.1794
31976	1153.6917		1179.8073			1211.8171
31977	1262.6562		1304.5079			1334.7301
31978	1364.2233		1403.7049			1410.2409
31979	1435.4336		1444.0005			1470.9171
31980	1488.1377		1505.8918			1659.3762
31981	1926.9583		3075.3539			3079.0864
31982	3099.6897		3138.4291			3157.2485
31983	3173.3593		3767.1018			3833.7370
31984	Zero-point correction (Hartree):			0.150595		
31985						
31986	TS.diHPCARP_Ib.15aldHshift.updmmuud					
31987	-----					
31988	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14244410		
31989	Electronic state : 2-A					
31990	Cartesian coordinates (Angs):					
31991	O	0.582941	1.826208	0.016241		
31992	O	1.124161	1.325058	1.184683		
31993	H	0.156379	0.478522	1.557422		
31994	C	-0.580349	-0.429928	1.106786		
31995	C	-0.848884	-0.076342	-0.378013		
31996	C	0.317606	0.775027	-0.906031		
31997	O	-0.912922	-1.385823	1.699273		
31998	C	-1.120722	-1.333138	-1.180248		
31999	O	-1.938271	0.835405	-0.397826		
32000	H	-2.012829	-1.817817	-0.790479		
32001	H	-0.291798	-2.031522	-1.087201		
32002	H	-1.268387	-1.075904	-2.229573		
32003	O	-3.049438	0.240242	0.256951		
32004	H	-3.668508	0.121679	-0.473902		
32005	H	-0.038220	1.306536	-1.791342		
32006	C	1.537169	-0.054801	-1.280704		
32007	O	1.851311	-1.031286	-0.304401		
32008	H	1.323531	-0.593018	-2.205782		
32009	H	2.396520	0.594228	-1.442336		
32010	O	2.967776	-0.604737	0.455686		
32011	H	2.569922	0.091857	1.007593		
32012	Rotational constants (GHz):			1.4469600	0.7284000	0.6975100
32013	Vibrational harmonic frequencies (cm-1):					
32014	i1656.4454		64.0861			86.0328

32015	129.3943	139.8858	168.2966		
32016	197.2830	205.7703	234.5486		
32017	255.0635	269.3638	290.2841		
32018	324.2293	340.8113	381.7776		
32019	420.0997	497.9128	522.4341		
32020	541.7390	546.3500	581.0701		
32021	622.2250	779.4854	811.7831		
32022	846.5593	930.7223	959.8993		
32023	981.3672	1028.7732	1047.7624		
32024	1055.1193	1112.8026	1128.4455		
32025	1144.6488	1163.7585	1218.6135		
32026	1244.7691	1294.6589	1341.1779		
32027	1369.9955	1393.9225	1404.0195		
32028	1407.0221	1468.9256	1478.0136		
32029	1486.3824	1508.9808	1667.8641		
32030	1963.8581	3073.5110	3078.5883		
32031	3096.9741	3140.0348	3157.4632		
32032	3170.6568	3675.1401	3826.0084		
32033	Zero-point correction (Hartree): 0.150989				
32034	-----				
32035	TS.diHPCARP_Ib.15aldHshift.upummuud				
32036	-----				
32037	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14377290				
32038	Electronic state : 2-A				
32039	Cartesian coordinates (Angs):				
32040	O	0.589430	1.818496	-0.131210	
32041	O	1.151072	1.416801	1.065482	
32042	H	0.209738	0.569121	1.496897	
32043	C	-0.587537	-0.327809	1.133832	
32044	C	-0.835463	-0.111581	-0.378563	
32045	C	0.332338	0.693365	-0.967208	
32046	O	-1.034065	-1.158591	1.833622	
32047	C	-1.098623	-1.431516	-1.076047	
32048	O	-1.930892	0.790404	-0.486578	
32049	H	-2.003791	-1.873224	-0.668867	
32050	H	-0.271225	-2.118553	-0.912004	
32051	H	-1.229674	-1.257979	-2.144195	
32052	O	-3.097869	0.169427	0.028925	
32053	H	-3.282432	0.712904	0.805648	
32054	H	-0.016246	1.146656	-1.897245	
32055	C	1.555490	-0.165039	-1.253219	
32056	O	1.846270	-1.058956	-0.191852	
32057	H	1.357202	-0.775025	-2.135928	
32058	H	2.420473	0.466481	-1.449167	
32059	O	2.977869	-0.599254	0.524674	
32060	H	2.604209	0.158495	1.007585	
32061	Rotational constants (GHz): 1.4546500			0.7194700	0.6934300
32062	Vibrational harmonic frequencies (cm-1):				
32063	i1663.8253	48.7542		80.3678	
32064	134.8011	140.4610		162.0019	
32065	201.7864	230.9735		250.7915	
32066	259.4145	279.2619		292.8231	
32067	324.7693	344.1322		381.0506	
32068	422.5016	499.0525		520.3633	
32069	526.8492	550.2484		565.9695	
32070	613.7968	778.5327		809.8586	
32071	846.8941	932.1699		958.4843	
32072	981.5393	1030.2893		1046.0667	
32073	1056.5983	1090.7842		1129.0599	
32074	1139.1793	1161.1339		1210.8868	
32075	1247.2920	1293.3997		1343.7188	
32076	1370.5612	1394.8503		1407.6621	
32077	1416.9604	1470.6337		1472.5171	
32078	1489.4646	1506.0803		1666.0174	
32079	1955.6481	3077.5696		3083.0969	
32080	3101.9506	3143.7941		3159.6905	
32081	3180.7664	3669.6880		3815.9553	
32082	Zero-point correction (Hartree): 0.150972				
32083	-----				
32084	TS.diHPCARP_Ib.15aldHshift.upupmudu				
32085	-----				
32086	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14249419				

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32087 Electronic state : 2-A
32088 Cartesian coordinates (Angs):
32089 O 0.710891 1.651809 -1.071136
32090 O 1.384341 2.188672 0.012276
32091 H 1.966506 1.121524 0.502624
32092 C 1.749541 -0.095453 0.802106
32093 C 0.712516 -0.577725 -0.209523
32094 C -0.166516 0.631222 -0.604474
32095 O 2.208460 -0.660456 1.725356
32096 C 1.497151 -1.121514 -1.399961
32097 O -0.033144 -1.574328 0.455030
32098 H 2.101415 -1.967153 -1.076721
32099 H 2.140366 -0.347593 -1.813718
32100 H 0.798474 -1.452971 -2.164226
32101 O -0.910459 -2.167790 -0.493253
32102 H -1.736224 -1.690539 -0.303979
32103 H -0.767924 0.361780 -1.473460
32104 C -1.084243 1.148967 0.510058
32105 O -2.458590 1.058347 0.182663
32106 H -0.898336 0.650181 1.463756
32107 H -0.913953 2.217736 0.626297
32108 O -2.856593 -0.303912 0.256190
32109 H -3.300271 -0.344673 1.113175
32110 Rotational constants (GHz): 1.1322700 0.8416900 0.6404000
32111 Vibrational harmonic frequencies (cm-1):
32112 i1889.8235 45.0709 67.7586
32113 115.8696 142.2946 189.5578
32114 193.4690 213.1991 244.6486
32115 251.5806 262.4403 312.8198
32116 322.4417 328.3185 354.0982
32117 413.0914 486.6043 507.3252
32118 541.2353 568.4949 616.6007
32119 632.7401 748.1548 793.2953
32120 919.3891 939.3669 966.9708
32121 976.9251 1032.3038 1038.8602
32122 1074.5217 1101.0168 1111.4645
32123 1121.4372 1174.8735 1217.6222
32124 1231.7871 1306.3193 1318.6596
32125 1362.4266 1391.8038 1400.6482
32126 1432.8646 1462.0255 1466.4799
32127 1487.9744 1498.4425 1666.0218
32128 1951.8483 3071.9281 3082.4046
32129 3112.3867 3152.0806 3165.1547
32130 3171.6142 3681.3519 3813.1136
32131 Zero-point correction (Hartree): 0.150936
32132
32133 TS.diHPCARP_Ib.15aldHshift.utdmmddu
32134 -----
32135 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14474011
32136 Electronic state : 2-A
32137 Cartesian coordinates (Angs):
32138 O 0.542285 1.991211 -0.147884
32139 O 1.571805 1.916242 -1.066227
32140 H 2.174859 0.823400 -0.607372
32141 C 1.972444 -0.299106 -0.081605
32142 C 0.514425 -0.322882 0.447790
32143 C -0.250307 0.815579 -0.251372
32144 O 2.752391 -1.176467 -0.046020
32145 C 0.577266 -0.168994 1.959798
32146 O -0.038779 -1.598680 0.229185
32147 H 0.939709 0.824553 2.219080
32148 H 1.248263 -0.918777 2.373416
32149 H -0.418385 -0.319399 2.373932
32150 O -0.104804 -1.849038 -1.166976
32151 H -1.051726 -1.711077 -1.324979
32152 H -0.376915 0.573533 -1.305620
32153 C -1.588406 1.176818 0.375300
32154 O -2.416546 0.050955 0.567607
32155 H -1.447593 1.580016 1.378549
32156 H -2.084538 1.926300 -0.244043
32157 O -2.647035 -0.517594 -0.720051
32158 H -3.610733 -0.520078 -0.759501

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32159 Rotational constants (GHz): 1.2273700 0.8252100 0.6582100
32160 Vibrational harmonic frequencies (cm-1):
32161 i1769.7307 60.9343 82.9679
32162 129.9127 167.4893 172.3897
32163 189.6415 212.2213 214.6970
32164 248.4746 260.0315 294.7265
32165 317.9342 360.7498 381.4888
32166 419.5573 455.6832 476.1938
32167 508.0915 518.0931 593.3584
32168 630.6789 668.1151 812.4215
32169 881.8000 938.0419 954.7794
32170 1002.1524 1040.6476 1058.0131
32171 1080.0579 1111.8143 1120.4304
32172 1133.8748 1194.6719 1211.5218
32173 1268.4484 1287.9473 1340.9791
32174 1387.0455 1389.8200 1404.0375
32175 1425.8683 1448.7915 1483.0759
32176 1492.7561 1513.2863 1672.5095
32177 1958.1525 3074.2022 3077.4655
32178 3119.2658 3138.4972 3160.7983
32179 3164.2157 3756.2191 3838.7325
32180 Zero-point correction (Hartree): 0.151056
32181
32182 TS.diHPCARP_Ib.15aldHshift.utdmpddu
32183 -----
32184 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14381445
32185 Electronic state : 2-A
32186 Cartesian coordinates (Angs):
32187 O 0.856243 1.945632 0.071962
32188 O 2.077136 1.783193 -0.561278
32189 H 2.388631 0.558702 -0.167087
32190 C 1.906580 -0.590945 0.052503
32191 C 0.416638 -0.374656 0.373162
32192 C -0.014025 0.912111 -0.357759
32193 O 2.491370 -1.604929 -0.037973
32194 C 0.302616 -0.283284 1.888581
32195 O -0.342574 -1.511156 0.001418
32196 H 0.876336 0.568741 2.248331
32197 H 0.692103 -1.195855 2.335961
32198 H -0.739102 -0.158723 2.178804
32199 O -0.360630 -1.643679 -1.410781
32200 H -1.189021 -1.189122 -1.637883
32201 H 0.121981 0.774062 -1.431720
32202 C -1.442693 1.364883 -0.096429
32203 O -2.361777 0.382404 -0.553081
32204 H -1.631361 1.584338 0.952828
32205 H -1.629492 2.264129 -0.683235
32206 O -2.822762 -0.382266 0.551272
32207 H -2.200821 -1.128523 0.551330
32208 Rotational constants (GHz): 1.2511500 0.8336300 0.6471600
32209 Vibrational harmonic frequencies (cm-1):
32210 i1859.2723 74.6439 95.5290
32211 116.8419 164.5225 195.8934
32212 203.3146 206.9143 238.1172
32213 250.4728 290.0054 336.0542
32214 361.8801 373.6043 420.1240
32215 456.3556 471.1438 486.5303
32216 531.8165 578.1013 593.8091
32217 625.5478 663.5485 816.5740
32218 884.6681 929.3238 959.5063
32219 1012.2155 1043.8989 1060.1398
32220 1087.1930 1111.9098 1120.4729
32221 1129.5808 1182.9362 1214.3723
32222 1262.4597 1288.6453 1345.9852
32223 1389.7276 1407.7303 1416.8181
32224 1445.2002 1469.5209 1487.7023
32225 1492.6067 1512.3532 1670.5246
32226 1962.1890 3080.0291 3093.3133
32227 3095.1333 3151.6565 3162.8797
32228 3166.0189 3710.8812 3724.5971
32229 Zero-point correction (Hartree): 0.151780
32230

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32231 TS.diHPCARP_Ib.15aldHshift.utummuud
32232 -----
32233 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14467415
32234 Electronic state : 2-A
32235 Cartesian coordinates (Angs):
32236 O -0.148172 -1.680769 -0.559481
32237 O -0.718941 -1.677357 0.702003
32238 H 0.001912 -0.693711 1.325249
32239 C 0.595169 0.381393 1.152681
32240 C 0.856592 0.491534 -0.371641
32241 C -0.171304 -0.363562 -1.122455
32242 O 0.863308 1.153373 1.992535
32243 C 0.882032 1.943029 -0.804090
32244 O 2.161185 -0.026513 -0.608449
32245 H 1.681809 2.451179 -0.271174
32246 H -0.063304 2.426139 -0.565968
32247 H 1.065773 2.006424 -1.876478
32248 O 2.426937 -1.109289 0.273840
32249 H 1.953140 -1.846783 -0.140750
32250 H 0.207292 -0.517758 -2.134710
32251 C -1.558108 0.255815 -1.190057
32252 O -1.944360 0.832479 0.046377
32253 H -1.542561 1.062611 -1.925063
32254 H -2.294720 -0.484883 -1.497564
32255 O -2.921095 0.019136 0.670660
32256 H -2.386530 -0.740956 0.959956
32257 Rotational constants (GHz): 1.3234300 0.8100700 0.7461400
32258 Vibrational harmonic frequencies (cm-1):
32259 11456.4588 69.5153 94.0514
32260 132.6335 173.0033 184.2496
32261 198.5891 233.7074 250.5547
32262 276.7884 299.7910 337.0723
32263 363.8318 364.6338 432.6905
32264 453.1348 479.6778 496.1841
32265 533.5638 564.9669 590.0213
32266 623.0622 776.8272 795.0839
32267 846.5129 932.7666 957.2124
32268 973.4781 1040.4926 1044.3579
32269 1052.0823 1074.2762 1124.8021
32270 1139.7332 1185.7755 1218.7654
32271 1230.5392 1291.4382 1345.6212
32272 1373.4527 1396.2573 1408.1398
32273 1439.5188 1469.6325 1476.6759
32274 1489.1376 1497.2959 1709.3545
32275 1970.9253 3076.5952 3079.3630
32276 3103.3121 3140.3116 3158.9296
32277 3174.5795 3707.7832 3758.8033
32278 Zero-point correction (Hartree): 0.151752
32279
32280 TS.diHPCARP_Ib.15aldHshift.utupppdu
32281 -----
32282 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14539983
32283 Electronic state : 2-A
32284 Cartesian coordinates (Angs):
32285 O -0.898924 1.327731 -0.299930
32286 O 0.036338 2.303086 -0.582917
32287 H 1.014536 1.909434 0.190140
32288 C 1.669203 0.862540 0.476990
32289 C 0.712773 -0.328896 0.333835
32290 C -0.385003 0.052603 -0.677805
32291 O 2.831178 0.826170 0.669955
32292 C 0.204157 -0.670141 1.727881
32293 O 1.430386 -1.468765 -0.095055
32294 H -0.437392 0.126328 2.098351
32295 H 1.052009 -0.806167 2.396728
32296 H -0.376096 -1.589078 1.689346
32297 O 2.096364 -1.169912 -1.313136
32298 H 2.996011 -0.994860 -1.002542
32299 H 0.069209 0.130492 -1.667167
32300 C -1.547338 -0.927258 -0.732460
32301 O -2.393036 -0.850280 0.396057
32302 H -2.137798 -0.762665 -1.633028

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32303      H      -1.145915      -1.942367      -0.745351
32304      O      -3.362515      0.160099      0.165930
32305      H      -2.875649      0.970759      0.375646
32306 Rotational constants (GHz):      1.4506300      0.6924500      0.5984800
32307 Vibrational harmonic frequencies (cm-1):
32308      i1929.6048      54.8086      75.5248
32309      129.2904      156.4167      171.8392
32310      190.6145      211.7905      253.2716
32311      260.0197      278.8582      291.4743
32312      322.9482      349.8783      398.7974
32313      408.4033      438.7854      458.1343
32314      491.7410      542.1850      610.4418
32315      638.9859      750.5341      831.8600
32316      884.3313      912.9415      944.5419
32317      998.7208      1015.3726      1050.3199
32318      1074.9420      1120.1424      1133.1278
32319      1140.0398      1166.1228      1216.2574
32320      1264.7037      1314.8639      1357.3560
32321      1381.2134      1402.9084      1410.0907
32322      1418.9516      1446.4540      1467.8738
32323      1480.8339      1501.7639      1660.9976
32324      1937.5461      3082.6509      3083.1131
32325      3100.3485      3138.1157      3165.3556
32326      3172.5841      3770.1641      3790.2366
32327 Zero-point correction (Hartree): 0.151092
32328
32329 TS.diHPCARP_Ib.15aldHshift.utuppudu
32330 -----
32331 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14225144
32332 Electronic state : 2-A
32333 Cartesian coordinates (Angs):
32334      O      -0.687129      1.591007      -0.381608
32335      O      0.415689      2.390549      -0.624698
32336      H      1.283240      1.841342      0.165661
32337      C      1.743926      0.691117      0.480995
32338      C      0.577803      -0.298337      0.353966
32339      C      -0.350589      0.255833      -0.744212
32340      O      2.879524      0.440512      0.676586
32341      C      -0.050582      -0.414827      1.737614
32342      O      1.066218      -1.585736      0.036797
32343      H      -0.730567      -1.261066      1.752361
32344      H      -0.612891      0.489319      1.961123
32345      H      0.730575      -0.561007      2.481636
32346      O      1.802654      -1.519777      -1.176190
32347      H      2.711089      -1.462241      -0.847520
32348      H      0.213939      0.298280      -1.679122
32349      C      -1.595564      -0.557107      -1.045706
32350      O      -2.365030      -0.986845      0.052590
32351      H      -2.212742      0.013755      -1.744489
32352      H      -1.280082      -1.488722      -1.517642
32353      O      -2.890364      0.164765      0.700042
32354      H      -3.825027      0.114467      0.463892
32355 Rotational constants (GHz):      1.3293500      0.7552600      0.6379700
32356 Vibrational harmonic frequencies (cm-1):
32357      i2035.2201      48.4705      77.6763
32358      126.8044      136.6814      169.9525
32359      183.3089      206.3059      220.1103
32360      241.8766      257.7416      306.1661
32361      313.1061      337.3238      347.9880
32362      396.2812      430.5822      452.7755
32363      464.7137      525.6969      614.1665
32364      635.0109      783.7885      845.2153
32365      859.1744      899.2709      948.8496
32366      981.1008      1023.3455      1048.6381
32367      1070.5255      1112.9414      1136.9918
32368      1153.5737      1176.9033      1223.3987
32369      1269.8120      1324.8381      1361.9140
32370      1390.5418      1396.7587      1407.7062
32371      1415.1615      1429.0819      1458.9958
32372      1490.9893      1502.8150      1658.0233
32373      1933.7106      3059.5634      3081.4407
32374      3085.7973      3127.9938      3165.4867

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32375          3187.3970          3788.4500          3819.1820
32376 Zero-point correction (Hartree): 0.150614
32377
32378 TS.diHPCARP_Ib.15aldHshift.utuppuud
32379 -----
32380 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14195250
32381 Electronic state : 2-A
32382 Cartesian coordinates (Angs):
32383 O -0.144109 1.731941 -0.384312
32384 O -0.603212 2.022734 0.892306
32385 H -1.371251 0.967711 1.132756
32386 C -1.473308 -0.278817 0.964239
32387 C -0.555784 -0.621345 -0.239797
32388 C 0.516431 0.465816 -0.353108
32389 O -2.065280 -1.017028 1.659105
32390 C -0.005422 -2.026745 -0.123349
32391 O -1.372139 -0.603048 -1.406186
32392 H -0.837705 -2.723490 -0.060366
32393 H 0.617899 -2.126720 0.762116
32394 H 0.602403 -2.253435 -0.998057
32395 O -2.381467 0.391239 -1.283057
32396 H -1.898603 1.210684 -1.472667
32397 H 0.991375 0.374229 -1.329974
32398 C 1.588134 0.450062 0.734698
32399 O 2.578280 -0.522956 0.477049
32400 H 2.025497 1.447134 0.810270
32401 H 1.186445 0.169973 1.709681
32402 O 3.254990 -0.139612 -0.714455
32403 H 4.127128 0.093932 -0.373461
32404 Rotational constants (GHz): 1.3157000 0.6978100 0.6402000
32405 Vibrational harmonic frequencies (cm-1):
32406 i1732.1246 55.5093 59.9479
32407 111.6693 153.8553 173.7917
32408 184.9193 197.4311 200.4697
32409 228.9859 260.3654 285.8937
32410 323.4333 348.9668 378.9363
32411 433.0305 453.2918 476.3313
32412 495.8507 527.8498 578.8120
32413 613.4910 732.1604 789.1078
32414 882.7657 928.8009 959.5254
32415 988.4416 1038.0297 1050.1729
32416 1079.4616 1093.6282 1113.1004
32417 1141.8186 1195.0494 1212.5975
32418 1233.8513 1284.6527 1327.6518
32419 1375.1589 1395.0089 1413.9625
32420 1419.4462 1438.6580 1476.6725
32421 1478.1772 1491.0517 1678.4474
32422 1960.7341 3073.8136 3083.4661
32423 3120.6433 3131.0214 3163.7394
32424 3175.8550 3752.6661 3826.2946
32425 Zero-point correction (Hartree): 0.150469
32426
32427 TS.diHPCARP_Ib.15aldHshift.ututmudu
32428 -----
32429 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14521631
32430 Electronic state : 2-A
32431 Cartesian coordinates (Angs):
32432 O -0.888223 1.295002 0.084552
32433 O -0.121959 2.193599 -0.634167
32434 H 1.059187 1.911922 -0.158024
32435 C 1.805000 0.913918 0.083224
32436 C 0.889086 -0.270706 0.428101
32437 C -0.475121 -0.032329 -0.243096
32438 O 2.971830 0.884813 -0.078056
32439 C 0.811863 -0.367231 1.945955
32440 O 1.485862 -1.477022 0.000607
32441 H 0.243801 0.472346 2.342663
32442 H 1.814177 -0.363571 2.369263
32443 H 0.319858 -1.297955 2.222654
32444 O 1.734612 -1.401464 -1.394749
32445 H 2.680148 -1.195893 -1.411245
32446 H -0.369108 -0.108008 -1.326148

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32447	C	-1.553923	-0.987737	0.228451		
32448	O	-2.735923	-0.830031	-0.523167		
32449	H	-1.212517	-2.008958	0.051193		
32450	H	-1.780972	-0.855773	1.286686		
32451	O	-3.511109	0.198476	0.074335		
32452	H	-3.096711	1.003421	-0.267696		
32453	Rotational constants (GHz):			1.4676400	0.6464500	0.5612000
32454	Vibrational harmonic frequencies (cm-1):					
32455	i1949.1076		52.9224			65.3386
32456	123.8621		138.4461			169.4476
32457	179.2312		209.6482			246.2564
32458	256.2013		286.8827			300.5033
32459	322.1835		349.6821			369.0692
32460	400.3057		410.1157			470.4787
32461	488.7977		548.7617			559.4855
32462	637.4793		743.5420			829.6044
32463	875.7223		913.7192			963.8012
32464	976.2580		1047.2103			1055.3737
32465	1102.4593		1117.4860			1131.7158
32466	1133.0242		1185.1969			1221.4633
32467	1268.2999		1315.1755			1333.6739
32468	1368.5880		1406.3418			1420.4027
32469	1422.4688		1441.1734			1467.6174
32470	1489.9237		1508.3806			1663.5334
32471	1938.4390		3077.5779			3081.3271
32472	3107.9140		3138.0302			3160.8179
32473	3165.3743		3784.8269			3789.6395
32474	Zero-point correction (Hartree): 0.150886					
32475						
32476	TS.diHPCARP_Ib.15aldHshift.ututpddu					
32477	-----					
32478	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14451910					
32479	Electronic state : 2-A					
32480	Cartesian coordinates (Angs):					
32481	O	-0.514466	1.694751	0.041268		
32482	O	0.273587	2.176519	-0.984285		
32483	H	1.410771	1.675846	-0.645262		
32484	C	1.937172	0.572532	-0.265521		
32485	C	0.848888	-0.214885	0.483201		
32486	C	-0.523336	0.272170	-0.015130		
32487	O	3.005580	0.181463	-0.573886		
32488	C	1.062244	0.006915	1.974418		
32489	O	1.033185	-1.599184	0.274440		
32490	H	0.836924	1.040707	2.230355		
32491	H	2.093398	-0.218041	2.238979		
32492	H	0.405728	-0.656068	2.535691		
32493	O	1.009449	-1.863668	-1.119789		
32494	H	1.954281	-1.930812	-1.318166		
32495	H	-0.667761	-0.050501	-1.046405		
32496	C	-1.667669	-0.213179	0.847707		
32497	O	-2.925758	0.058951	0.277974		
32498	H	-1.558287	-1.284177	1.033694		
32499	H	-1.686171	0.324463	1.796451		
32500	O	-3.069062	-0.807489	-0.843398		
32501	H	-3.232798	-0.173466	-1.551977		
32502	Rotational constants (GHz):			1.3121700	0.6808100	0.5964500
32503	Vibrational harmonic frequencies (cm-1):					
32504	i2041.6522		45.3400			53.5478
32505	116.2720		146.2628			170.2449
32506	171.7383		214.7311			237.9133
32507	244.0931		261.9109			282.0584
32508	297.3066		320.1204			360.1110
32509	404.7991		409.0220			464.5707
32510	485.3623		553.4745			559.9608
32511	636.4102		745.6365			829.0043
32512	880.1249		911.0877			962.7048
32513	979.2106		1047.9203			1059.1243
32514	1097.5850		1113.8287			1121.6612
32515	1151.7769		1181.8483			1215.7132
32516	1267.6973		1308.1243			1335.8316
32517	1366.0459		1403.4649			1407.6117
32518	1422.7041		1435.4119			1468.7656


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32519      1490.4928      1508.2038      1656.3334
32520      1935.5932      3070.8546      3077.7591
32521      3116.5748      3134.6490      3158.7344
32522      3164.6511      3789.9323      3832.2726
32523 Zero-point correction (Hartree): 0.150551
32524
32525
32526
32527 1,6-aldehyde-H-shift in (2R,3R)-2-Me-2,3-diOOH-butanal-4-peroxyl (C, R,R-di-HPCARP-Ic)
32528 =====
32529
32530 TS.diHPCARP_Ic.16aldHshift.a.mppmmu
32531 -----
32532 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14835611
32533 Electronic state : 2-A
32534 Cartesian coordinates (Angs):
32535 O      1.881584      -1.568288      0.667349
32536 H      0.735516      -1.238708      1.082096
32537 C     -0.423989      -0.679460      1.000393
32538 O      2.420461      -0.358272      0.297542
32539 C     -0.628212      -0.208456     -0.447428
32540 C      1.925638      0.010956     -0.972796
32541 C      0.541301      0.660320     -0.953348
32542 O     -1.222242      -0.632783      1.871027
32543 C     -0.789901      -1.457023     -1.311049
32544 O     -1.744853      0.659347     -0.512647
32545 H     -1.698151      -1.982852     -1.031877
32546 H      0.061758      -2.120885     -1.180997
32547 H     -0.865050      -1.158779     -2.356270
32548 O     -2.937066      -0.061031     -0.256786
32549 H     -2.966670      -0.058032      0.712286
32550 O      0.569806      1.928749     -0.329592
32551 H      0.294671      0.913108     -1.989384
32552 O      0.582697      1.740838      1.079077
32553 H     -0.280987      2.105653      1.317832
32554 H      2.621992      0.766410     -1.336007
32555 H      1.944811      -0.852418     -1.640084
32556 Rotational constants (GHz):      1.313990      0.8096500      0.7470100
32557 Vibrational harmonic frequencies (cm-1):
32558 i2066.9004      77.2832      90.3990
32559      132.1480      153.5204      177.7346
32560      203.7162      216.4589      264.9110
32561      278.9355      312.7415      326.5826
32562      327.9620      363.0367      393.0234
32563      414.2038      460.0885      481.2283
32564      496.1959      535.1249      593.9462
32565      624.7900      822.0709      835.4768
32566      864.4308      923.2438      941.3612
32567      981.4974      1006.5180      1050.8701
32568      1077.9381      1120.3121      1150.8471
32569      1156.8359      1181.7212      1221.9233
32570      1253.7510      1310.8913      1347.0323
32571      1377.0362      1400.3816      1407.2673
32572      1419.3553      1444.3005      1466.8549
32573      1490.3103      1506.5262      1509.8891
32574      1916.6635      3069.9315      3079.7816
32575      3084.3638      3138.2884      3163.2106
32576      3181.7054      3755.0952      3793.2260
32577 Zero-point correction (Hartree): 0.151213
32578
32579 TS.diHPCARP_Ic.16aldHshift.a.mppmu
32580 -----
32581 IRC pathway available
32582 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17664245
32583 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05444034
32584 T1 diagnostic: 0.022645
32585 E(MP2/Aug-CC-pVTZ) (Hartree): -721.01200415
32586 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02911721
32587 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01875681
32588 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03329845
32589 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48013986
32590 E(UHF/Aug-CC-pVTZ) (Hartree): -718.47053628

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32591 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15081632
32592 Electronic state : 2-A
32593 Cartesian coordinates (Angs):
32594 O 1.840680 -1.532105 0.698886
32595 H 0.661185 -1.126021 1.111091
32596 C -0.482823 -0.594994 1.026050
32597 O 2.416914 -0.398463 0.169170
32598 C -0.692441 -0.165159 -0.433296
32599 C 1.836082 -0.107238 -1.091177
32600 C 0.506502 0.638708 -0.971172
32601 O -1.272978 -0.561255 1.901200
32602 C -0.904018 -1.441236 -1.247175
32603 O -1.774726 0.734248 -0.537101
32604 H -1.865532 -1.875301 -0.989659
32605 H -0.118499 -2.165528 -1.042449
32606 H -0.902154 -1.193601 -2.308716
32607 O -2.985654 0.077468 -0.211365
32608 H -3.016494 0.189696 0.750855
32609 O 0.689739 1.863005 -0.283866
32610 H 0.216020 0.960925 -1.975461
32611 O 0.768372 1.608818 1.109984
32612 H 1.695023 1.349413 1.228553
32613 H 2.543430 0.568444 -1.571768
32614 H 1.748422 -1.022243 -1.677086
32615 Rotational constants (GHz): 1.3600100 0.7870800 0.7501900
32616 Vibrational harmonic frequencies (cm-1):
32617 i1777.1147 89.7126 113.5727
32618 155.2752 169.8861 194.3450
32619 208.7569 227.0013 275.5292
32620 289.7158 310.8020 327.8918
32621 333.7367 362.6664 400.9822
32622 446.4646 461.9513 478.8721
32623 493.4472 536.1084 600.6000
32624 625.4606 822.7895 839.9474
32625 871.2425 922.3119 945.8727
32626 978.7816 1003.1516 1052.6062
32627 1079.8609 1114.8387 1143.2382
32628 1149.6961 1183.6791 1216.6187
32629 1255.7566 1306.4550 1345.1071
32630 1374.9400 1396.6392 1404.3288
32631 1435.6822 1445.1755 1473.0977
32632 1490.5838 1508.9213 1517.7173
32633 1929.5343 3077.4175 3078.9054
32634 3091.0189 3144.0989 3159.1381
32635 3182.8701 3755.3065 3764.7927
32636 Zero-point correction (Hartree): 0.151646
32637
32638 TS.diHPCARP_Ic.16aldHshift.a.mppmuu
32639 -----
32640 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14902797
32641 Electronic state : 2-A
32642 Cartesian coordinates (Angs):
32643 O 1.395974 -1.998726 0.495691
32644 H 0.324963 -1.457426 0.974264
32645 C -0.701598 -0.693412 0.980829
32646 O 2.196165 -0.923025 0.184200
32647 C -0.800088 -0.048231 -0.412730
32648 C 1.723925 -0.297437 -0.993235
32649 C 0.547239 0.636745 -0.702837
32650 O -1.435343 -0.550851 1.891213
32651 C -1.152921 -1.120576 -1.436367
32652 O -1.729627 1.015108 -0.404582
32653 H -2.197242 -1.394010 -1.318218
32654 H -0.532088 -2.003841 -1.306603
32655 H -1.005182 -0.718336 -2.438658
32656 O -3.030361 0.508776 -0.166744
32657 H -3.079837 0.549881 0.799918
32658 O 0.785149 1.409090 0.461818
32659 H 0.394430 1.291767 -1.567744
32660 O 2.039621 2.053499 0.341610
32661 H 2.592460 1.499589 0.911283
32662 H 2.559174 0.302069 -1.347852

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32663      H      1.471357      -1.043203      -1.746011
32664 Rotational constants (GHz):      1.3023000      0.7684400      0.6683300
32665 Vibrational harmonic frequencies (cm-1):
32666      i1941.9876      62.6891      91.1996
32667      122.6220      149.1668      177.1601
32668      195.3820      239.2130      268.1540
32669      290.3942      311.2500      334.9297
32670      349.4697      377.8902      388.0424
32671      411.1222      414.2900      462.7310
32672      483.1837      518.1681      611.0325
32673      660.4083      762.7281      821.1365
32674      874.5178      913.3128      964.4200
32675      984.6756      1038.2411      1055.3811
32676      1074.6085      1125.6418      1143.4791
32677      1157.4281      1186.9727      1216.3346
32678      1261.7894      1292.8332      1349.8539
32679      1370.8907      1395.0979      1404.7550
32680      1422.9381      1441.3921      1480.5659
32681      1491.1301      1506.8230      1511.9505
32682      1941.8476      3052.3263      3080.0536
32683      3104.7620      3159.1431      3162.1076
32684      3183.9639      3771.7136      3779.8109
32685 Zero-point correction (Hartree): 0.151277
32686
32687 TS.diHPCARP_Ic.16aldHshift.a.mppuu
32688 -----
32689 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14802626
32690 Electronic state : 2-A
32691 Cartesian coordinates (Angs):
32692      O      -1.259744      -2.191241      -0.335837
32693      H      -0.211810      -1.683072      -0.844826
32694      C      0.744551      -0.819158      -0.914648
32695      O      -2.117259      -1.117047      -0.286443
32696      C      0.740775      -0.036046      0.407426
32697      C      -1.817524      -0.310093      0.834398
32698      C      -0.634511      0.627790      0.594471
32699      O      1.491095      -0.688776      -1.817353
32700      C      1.073496      -0.987947      1.551369
32701      O      1.637591      1.055345      0.341969
32702      H      2.119833      -1.272028      1.486865
32703      H      0.452875      -1.879028      1.510220
32704      H      0.907556      -0.472735      2.497343
32705      O      2.962859      0.574369      0.212244
32706      H      3.052981      0.515892      -0.750737
32707      O      -0.835555      1.391465      -0.579011
32708      H      -0.538297      1.296467      1.457267
32709      O      -1.945182      2.245417      -0.342725
32710      H      -1.529961      3.112467      -0.429405
32711      H      -2.702194      0.308837      0.974451
32712      H      -1.662134      -0.930328      1.717962
32713 Rotational constants (GHz):      1.1954100      0.8094900      0.6539000
32714 Vibrational harmonic frequencies (cm-1):
32715      i2055.6250      68.1264      90.2615
32716      117.8291      146.2103      178.2234
32717      192.1542      214.4867      220.9790
32718      267.6545      283.6372      287.1799
32719      321.5535      349.9723      381.8718
32720      404.9244      414.2648      464.1277
32721      486.2235      510.4536      606.4428
32722      665.9026      765.1655      820.9614
32723      876.7497      915.5678      961.8640
32724      987.7449      1038.4918      1054.7331
32725      1072.7594      1126.6905      1143.8364
32726      1165.1532      1185.4006      1223.6674
32727      1265.7118      1300.3970      1353.6508
32728      1369.0707      1396.5403      1405.7406
32729      1417.7815      1438.8021      1473.0603
32730      1489.6066      1506.0955      1510.2225
32731      1937.4014      3045.9569      3082.3039
32732      3091.7148      3151.8860      3164.3002
32733      3185.5750      3766.6166      3826.2989
32734 Zero-point correction (Hartree): 0.150792

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32735
32736 TS.diHPCARP_Ic.16aldHshift.a.mptpuu
32737 -----
32738 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15000986
32739 Electronic state : 2-A
32740 Cartesian coordinates (Angs):
32741 O -2.185595 -1.496543 -0.357827
32742 H -1.001596 -1.498072 -0.802118
32743 C 0.214320 -1.069132 -0.859775
32744 O -2.500660 -0.158125 -0.393372
32745 C 0.506429 -0.311259 0.442364
32746 C -1.954090 0.489977 0.739439
32747 C -0.485105 0.868673 0.570995
32748 O 0.956158 -1.240127 -1.760696
32749 C 0.428133 -1.269582 1.622244
32750 O 1.771516 0.324945 0.346399
32751 H 1.273507 -1.951505 1.597649
32752 H -0.496551 -1.841026 1.591978
32753 H 0.467849 -0.694796 2.547489
32754 O 2.798860 -0.643554 0.241912
32755 H 2.816023 -0.810211 -0.713284
32756 O -0.405056 1.704961 -0.565888
32757 H -0.178971 1.439822 1.452259
32758 O 0.575445 2.705523 -0.346271
32759 H 1.399542 2.233741 -0.536903
32760 H -2.516522 1.417997 0.830311
32761 H -2.106752 -0.124649 1.626970
32762 Rotational constants (GHz): 1.1642200 0.8588500 0.6722500
32763 Vibrational harmonic frequencies (cm-1):
32764 i2066.2125 72.9842 91.7542
32765 142.9159 160.6523 176.9005
32766 195.2599 217.5667 235.8771
32767 289.6800 309.4033 320.1269
32768 353.5493 380.2539 400.2567
32769 420.3365 454.8358 477.6461
32770 498.8379 520.2109 593.5051
32771 625.7432 753.3710 823.7579
32772 894.7287 913.2263 955.2540
32773 986.3647 1033.8588 1058.2274
32774 1079.7972 1132.7161 1144.7461
32775 1163.3593 1177.9718 1207.9691
32776 1256.3854 1311.1559 1340.8909
32777 1366.2984 1396.3032 1405.7224
32778 1441.5226 1448.0916 1469.3108
32779 1489.5361 1506.5184 1508.2546
32780 1933.2975 3070.7719 3080.0831
32781 3091.0124 3150.4148 3160.2895
32782 3180.2185 3755.1476 3775.2175
32783 Zero-point correction (Hartree): 0.151271
32784
32785 TS.diHPCARP_Ic.16aldHshift.a.pmmuu
32786 -----
32787 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14926425
32788 Electronic state : 2-A
32789 Cartesian coordinates (Angs):
32790 O 2.127024 -1.081957 0.851304
32791 H 0.909995 -1.065536 1.147780
32792 C -0.361029 -0.915482 0.929604
32793 O 2.366571 0.217629 0.473072
32794 C -0.532376 -0.515247 -0.537329
32795 C 1.901277 0.417687 -0.844850
32796 C 0.391050 0.646093 -0.966768
32797 O -1.221943 -1.172029 1.696336
32798 C -0.231367 -1.773099 -1.353820
32799 O -1.888066 -0.233200 -0.836185
32800 H -0.969005 -2.536841 -1.117103
32801 H 0.762562 -2.149319 -1.125649
32802 H -0.297691 -1.535713 -2.414777
32803 O -2.435634 0.709660 0.074222
32804 H -2.856356 0.119285 0.716714
32805 O 0.009358 1.879618 -0.401936
32806 H 0.184370 0.798546 -2.031178

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32807	O	-0.005618	1.747239	1.012206	
32808	H	-0.963400	1.747517	1.163030	
32809	H	2.385102	1.336992	-1.173935	
32810	H	2.225550	-0.410315	-1.478064	
32811	Rotational constants (GHz):		1.2633000	0.8768600	0.7823000
32812	Vibrational harmonic frequencies (cm-1):				
32813	i2113.4557		89.5911		104.7922
32814	168.0532		184.9948		199.4583
32815	205.8889		241.1481		262.8811
32816	275.1963		309.7896		322.4085
32817	330.0402		387.2997		398.9567
32818	424.4040		464.6870		508.6949
32819	523.9141		561.3859		608.4747
32820	626.0240		813.2196		833.2258
32821	879.2722		928.8064		946.1448
32822	980.8727		1008.4236		1045.2669
32823	1074.3089		1110.3730		1151.3681
32824	1163.1921		1201.4527		1223.4126
32825	1233.0840		1309.5530		1339.7052
32826	1381.6298		1398.1441		1407.5371
32827	1430.3979		1447.6140		1469.1103
32828	1488.8884		1504.1651		1505.1491
32829	1922.0977		3063.8824		3075.9835
32830	3082.0396		3137.2632		3159.4236
32831	3178.2835		3767.4762		3773.3497
32832	Zero-point correction (Hartree): 0.151799				
32833					
32834	TS.diHPCARP_Ic.16aldHshift.a.pmpdd				
32835	-----				
32836	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14421827				
32837	Electronic state : 2-A				
32838	Cartesian coordinates (Angs):				
32839	O	1.033403	2.267735	-0.308392	
32840	H	1.551303	1.243107	0.264235	
32841	C	1.427435	0.112818	0.847132	
32842	O	-0.212454	2.308146	0.278436	
32843	C	0.369683	-0.712619	0.067065	
32844	C	-1.083192	1.386009	-0.354380	
32845	C	-0.985490	-0.007015	0.273186	
32846	O	1.945119	-0.185295	1.858900	
32847	C	0.377924	-2.155337	0.534765	
32848	O	0.657464	-0.588296	-1.308937	
32849	H	0.103397	-2.203727	1.587121	
32850	H	1.376211	-2.569659	0.416360	
32851	H	-0.332456	-2.729346	-0.052776	
32852	O	2.018924	-0.965258	-1.487880	
32853	H	2.367801	-0.172530	-1.916558	
32854	O	-1.961469	-0.862756	-0.289974	
32855	H	-1.156303	0.065599	1.351413	
32856	O	-3.209903	-0.490395	0.288094	
32857	H	-3.751100	-0.363751	-0.500583	
32858	H	-2.088253	1.765280	-0.175253	
32859	H	-0.877428	1.350853	-1.422534	
32860	Rotational constants (GHz):		1.0904800	0.8288800	0.6510800
32861	Vibrational harmonic frequencies (cm-1):				
32862	i1965.1093		61.2974		82.7643
32863	91.5830		119.5439		149.2601
32864	176.2412		195.4772		205.2662
32865	233.5291		260.9956		278.1984
32866	281.6495		301.0799		363.8824
32867	408.4931		442.9563		462.7538
32868	481.2144		532.3768		577.1744
32869	620.1069		694.2565		785.7647
32870	900.4932		947.8787		984.1390
32871	1020.5981		1037.3987		1068.5890
32872	1097.0940		1115.7745		1133.1391
32873	1174.3667		1176.5518		1209.6887
32874	1245.3424		1292.1785		1337.2978
32875	1374.9146		1404.1944		1408.6658
32876	1410.1992		1422.0784		1481.6092
32877	1484.2478		1493.7486		1540.1011
32878	1955.3758		3067.6502		3090.4962

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32879          3100.2624          3160.8715          3168.2222
32880          3186.3374          3812.0853          3833.3438
32881 Zero-point correction (Hartree): 0.150224
32882
32883 TS.diHPCARP_Ic.16aldHshift.a.pmpmpuu
32884 -----
32885 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14893493
32886 Electronic state : 2-A
32887 Cartesian coordinates (Angs):
32888 O          2.053735          -1.052261          0.922459
32889 H          0.794977          -0.923960          1.229678
32890 C         -0.451191          -0.754983          1.027655
32891 O          2.378649          0.130053          0.292853
32892 C         -0.638296          -0.522935          -0.475562
32893 C          1.831918          0.145182          -1.015359
32894 C          0.348022          0.529123          -1.026986
32895 O         -1.296984          -0.888649          1.837509
32896 C         -0.415281          -1.881449          -1.143562
32897 O         -1.978311          -0.215870          -0.776436
32898 H         -1.240665          -2.538139          -0.877682
32899 H          0.519727          -2.329310          -0.816965
32900 H         -0.400632          -1.755463          -2.225712
32901 O         -2.398392          0.940546          -0.073259
32902 H         -2.724506          0.557342          0.754702
32903 O          0.189910          1.812762          -0.452497
32904 H          0.053279          0.683247          -2.069353
32905 O          0.222971          1.697382          0.961262
32906 H          1.174112          1.695701          1.149901
32907 H          2.375157          0.937565          -1.529902
32908 H          2.024895          -0.808322          -1.506910
32909 Rotational constants (GHz):      1.2866700      0.8658500      0.7947400
32910 Vibrational harmonic frequencies (cm-1):
32911 i1838.3612          94.7440          119.6354
32912 152.3114          174.1540          195.2186
32913 221.1688          228.0122          266.8587
32914 290.5639          311.8494          322.0143
32915 332.0323          391.3678          397.5333
32916 414.7970          445.4665          469.6604
32917 506.6717          545.5018          613.2693
32918 627.8507          810.7687          832.6329
32919 886.7636          927.9800          952.4173
32920 979.3717          1003.7742          1056.3535
32921 1073.0053          1107.6066          1139.2235
32922 1155.0036          1207.4299          1220.3654
32923 1234.3157          1301.7672          1335.2551
32924 1373.8043          1393.4355          1406.9672
32925 1434.8109          1443.3612          1474.9135
32926 1492.8765          1508.1867          1515.8573
32927 1933.8805          3074.3958          3079.0884
32928 3090.1538          3143.6251          3158.6173
32929 3176.7168          3751.9565          3772.4755
32930 Zero-point correction (Hartree): 0.151657
32931
32932 TS.diHPCARP_Ic.16aldHshift.a.pmpmdd
32933 -----
32934 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14406534
32935 Electronic state : 2-A
32936 Cartesian coordinates (Angs):
32937 O         -1.525489          1.861327          0.594944
32938 H         -1.834397          0.734253          0.050399
32939 C         -1.513603          -0.305605          -0.620489
32940 O         -0.546305          2.322319          -0.257857
32941 C         -0.091671          -0.721293          -0.163980
32942 C          0.704989          1.728022          0.048147
32943 C          0.855681          0.390011          -0.684322
32944 O         -2.136968          -0.765305          -1.504324
32945 C          0.266508          -2.098940          -0.680644
32946 O         -0.070274          -0.657077          1.246261
32947 H          0.261931          -2.104652          -1.769343
32948 H         -0.463218          -2.821833          -0.323075
32949 H          1.256666          -2.364675          -0.319019
32950 O         -1.205776          -1.381870          1.711657

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32951	H	-1.647629	-0.699942	2.235203	
32952	O	2.196516	-0.031734	-0.746304	
32953	H	0.611573	0.548825	-1.738354	
32954	O	2.632745	-0.284612	0.590698	
32955	H	3.457459	0.215588	0.610979	
32956	H	1.456696	2.413312	-0.343744	
32957	H	0.813903	1.621568	1.124084	
32958	Rotational constants (GHz):		1.0662500	0.9167200	0.7132200
32959	Vibrational harmonic frequencies (cm-1):				
32960	i1940.3240		62.1305		90.5301
32961	108.7469		110.5899		134.5505
32962	169.0485		186.8710		211.9187
32963	228.3340		267.5197		286.3333
32964	299.0572		315.7095		353.6774
32965	413.9897		445.6176		469.6099
32966	495.3808		552.2618		575.4394
32967	600.0734		733.9066		792.3460
32968	894.0840		948.3287		965.0326
32969	981.9259		1030.9893		1055.5717
32970	1095.9371		1122.2865		1134.9543
32971	1166.6122		1187.0825		1213.4256
32972	1246.2563		1287.2022		1329.0677
32973	1372.9898		1392.1416		1407.1879
32974	1410.8318		1425.9574		1481.9722
32975	1484.9632		1493.9763		1540.3682
32976	1954.6359		3080.7592		3086.0186
32977	3096.3120		3165.8811		3169.2389
32978	3177.9502		3807.2394		3836.5292
32979	Zero-point correction (Hartree): 0.150239				
32980					
32981	TS.diHPCARP_Ic.16aldHshift.a.pmpdd				
32982	-----				
32983	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14631205				
32984	Electronic state : 2-A				
32985	Cartesian coordinates (Angs):				
32986	O	-1.317323	1.979312	0.761570	
32987	H	-1.757363	0.881968	0.283266	
32988	C	-1.589650	-0.132526	-0.483918	
32989	O	-0.405604	2.349738	-0.202825	
32990	C	-0.172217	-0.700229	-0.229414	
32991	C	0.829455	1.683952	0.010623	
32992	C	0.854064	0.346550	-0.736512	
32993	O	-2.335692	-0.467185	-1.328380	
32994	C	-0.014517	-2.049614	-0.902640	
32995	O	0.022080	-0.776649	1.171023	
32996	H	-0.171341	-1.947484	-1.974925	
32997	H	-0.750701	-2.745732	-0.508429	
32998	H	0.987256	-2.434947	-0.726446	
32999	O	-1.048866	-1.545939	1.710184	
33000	H	-1.419467	-0.916775	2.343576	
33001	O	2.154685	-0.197254	-0.783818	
33002	H	0.618614	0.530035	-1.788086	
33003	O	2.701310	-0.233145	0.527889	
33004	H	2.284594	-1.014290	0.921006	
33005	H	1.599456	2.323299	-0.419405	
33006	H	1.001432	1.564108	1.075468	
33007	Rotational constants (GHz):		1.0518500	0.9247000	0.7078700
33008	Vibrational harmonic frequencies (cm-1):				
33009	i2006.4975		59.7457		88.3722
33010	111.8054		136.5508		160.6920
33011	175.8855		206.8978		221.7542
33012	269.8847		280.7770		296.1773
33013	317.7598		326.0174		360.1938
33014	415.5246		443.7826		477.7119
33015	501.9757		556.3834		583.7006
33016	603.5872		734.3212		788.1620
33017	892.0616		948.9361		965.6507
33018	977.5702		1029.5144		1059.2098
33019	1098.1021		1122.4167		1135.5192
33020	1166.5033		1176.4166		1208.6656
33021	1232.1119		1292.6494		1327.2893
33022	1377.0180		1401.2014		1409.7711

33023	1415.4185	1438.2650	1481.9458			
33024	1484.9312	1492.8142	1553.9035			
33025	1952.9261	3084.7402	3087.4622			
33026	3108.9503	3166.1658	3175.0733			
33027	3183.4170	3765.7332	3809.3701			
33028	Zero-point correction (Hartree): 0.150677					
33029						
33030	TS.diHPCARP_Ic.16aldHshift.a.pmpuu					
33031	-----					
33032	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15005785					
33033	Electronic state : 2-A					
33034	Cartesian coordinates (Angs):					
33035	O	-2.527042	-0.694529	-0.552019		
33036	H	-1.398129	-1.154596	-0.846951		
33037	C	-0.111254	-1.289251	-0.728552		
33038	O	-2.315877	0.662788	-0.609284		
33039	C	0.308951	-0.583522	0.564083		
33040	C	-1.683516	1.096693	0.580267		
33041	C	-0.167611	0.890182	0.561120		
33042	O	0.584181	-1.893520	-1.466438		
33043	C	-0.291527	-1.363239	1.732433		
33044	O	1.706092	-0.716185	0.772050		
33045	H	0.198458	-2.331655	1.806257		
33046	H	-1.359005	-1.507933	1.590833		
33047	H	-0.119025	-0.811360	2.655854		
33048	O	2.454794	-0.215488	-0.321869		
33049	H	2.409053	-0.946597	-0.957507		
33050	O	0.307254	1.602869	-0.563238		
33051	H	0.246748	1.345695	1.464732		
33052	O	1.482277	2.311373	-0.211499		
33053	H	2.166161	1.650230	-0.404551		
33054	H	-1.856730	2.171305	0.611204		
33055	H	-2.151225	0.621283	1.442397		
33056	Rotational constants (GHz):			1.1662400	0.8904800	0.6915300
33057	Vibrational harmonic frequencies (cm-1):					
33058	i2115.1702		63.3288			97.2718
33059	142.0548		155.1706			195.3856
33060	225.9799		240.0649			260.5857
33061	278.4770		309.8615			327.2616
33062	359.2743		395.4104			403.0243
33063	416.7986		453.5439			510.8538
33064	524.7198		562.2338			594.9857
33065	625.5770		746.8457			818.9896
33066	891.1059		927.5135			956.0365
33067	989.5912		1036.0711			1054.2932
33068	1081.2952		1116.4452			1139.6845
33069	1163.6172		1196.6860			1208.7105
33070	1236.0320		1307.7443			1329.8183
33071	1368.2148		1393.9058			1407.7429
33072	1431.3278		1454.0209			1470.8653
33073	1489.9256		1504.8846			1506.9995
33074	1928.6090		3074.2095			3080.3810
33075	3092.4502		3150.2301			3158.3782
33076	3180.6115		3719.6406			3749.4204
33077	Zero-point correction (Hartree): 0.151508					
33078						
33079	TS.diHPCARP_Ic.16aldHshift.a.ppmuu					
33080	-----					
33081	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14685391					
33082	Electronic state : 2-A					
33083	Cartesian coordinates (Angs):					
33084	O	2.215517	-1.007835	0.736303		
33085	H	0.990573	-1.061078	1.097192		
33086	C	-0.280446	-0.969768	0.951561		
33087	O	2.368363	0.313158	0.388519		
33088	C	-0.538689	-0.559035	-0.506271		
33089	C	1.826948	0.524736	-0.895831		
33090	C	0.302346	0.659418	-0.945764		
33091	O	-1.077253	-1.266435	1.764247		
33092	C	-0.198852	-1.785554	-1.352858		
33093	O	-1.915036	-0.350215	-0.757760		
33094	H	-0.903803	-2.580696	-1.120047		


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33095      H      0.811934      -2.125511      -1.142138
33096      H      -0.286517      -1.533396      -2.408946
33097      O      -2.461873      0.621487      0.125016
33098      H      -2.454818      1.413108      -0.431015
33099      O      -0.136551      1.860025      -0.334431
33100      H      0.043788      0.824215      -1.997505
33101      O      -0.032925      1.718721      1.075285
33102      H      -0.953186      1.517478      1.311914
33103      H      2.238753      1.480254      -1.220531
33104      H      2.163492      -0.264403      -1.571377
33105      Rotational constants (GHz):      1.2507400      0.8809600      0.7814300
33106      Vibrational harmonic frequencies (cm-1):
33107      i1989.3117      87.3139      102.0688
33108      162.0051      167.8401      200.0444
33109      209.1096      242.8704      255.4796
33110      274.5811      303.7042      320.1187
33111      326.5870      388.1201      396.8433
33112      421.1155      461.2714      509.1882
33113      530.9518      570.8654      610.9904
33114      624.2869      804.7003      825.8157
33115      879.1933      929.9597      945.2343
33116      982.4429      1008.1864      1044.2300
33117      1075.1850      1112.1314      1154.4404
33118      1158.1198      1202.5297      1221.1616
33119      1239.7927      1310.3089      1344.8184
33120      1381.0989      1399.3744      1407.7379
33121      1427.7127      1449.2286      1468.0848
33122      1487.3832      1504.5585      1505.3310
33123      1947.2597      3057.3397      3073.2558
33124      3080.6746      3134.2548      3159.1577
33125      3177.6704      3735.4270      3793.0165
33126      Zero-point correction (Hartree): 0.151708
33127
33128      TS.diHPCARP_Ic.16aldHshift.a.pppuu
33129      -----
33130      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14857994
33131      Electronic state : 2-A
33132      Cartesian coordinates (Angs):
33133      O      2.076705      -1.129434      0.815982
33134      H      0.773337      -1.039114      1.134188
33135      C      -0.453310      -0.905598      0.953786
33136      O      2.384758      0.106899      0.295220
33137      C      -0.665211      -0.480323      -0.506784
33138      C      1.828914      0.225791      -1.001529
33139      C      0.343427      0.587429      -0.979891
33140      O      -1.265867      -1.218541      1.741045
33141      C      -0.511767      -1.760827      -1.327931
33142      O      -1.981158      -0.047469      -0.757602
33143      H      -1.341859      -2.422815      -1.092284
33144      H      0.425325      -2.261645      -1.093940
33145      H      -0.540010      -1.520883      -2.390520
33146      O      -2.399545      0.907199      0.204012
33147      H      -1.953537      1.716688      -0.085994
33148      O      0.155257      1.834226      -0.320665
33149      H      0.052940      0.814849      -2.010363
33150      O      0.247824      1.639877      1.085644
33151      H      1.206180      1.597481      1.232350
33152      H      2.362013      1.059636      -1.458869
33153      H      2.019495      -0.685097      -1.569562
33154      Rotational constants (GHz):      1.2629500      0.8708000      0.7844500
33155      Vibrational harmonic frequencies (cm-1):
33156      i1570.3174      88.7549      118.9913
33157      155.3756      174.2447      202.9052
33158      215.5625      229.4321      262.7245
33159      293.1230      310.9030      319.1481
33160      334.0632      377.2610      403.2141
33161      431.5113      442.6008      467.2753
33162      505.8798      546.7713      608.9737
33163      626.8374      808.4790      830.7258
33164      887.1157      924.6052      945.7850
33165      980.1213      1004.3432      1053.9105
33166      1079.8713      1104.8002      1140.8734

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33167      1154.2211          1210.7470          1220.1360
33168      1236.7795          1306.4467          1346.4090
33169      1375.1426          1395.3154          1407.5635
33170      1442.4481          1450.0629          1472.0847
33171      1491.5634          1504.2249          1521.6972
33172      1959.3708          3068.5397          3075.6933
33173      3085.4515          3138.5761          3157.0588
33174      3171.0087          3744.5979          3774.3290
33175      Zero-point correction (Hartree): 0.151693
33176
33177      TS.diHPCARP_Ic.16aldHshift.a.ttmpuu
33178      -----
33179      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14739164
33180      Electronic state : 2-A
33181      Cartesian coordinates (Angs):
33182      O      2.336258      1.066853      0.309035
33183      H      1.210964      1.374076      -0.314078
33184      C      -0.003325      1.348876      -0.611698
33185      O      2.396370      -0.302187      0.189691
33186      C      -0.721049      0.368120      0.319261
33187      C      1.461211      -0.893656      1.075839
33188      C      0.046121      -0.955881      0.506906
33189      O      -0.489974      2.074499      -1.398482
33190      C      -0.903320      1.093816      1.651853
33191      O      -1.963926      0.137440      -0.319007
33192      H      -1.549076      1.955322      1.494892
33193      H      0.051308      1.432930      2.050932
33194      H      -1.377695      0.421606      2.365476
33195      O      -2.678659      -0.842307      0.418978
33196      H      -2.611783      -1.599872      -0.178839
33197      O      0.010097      -1.738342      -0.673849
33198      H      -0.543141      -1.546390      1.212415
33199      O      0.488781      -0.955483      -1.758344
33200      H      1.451176      -1.028926      -1.665725
33201      H      1.805477      -1.920472      1.200902
33202      H      1.493370      -0.379707      2.036871
33203      Rotational constants (GHz): 1.2294100      0.8462100      0.7597700
33204      Vibrational harmonic frequencies (cm-1):
33205      i1700.9473          56.9338          93.4195
33206      123.5468          153.3974          173.8431
33207      202.5346          222.7524          253.6372
33208      275.2230          290.5223          318.8552
33209      335.4199          363.1770          399.3793
33210      411.5223          440.2424          489.4504
33211      506.9565          531.6300          588.8115
33212      657.6572          755.5640          839.9352
33213      904.0455          926.8516          953.0726
33214      979.3847          1007.8671          1046.9638
33215      1086.7350          1099.1380          1144.6485
33216      1155.3129          1176.5787          1214.9051
33217      1251.4907          1310.6074          1350.8024
33218      1382.6357          1398.1217          1405.8953
33219      1415.2595          1439.2738          1470.6150
33220      1489.8955          1502.1703          1511.9314
33221      1948.8304          3074.6777          3083.0303
33222      3093.6449          3140.2916          3157.1372
33223      3162.7029          3756.6834          3793.6960
33224      Zero-point correction (Hartree): 0.151087
33225
33226      TS.diHPCARP_Ic.16aldHshift.a.tmtpuu
33227      -----
33228      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14771108
33229      Electronic state : 2-A
33230      Cartesian coordinates (Angs):
33231      O      2.682469      -0.522226      0.022756
33232      H      1.688227      -1.038756      0.645187
33233      C      0.449642      -1.158451      0.936254
33234      O      2.383896      0.819158      0.084065
33235      C      -0.353866      -0.653910      -0.264766
33236      C      1.436535      1.137599      -0.916010
33237      C      -0.004427      0.831362      -0.517683
33238      O      0.040208      -1.571551      1.957689

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33239	C	-0.053466	-1.536765	-1.469765	
33240	O	-1.709852	-0.783709	0.143796	
33241	H	-0.470536	-2.526627	-1.294430	
33242	H	1.018128	-1.619814	-1.635140	
33243	H	-0.525925	-1.113552	-2.354479	
33244	O	-2.545915	-0.323719	-0.905357	
33245	H	-2.713681	0.589112	-0.621827	
33246	O	-0.258220	1.625155	0.628519	
33247	H	-0.639870	1.174211	-1.339459	
33248	O	-1.658092	1.848942	0.747260	
33249	H	-1.891847	1.233533	1.456956	
33250	H	1.517760	2.215616	-1.048760	
33251	H	1.695306	0.630865	-1.846055	
33252	Rotational constants (GHz):		1.2148600	0.8275000	0.7138200
33253	Vibrational harmonic frequencies (cm-1):				
33254	i1978.8232		65.7305		93.4948
33255	140.0516		166.4185		175.1519
33256	207.6152		218.6541		228.4810
33257	264.5837		304.4683		315.5038
33258	330.7195		390.7330		421.6736
33259	438.7492		469.3075		500.0725
33260	522.5725		537.4554		603.5014
33261	650.5478		719.1107		782.3334
33262	897.2960		943.7717		964.2212
33263	982.0357		1038.3412		1049.8628
33264	1077.4727		1123.9642		1148.3712
33265	1166.4861		1175.6282		1224.6909
33266	1240.3340		1315.8123		1352.8977
33267	1370.8921		1399.8323		1409.7669
33268	1423.7155		1446.4187		1467.7126
33269	1493.0000		1502.3520		1512.0884
33270	1952.4831		3069.2172		3081.7583
33271	3091.0665		3148.4082		3159.3417
33272	3174.1846		3734.9897		3786.0651
33273	Zero-point correction (Hartree):		0.151433		
33274	-----				
33275	TS.diHPCARP_Ic.16aldHshift.b.mppmmu				
33276	-----				
33277	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.14609284		
33278	Electronic state : 2-A				
33279	Cartesian coordinates (Angs):				
33280	O	2.063128	-0.930280	1.175189	
33281	H	0.812573	-0.830883	1.356763	
33282	C	-0.397277	-0.524520	1.095640	
33283	O	2.119277	-1.161132	-0.177532	
33284	C	-0.600810	-0.259362	-0.408562	
33285	C	1.969215	0.054419	-0.885263	
33286	C	0.525662	0.609535	-1.002712	
33287	O	-1.240117	-0.443204	1.922533	
33288	C	-0.714249	-1.591701	-1.143307	
33289	O	-1.757179	0.545854	-0.570223	
33290	H	-1.525274	-2.181980	-0.727141	
33291	H	0.214463	-2.149994	-1.067712	
33292	H	-0.940202	-1.385291	-2.189188	
33293	O	-2.920050	-0.208779	-0.281980	
33294	H	-2.974270	-0.125964	0.682432	
33295	O	0.464409	1.942778	-0.540569	
33296	H	0.273038	0.733337	-2.057940	
33297	O	0.613328	1.914744	0.874167	
33298	H	-0.238398	2.277313	1.153888	
33299	H	2.585405	0.823313	-0.420090	
33300	H	2.355041	-0.169926	-1.878461	
33301	Rotational constants (GHz):		1.2728200	0.8111100	0.7555200
33302	Vibrational harmonic frequencies (cm-1):				
33303	i2013.2022		45.0567		75.5634
33304	123.1321		153.4538		165.4286
33305	186.2710		227.3497		263.2453
33306	282.0196		290.6909		318.9931
33307	343.4575		353.3109		388.2555
33308	399.0158		436.4445		467.2115
33309	522.1353		536.4904		594.6628
33310	628.9761		728.0590		842.2539

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33311      860.4695          919.1937          967.4907
33312      993.0474          1032.0276         1041.1042
33313     1070.1398          1087.7411         1129.4112
33314     1156.0626          1169.2043         1193.9724
33315     1247.0184          1318.6015         1334.8691
33316     1368.0698          1395.3251         1403.8532
33317     1421.0462          1446.0466         1474.0407
33318     1492.0326          1506.2711         1572.4709
33319     1910.1844          3084.3725         3088.0701
33320     3094.7023          3149.4878         3166.5853
33321     3186.7952          3757.9138         3802.2058
33322 Zero-point correction (Hartree): 0.150840
33323
33324 TS.diHPCARP_Ic.16aldHshift.b.mppmuu
33325 -----
33326 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14784566
33327 Electronic state : 2-A
33328 Cartesian coordinates (Angs):
33329 O      2.044777      -0.150948      1.332640
33330 H      0.747488      -0.050792      1.540301
33331 C     -0.458554      0.055143      1.200127
33332 O      2.054763     -1.171186      0.412819
33333 C     -0.653065     -0.359100     -0.277655
33334 C      1.856476     -0.659438     -0.891824
33335 C      0.530720      0.082114     -1.152924
33336 O     -1.309495      0.418520      1.932010
33337 C     -0.842637     -1.873118     -0.336208
33338 O     -1.753981      0.343696     -0.817007
33339 H     -1.737911     -2.151066      0.211564
33340 H      0.014440     -2.386315      0.092244
33341 H     -0.968428     -2.167065     -1.378349
33342 O     -2.961551     -0.119549     -0.243064
33343 H     -3.026374      0.431319      0.551636
33344 O      0.693969      1.487744     -1.201311
33345 H      0.237601     -0.136906     -2.182832
33346 O      0.723221      2.029267      0.106054
33347 H      1.617604      1.816282      0.418360
33348 H      2.672621      0.017025     -1.157082
33349 H      1.911685     -1.546446     -1.522070
33350 Rotational constants (GHz): 1.3222400      0.7925100      0.7701800
33351 Vibrational harmonic frequencies (cm-1):
33352 i1800.3096          85.7243          126.6720
33353      141.3296          168.8017          180.0090
33354      191.2698          232.2924          265.1172
33355      280.0564          289.1635          322.0334
33356      348.7840          383.2630          401.0609
33357      408.7142          449.6479          461.3970
33358      529.9095          558.0695          587.0475
33359      637.3736          759.2474          827.8912
33360      848.4991          926.0590          966.2020
33361      992.3554          1035.3003         1053.0618
33362     1061.2092          1113.4808         1136.5191
33363     1167.6558          1191.4690         1202.6905
33364     1257.9372          1297.1277         1347.4232
33365     1377.0759          1398.6375         1408.9647
33366     1447.4197          1449.6986         1478.0045
33367     1492.2842          1505.9374         1553.0096
33368     1926.8445          3067.3349         3080.6402
33369     3085.3166          3135.3623         3163.6890
33370     3185.4818          3730.7948         3766.6327
33371 Zero-point correction (Hartree): 0.151464
33372
33373 TS.diHPCARP_Ic.16aldHshift.b.mppmuu
33374 -----
33375 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14759946
33376 Electronic state : 2-A
33377 Cartesian coordinates (Angs):
33378 O     -1.841881      0.720497      1.269752
33379 H     -0.571671      0.494630      1.492075
33380 C      0.622600      0.189164      1.189433
33381 O     -1.744673      1.506572      0.144269
33382 C      0.799198      0.187379     -0.356306

```

33383	C	-1.624142	0.692544	-1.012533	
33384	C	-0.513851	-0.348878	-0.943664	
33385	O	1.443028	-0.107242	1.981299	
33386	C	1.182707	1.576280	-0.846013	
33387	O	1.757137	-0.791106	-0.710691	
33388	H	2.167642	1.833736	-0.468571	
33389	H	0.462704	2.317977	-0.509710	
33390	H	1.220747	1.565290	-1.935464	
33391	O	3.047721	-0.387069	-0.294463	
33392	H	3.082308	-0.733403	0.609744	
33393	O	-0.795492	-1.478488	-0.113262	
33394	H	-0.321822	-0.693665	-1.964833	
33395	O	-2.162130	-1.821963	-0.145929	
33396	H	-2.502899	-1.286604	0.589970	
33397	H	-2.568905	0.199040	-1.232667	
33398	H	-1.396865	1.394458	-1.813837	
33399	Rotational constants (GHz):		1.3886900	0.7454400	0.7068000
33400	Vibrational harmonic frequencies (cm-1):				
33401	i1904.4792		74.7139		110.8834
33402	148.2499		164.9981		197.5490
33403	200.5192		235.8049		243.9329
33404	290.2955		303.2871		349.5650
33405	362.1176		388.1302		396.8564
33406	408.7507		416.9603		484.6863
33407	545.7338		567.3251		575.9751
33408	643.0920		769.4270		818.0470
33409	850.5369		926.4543		936.6944
33410	995.8131		1025.9453		1044.0971
33411	1057.8691		1111.4720		1142.5107
33412	1173.9895		1178.1031		1192.4866
33413	1258.0510		1292.9415		1353.1617
33414	1374.4488		1398.3477		1407.2246
33415	1444.8473		1449.8712		1484.4803
33416	1500.1238		1507.8227		1556.5829
33417	1938.2643		3058.4402		3080.6949
33418	3105.7206		3152.5953		3162.6113
33419	3185.7320		3714.3589		3768.8069
33420	Zero-point correction (Hartree): 0.151562				
33421					
33422	TS.diHPCARP_Ic.16aldHshift.b.mpppuu				
33423	-----				
33424	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14645057				
33425	Electronic state : 2-A				
33426	Cartesian coordinates (Angs):				
33427	O	1.658995	-1.515962	1.029556	
33428	H	0.429658	-1.261945	1.227731	
33429	C	-0.710111	-0.706807	1.013372	
33430	O	1.689056	-1.632849	-0.338684	
33431	C	-0.727140	-0.064243	-0.393593	
33432	C	1.788310	-0.352473	-0.939787	
33433	C	0.634555	0.603658	-0.623505	
33434	O	-1.575868	-0.642635	1.812784	
33435	C	-1.060705	-1.105903	-1.454310	
33436	O	-1.642048	1.018112	-0.405516	
33437	H	-2.082677	-1.445711	-1.315990	
33438	H	-0.384656	-1.953809	-1.394800	
33439	H	-0.980442	-0.637839	-2.435642	
33440	O	-2.968065	0.536770	-0.293003	
33441	H	-3.069261	0.462947	0.668140	
33442	O	0.871214	1.348687	0.561111	
33443	H	0.517194	1.300139	-1.459192	
33444	O	1.961843	2.218579	0.308272	
33445	H	1.528042	3.080147	0.352692	
33446	H	2.719221	0.132135	-0.644292	
33447	H	1.812460	-0.567073	-2.007871	
33448	Rotational constants (GHz):		1.2147400	0.7901200	0.6770700
33449	Vibrational harmonic frequencies (cm-1):				
33450	i2073.0138		73.9298		84.2923
33451	137.0914		159.0744		173.7870
33452	174.4931		223.1153		227.3275
33453	244.5730		294.4097		298.5866
33454	332.5772		352.7447		373.9050

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33455      393.3443      408.5505      427.4109
33456      449.9232      561.4046      565.7363
33457      642.8678      768.4049      827.9728
33458      859.2236      927.4030      956.2238
33459      1010.0060     1024.5994     1051.4197
33460      1055.9912     1096.1241     1135.9219
33461      1159.5384     1177.1690     1196.6982
33462      1254.7701     1303.2684     1356.2701
33463      1373.4925     1398.9305     1406.1832
33464      1414.9984     1445.7395     1475.5907
33465      1494.4411     1504.5013     1570.1541
33466      1929.6876     3060.4253     3081.8976
33467      3090.9406     3144.6654     3165.3279
33468      3188.6841     3760.9421     3817.5781
33469      Zero-point correction (Hartree): 0.150551
33470
33471      TS.diHPCARP_Ic.16aldHshift.b.mptpuu
33472      -----
33473      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14896985
33474      Electronic state : 2-A
33475      Cartesian coordinates (Angs):
33476      O      2.185804      -0.812128      1.116279
33477      H      0.940344      -0.997190      1.274281
33478      C     -0.306573      -0.880186      1.001910
33479      O      2.290930      -0.960986     -0.244334
33480      C     -0.504872      -0.311552     -0.423363
33481      C      1.975022      0.260420     -0.886247
33482      C      0.556606      0.782303     -0.633356
33483      O     -1.167934     -1.094954      1.781080
33484      C     -0.467796     -1.411617     -1.472182
33485      O     -1.732714      0.408277     -0.442375
33486      H     -1.313655     -2.079567     -1.338635
33487      H      0.456136     -1.979030     -1.399066
33488      H     -0.540561     -0.952855     -2.458650
33489      O     -2.833444     -0.475717     -0.339219
33490      H     -2.874178     -0.635142      0.616975
33491      O      0.582379      1.637165      0.499760
33492      H      0.254621      1.378521     -1.497431
33493      O     -0.328794      2.705434      0.294542
33494      H     -1.185404      2.294655      0.483889
33495      H      2.675882      1.038431     -0.582493
33496      H      2.102670      0.039241     -1.945300
33497      Rotational constants (GHz):      1.1842900      0.8390300      0.7017600
33498      Vibrational harmonic frequencies (cm-1):
33499      i2068.5537      67.3371      96.7734
33500      146.4118      161.9170      170.5520
33501      180.5816      223.5147      244.6295
33502      278.4485      308.8443      319.3837
33503      353.9998      368.9376      397.8569
33504      402.8962      425.9499      455.4922
33505      466.2860      545.0913      582.6006
33506      612.9484      769.9701      826.5070
33507      873.4077      926.4515      942.2659
33508      989.5658      1030.8723     1048.7110
33509      1068.7214     1093.6769     1145.9553
33510      1161.8194     1168.5583     1187.0354
33511      1251.3897     1302.3127     1354.7649
33512      1358.4509     1399.9147     1407.2430
33513      1447.9234     1453.6765     1471.6428
33514      1492.1731     1503.9612     1568.7341
33515      1925.0231     3080.0717     3081.1894
33516      3090.3849     3146.6916     3161.9885
33517      3184.5833     3746.1029     3769.8891
33518      Zero-point correction (Hartree): 0.150911
33519
33520      TS.diHPCARP_Ic.16aldHshift.b.pmmuu
33521      -----
33522      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14790371
33523      Electronic state : 2-A
33524      Cartesian coordinates (Angs):
33525      O      2.166549      -0.557680      1.238708
33526      H      0.950127      -0.864761      1.266965

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33527	C	-0.275899	-0.966513	0.900182		
33528	O	2.400212	-0.454031	-0.111650		
33529	C	-0.445861	-0.513568	-0.553855		
33530	C	1.868272	0.764561	-0.597345		
33531	C	0.347456	0.765382	-0.908773		
33532	O	-1.132708	-1.384595	1.598882		
33533	C	-0.017241	-1.679349	-1.446053		
33534	O	-1.821119	-0.355636	-0.863481		
33535	H	-0.595520	-2.564134	-1.188444		
33536	H	1.042408	-1.886206	-1.328954		
33537	H	-0.228239	-1.413244	-2.481153		
33538	O	-2.483989	0.459859	0.091850		
33539	H	-2.852218	-0.214226	0.682017		
33540	O	-0.241865	1.930643	-0.381697		
33541	H	0.192942	0.901930	-1.981535		
33542	O	-0.224222	1.819754	1.034384		
33543	H	-1.163261	1.636731	1.193060		
33544	H	2.063423	1.552716	0.127915		
33545	H	2.427100	0.961610	-1.510766		
33546	Rotational constants (GHz):			1.2394900	0.8737200	0.7775800
33547	Vibrational harmonic frequencies (cm-1):					
33548	i2042.5424		36.6406			91.4273
33549	166.9669		182.1763			204.2375
33550	207.8537		220.5854			259.9789
33551	265.8385		298.4766			326.6601
33552	351.2161		367.4503			418.5716
33553	423.7733		450.1705			480.5607
33554	514.8403		558.2004			580.1277
33555	656.8754		717.6970			834.3674
33556	877.6126		927.4285			968.6383
33557	994.3875		1017.5394			1044.9309
33558	1060.8746		1083.5657			1128.0873
33559	1147.1964		1165.4767			1201.1291
33560	1231.7106		1324.3180			1337.8160
33561	1369.8029		1400.6092			1411.9915
33562	1423.0508		1443.0369			1475.4453
33563	1495.7376		1500.7291			1571.0751
33564	1919.0533		3081.0991			3085.4333
33565	3096.1886		3154.3237			3157.6767
33566	3187.5224		3748.0889			3774.1877
33567	Zero-point correction (Hartree):			0.151317		
33568						
33569	TS.diHPCARP_Ic.16aldHshift.b.pmpuu					
33570	-----					
33571	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14624363					
33572	Electronic state : 2-A					
33573	Cartesian coordinates (Angs):					
33574	O	-2.020877	-0.038436	1.290869		
33575	H	-0.779765	0.302764	1.490150		
33576	C	0.431068	0.509391	1.171469		
33577	O	-2.296596	0.688212	0.157042		
33578	C	0.563676	0.625863	-0.360183		
33579	C	-1.874499	-0.017310	-0.996136		
33580	C	-0.370307	-0.354290	-1.095208		
33581	O	1.311053	0.606840	1.949000		
33582	C	0.246682	2.072945	-0.744035		
33583	O	1.911588	0.481152	-0.740901		
33584	H	0.986070	2.725239	-0.284691		
33585	H	-0.746519	2.362855	-0.414691		
33586	H	0.321335	2.171360	-1.826616		
33587	O	2.430521	-0.762157	-0.303891		
33588	H	2.795284	-0.526433	0.561861		
33589	O	-0.118319	-1.719141	-0.821731		
33590	H	-0.094508	-0.287710	-2.150894		
33591	O	-0.074811	-1.944371	0.574526		
33592	H	-1.011492	-1.954497	0.828943		
33593	H	-2.430060	-0.953962	-1.085233		
33594	H	-2.160536	0.644010	-1.813576		
33595	Rotational constants (GHz):			1.2655500	0.8673000	0.8117200
33596	Vibrational harmonic frequencies (cm-1):					
33597	i1865.2318		94.8367			116.8807
33598	160.6609		166.6167			201.3144

33599	204.8123	215.2827	240.6493			
33600	271.8464	297.9543	320.9074			
33601	351.8192	365.8741	390.5865			
33602	427.7716	446.1749	454.1513			
33603	498.8141	551.0255	591.6330			
33604	664.6190	760.4594	813.3883			
33605	853.8692	942.9297	963.8819			
33606	997.5100	1039.5664	1051.6720			
33607	1058.0680	1100.6776	1133.3785			
33608	1175.9258	1192.8838	1197.3679			
33609	1240.9424	1293.8852	1341.5437			
33610	1375.0808	1399.5720	1410.6863			
33611	1435.8330	1448.4089	1479.9213			
33612	1496.3718	1505.1714	1553.6768			
33613	1934.5243	3068.5180	3081.9192			
33614	3084.8303	3133.3500	3158.4050			
33615	3189.0141	3737.3265	3774.9121			
33616	Zero-point correction (Hartree): 0.151406					
33617						
33618	TS.diHPCARP_Ic.16aldHshift.b.pmpuu					
33619	-----					
33620	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14985104					
33621	Electronic state : 2-A					
33622	Cartesian coordinates (Angs):					
33623	O	-2.153132	-0.170827	-1.303909		
33624	H	-1.066457	-0.805520	-1.298702		
33625	C	0.095675	-1.164430	-0.862207		
33626	O	-2.479234	-0.202090	0.029714		
33627	C	0.326132	-0.583817	0.547171		
33628	C	-1.816513	0.848233	0.712370		
33629	C	-0.285583	0.829813	0.603780		
33630	O	0.879632	-1.788098	-1.486013		
33631	C	-0.259821	-1.529402	1.592412		
33632	O	1.712926	-0.605389	0.851937		
33633	H	0.277861	-2.474371	1.558464		
33634	H	-1.315693	-1.705203	1.411015		
33635	H	-0.124369	-1.086732	2.579059		
33636	O	2.477398	0.052062	-0.143516		
33637	H	2.624798	-0.656932	-0.787830		
33638	O	0.086165	1.590612	-0.535577		
33639	H	0.120233	1.328422	1.486336		
33640	O	1.161633	2.448860	-0.196051		
33641	H	1.925292	1.866167	-0.334618		
33642	H	-2.161789	1.813780	0.342499		
33643	H	-2.122308	0.716963	1.749944		
33644	Rotational constants (GHz):			1.1697800	0.8881100	0.7239900
33645	Vibrational harmonic frequencies (cm-1):					
33646	i2092.7960		66.5901			101.4329
33647	137.5864		178.6831			197.9782
33648	220.1645		235.7665			252.0465
33649	264.7065		304.3437			333.7457
33650	354.6889		375.0974			387.5635
33651	441.5735		456.9633			460.7342
33652	488.0293		569.6814			588.8517
33653	630.0633		765.2651			826.9451
33654	878.9554		929.9574			956.3084
33655	987.7690		1029.9266			1048.1817
33656	1069.5959		1081.8229			1135.3433
33657	1156.4152		1172.8515			1194.7178
33658	1234.5234		1294.3303			1344.6737
33659	1357.9370		1397.3905			1407.2778
33660	1422.6276		1457.1079			1475.0939
33661	1495.9270		1502.6467			1566.6142
33662	1930.2049		3080.1401			3083.8731
33663	3091.7498		3145.2168			3156.6913
33664	3186.7532		3726.9928			3761.6523
33665	Zero-point correction (Hartree): 0.151270					
33666						
33667	TS.diHPCARP_Ic.16aldHshift.b.ppmuu					
33668	-----					
33669	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14538694					
33670	Electronic state : 2-A					


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33671 Cartesian coordinates (Angs):
33672 O 2.207411 -0.418451 1.188140
33673 H 0.983526 -0.793665 1.270598
33674 C -0.229563 -0.972053 0.951159
33675 O 2.394995 -0.396894 -0.172451
33676 C -0.463344 -0.562633 -0.514750
33677 C 1.813377 0.769569 -0.718935
33678 C 0.276162 0.731531 -0.919669
33679 O -1.033884 -1.418134 1.685899
33680 C -0.023812 -1.739169 -1.385688
33681 O -1.848587 -0.457154 -0.789237
33682 H -0.616450 -2.612995 -1.123647
33683 H 1.030794 -1.953461 -1.239734
33684 H -0.207255 -1.491233 -2.430574
33685 O -2.491071 0.429753 0.118959
33686 H -2.555840 1.233543 -0.415420
33687 O -0.316863 1.887008 -0.352361
33688 H 0.048626 0.867349 -1.980008
33689 O -0.187870 1.800398 1.058984
33690 H -1.064679 1.465246 1.309155
33691 H 2.047413 1.622032 -0.082576
33692 H 2.303893 0.887507 -1.683957
33693 Rotational constants (GHz): 1.2327500 0.8764100 0.7825200
33694 Vibrational harmonic frequencies (cm-1):
33695 i1926.7084 42.4011 90.5799
33696 155.6656 169.6329 199.0755
33697 205.9605 216.8488 251.4486
33698 264.6911 289.8476 321.5769
33699 348.9112 369.9527 419.6749
33700 430.2474 448.8333 481.7280
33701 550.4143 576.6198 592.5376
33702 660.8301 716.2522 824.9324
33703 867.6768 929.6736 968.4659
33704 992.6743 1021.3144 1045.4543
33705 1064.7919 1079.8394 1124.0865
33706 1153.9285 1169.7913 1199.2458
33707 1231.6712 1322.0433 1336.7573
33708 1371.0957 1400.8308 1416.4270
33709 1424.1893 1439.6337 1472.6381
33710 1494.9088 1500.2784 1569.1254
33711 1942.7522 3078.1495 3081.6650
33712 3093.9803 3151.8363 3158.3359
33713 3187.0359 3725.5602 3794.2685
33714 Zero-point correction (Hartree): 0.151359
33715
33716 TS.diHPCARP_Ic.16aldHshift.b.pmpuu
33717 -----
33718 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14658155
33719 Electronic state : 2-A
33720 Cartesian coordinates (Angs):
33721 O 2.018841 -0.162891 1.269878
33722 H 0.733294 -0.520900 1.429398
33723 C -0.437991 -0.752009 1.078996
33724 O 2.266422 -0.743175 0.050147
33725 C -0.601278 -0.547309 -0.447483
33726 C 1.865253 0.127380 -0.989452
33727 C 0.370252 0.493334 -1.032405
33728 O -1.265605 -1.136447 1.816592
33729 C -0.382724 -1.909013 -1.106147
33730 O -1.931361 -0.213058 -0.769270
33731 H -1.136883 -2.598696 -0.734504
33732 H 0.607128 -2.298228 -0.881310
33733 H -0.502002 -1.805087 -2.184379
33734 O -2.409408 0.837244 0.054154
33735 H -1.990589 1.622191 -0.329707
33736 O 0.122672 1.816136 -0.572819
33737 H 0.094734 0.585230 -2.086496
33738 O 0.153859 1.872314 0.844847
33739 H 1.092574 1.738325 1.059533
33740 H 2.441575 1.055312 -0.945993
33741 H 2.135753 -0.413424 -1.895828
33742 Rotational constants (GHz): 1.2346300 0.8808600 0.8047900

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33743 Vibrational harmonic frequencies (cm-1):
33744 i1602.9261 77.4471 136.7675
33745 161.2931 177.3290 201.2592
33746 216.3153 223.8948 239.8440
33747 262.9858 294.9721 323.7111
33748 349.1683 374.1908 403.2251
33749 429.5648 445.4065 468.8907
33750 507.5776 541.4990 589.7356
33751 659.1129 760.0538 810.6859
33752 849.5594 936.9943 964.6595
33753 994.5639 1048.7378 1051.7462
33754 1058.3574 1096.1659 1136.4607
33755 1181.3301 1195.1746 1199.5662
33756 1240.6569 1296.5492 1349.2982
33757 1381.2964 1400.8864 1412.3730
33758 1446.4025 1463.5930 1482.1483
33759 1495.3929 1503.1420 1559.9426
33760 1959.6568 3063.7164 3078.1511
33761 3080.7605 3133.8298 3158.8510
33762 3178.5350 3709.9454 3764.0255
33763 Zero-point correction (Hartree): 0.151561
33764
33765 TS.diHPCARP_Ic.16aldHshift.c.mpmuu
33766 -----
33767 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14620475
33768 Electronic state : 2-A
33769 Cartesian coordinates (Angs):
33770 O 2.170010 -1.309277 0.874072
33771 H 0.923197 -1.220485 1.073439
33772 C -0.289089 -0.811581 0.958057
33773 O 2.311260 -0.826830 -0.407930
33774 C -0.529807 -0.245940 -0.447041
33775 C 1.978036 0.550109 -0.438163
33776 C 0.513693 0.834200 -0.833204
33777 O -1.092260 -0.897705 1.821438
33778 C -0.497339 -1.412413 -1.430899
33779 O -1.767205 0.445769 -0.464360
33780 H -1.210287 -2.178127 -1.138617
33781 H 0.501039 -1.840292 -1.472236
33782 H -0.776505 -1.034559 -2.413658
33783 O -2.833863 -0.476293 -0.332529
33784 H -2.896271 -0.570818 0.630334
33785 O 0.166232 2.110253 -0.337148
33786 H 0.422922 0.965157 -1.913205
33787 O 0.056246 2.006752 1.075588
33788 H -0.906122 1.975885 1.180931
33789 H 2.171709 0.983122 0.541490
33790 H 2.633994 1.012516 -1.174021
33791 Rotational constants (GHz): 1.2158700 0.8420700 0.7249000
33792 Vibrational harmonic frequencies (cm-1):
33793 i2063.5494 44.8572 101.5307
33794 141.3353 153.7801 164.4672
33795 203.5829 222.3401 269.8434
33796 282.1583 298.7535 324.4656
33797 350.7533 374.0286 382.3595
33798 422.1632 438.5863 480.2367
33799 504.3367 515.4376 598.4878
33800 614.4008 718.4399 851.6370
33801 882.7825 914.0865 967.8436
33802 994.1844 1025.0092 1041.8568
33803 1070.1779 1099.7231 1117.2748
33804 1139.7673 1168.4566 1204.3635
33805 1236.2396 1305.7411 1348.0040
33806 1363.9972 1402.6222 1408.1319
33807 1414.3051 1442.3070 1483.2519
33808 1490.1721 1502.4672 1575.0351
33809 1918.1823 3084.8512 3094.2025
33810 3098.7224 3158.7593 3166.7360
33811 3183.4110 3760.2482 3775.0932
33812 Zero-point correction (Hartree): 0.151033
33813
33814 TS.diHPCARP_Ic.16aldHshift.e.tmtpuu

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33815 -----
33816 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14630172
33817 Electronic state : 2-A
33818 Cartesian coordinates (Angs):
33819   O      2.511672      -0.054599      -0.753339
33820   H      1.503136      0.684253      -1.055632
33821   C      0.356516      1.206903      -0.917278
33822   O      2.402541      -0.051613      0.615429
33823   C     -0.388124      0.592527      0.290450
33824   C      1.481194     -1.047959      1.014071
33825   C      0.057891     -0.863278      0.483121
33826   O     -0.065106      2.040394     -1.631811
33827   C     -0.173742      1.464181      1.519837
33828   O     -1.749045      0.641866     -0.139598
33829   H     -0.593210      2.449709      1.327596
33830   H      0.884456      1.560104      1.752001
33831   H     -0.696557      1.019785      2.365599
33832   O     -2.567397      0.056056      0.858279
33833   H     -2.664265     -0.846176      0.515268
33834   O     -0.050138     -1.580567     -0.740952
33835   H     -0.610902     -1.333176      1.206499
33836   O     -1.411414     -1.963391     -0.916285
33837   H     -1.703419     -1.339934     -1.595765
33838   H      1.835297     -2.033091      0.708015
33839   H      1.474133     -0.980889      2.101423
33840 Rotational constants (GHz):      1.1738600      0.8479600      0.7285000
33841 Vibrational harmonic frequencies (cm-1):
33842   i1951.4072      44.0407      105.6047
33843      151.8331      167.8254      174.7180
33844      198.5489      208.3950      226.7497
33845      264.3445      269.6837      300.2303
33846      342.9958      366.7158      407.7726
33847      421.3829      457.7599      484.0045
33848      498.3966      513.3254      586.4209
33849      649.4680      734.9657      797.7995
33850      889.5540      932.8584      966.8157
33851      985.9879     1029.0934     1047.2770
33852     1062.1200     1087.2631     1145.4701
33853     1163.6240     1168.4252     1185.3416
33854     1254.1591     1306.4572     1365.9511
33855     1376.1189     1399.8625     1412.0061
33856     1419.2093     1439.5998     1471.7785
33857     1494.2652     1497.9368     1566.8392
33858     1949.5530     3079.2397     3084.0642
33859     3094.7377     3144.2024     3158.7754
33860     3170.8482     3744.7221     3794.3356
33861 Zero-point correction (Hartree): 0.150955
33862
33863
33864
33865 1,6-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
33866 HPCARP-Ia), forming B (di-HPCARP-Ib)
33867 =====
33868 =====
33869
33870 TS.diHPCARP_I.16OOHHshift.a.htppuu
33871 -----
33872 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14371098
33873 Electronic state : 2-A
33874 Cartesian coordinates (Angs):
33875   O     -2.432955      1.047232      0.217663
33876   H     -1.629722      1.908130      0.009524
33877   O     -0.578433      2.345941     -0.192418
33878   O     -1.801193      0.225381      1.099813
33879   O      0.045481      1.338383     -0.856258
33880   C     -0.806226     -0.575522      0.424432
33881   C      0.403631      0.283790      0.055018
33882   C     -0.439279     -1.640507      1.450280
33883   H     -1.350813     -2.089265      1.842290
33884   H      0.113351     -1.189420      2.273467
33885   H      0.165716     -2.418476      0.992694
33886   C     -1.467602     -1.250595     -0.772952

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33887	O	-0.829635	-1.794600	-1.627359	
33888	H	-2.570194	-1.253112	-0.762929	
33889	H	0.773664	0.751359	0.970124	
33890	C	1.544591	-0.451781	-0.636572	
33891	O	2.755446	0.249553	-0.466341	
33892	H	1.648549	-1.474449	-0.278376	
33893	H	1.374960	-0.468812	-1.711691	
33894	O	3.103329	0.130022	0.911860	
33895	H	3.967479	-0.293556	0.847982	
33896	Rotational constants (GHz):		1.2269000	0.7401500	0.6288100
33897	Vibrational harmonic frequencies (cm-1):				
33898	i2948.3878		44.6813		67.3204
33899	92.6769		138.1581		144.7021
33900	172.6875		174.4118		212.5837
33901	254.2552		285.3297		293.0400
33902	321.8742		340.8845		373.2317
33903	423.2048		447.9576		525.9370
33904	567.0498		591.3511		652.3408
33905	695.9526		866.9319		883.1681
33906	918.7516		953.8647		977.3271
33907	1000.1394		1053.8434		1082.3542
33908	1100.4364		1127.1796		1148.8912
33909	1158.6647		1160.2417		1207.1061
33910	1278.6304		1294.2281		1331.7423
33911	1373.2792		1392.5093		1405.0555
33912	1420.9035		1427.4698		1460.4338
33913	1490.8918		1496.9667		1502.1240
33914	1867.4618		3006.6676		3077.5256
33915	3092.6191		3106.6617		3152.9413
33916	3162.0021		3177.4431		3836.6863
33917	Zero-point correction (Hartree): 0.149933				
33918					
33919	TS.diHPCARP_I.1600HHshift.a.tmmuu				
33920	-----				
33921	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14336503				
33922	Electronic state : 2-A				
33923	Cartesian coordinates (Angs):				
33924	O	2.583414	0.324420	-0.528689	
33925	H	2.177761	1.388072	-0.212629	
33926	O	1.394050	2.174030	0.158488	
33927	O	1.571322	-0.211487	-1.265483	
33928	O	0.553700	1.423700	0.918599	
33929	C	0.483419	-0.631796	-0.406054	
33930	C	-0.277256	0.603256	0.077178	
33931	C	-0.370634	-1.521854	-1.297653	
33932	H	0.266732	-2.272663	-1.763309	
33933	H	-0.846822	-0.925370	-2.074681	
33934	H	-1.142592	-2.008732	-0.709146	
33935	C	1.085900	-1.491566	0.704141	
33936	O	0.491321	-1.792219	1.698042	
33937	H	2.097732	-1.872857	0.485614	
33938	H	-0.543536	1.195066	-0.800894	
33939	C	-1.527033	0.359936	0.922895	
33940	O	-2.573701	-0.238852	0.193994	
33941	H	-1.326157	-0.332095	1.737572	
33942	H	-1.841278	1.325904	1.324316	
33943	O	-2.941486	0.657220	-0.850396	
33944	H	-3.837174	0.900328	-0.586322	
33945	Rotational constants (GHz):		1.2351000	0.7612000	0.6612100
33946	Vibrational harmonic frequencies (cm-1):				
33947	i2990.5218		18.7813		53.8681
33948	89.9893		142.0113		188.2130
33949	193.8475		212.5898		233.3050
33950	246.6214		273.7255		295.5919
33951	315.6741		330.4758		389.3006
33952	414.7979		440.0135		507.9847
33953	550.8110		601.1669		663.0414
33954	694.8292		781.3538		911.6598
33955	939.7473		957.2243		967.6722
33956	1031.7086		1050.8008		1069.0678
33957	1112.4997		1124.5668		1134.2631
33958	1153.7534		1176.9805		1211.0394

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33959      1276.6741      1294.9770      1342.2425
33960      1382.3910      1390.3787      1408.3682
33961      1421.4492      1431.0665      1482.6803
33962      1484.3994      1495.5937      1498.8698
33963      1869.1504      3000.4282      3070.8188
33964      3076.4527      3096.0384      3151.2919
33965      3163.4333      3182.8511      3827.7159
33966 Zero-point correction (Hartree): 0.149963
33967
33968 TS.diHPCARP_I.1600HHshift.a.tppmdd
33969 -----
33970 IRC pathway available
33971 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17327212
33972 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05050651
33973 T1 diagnostic: 0.024541
33974 E(MP2/Aug-CC-pVTZ) (Hartree): -721.00600657
33975 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02399835
33976 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01625105
33977 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02984282
33978 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48013165
33979 E(UHF/Aug-CC-pVTZ) (Hartree): -718.46577254
33980 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14783201
33981 Electronic state : 2-A
33982 Cartesian coordinates (Angs):
33983 O      -2.422596      0.410872      -0.857009
33984 H      -2.397229      -0.688440      -0.423892
33985 O      -1.981528      -1.645456      0.115699
33986 O      -1.124566      0.663445      -1.171904
33987 O      -1.220388      -1.163194      1.139681
33988 C      -0.327656      0.821599      0.025771
33989 C      -0.022422      -0.553274      0.633112
33990 C      -0.987721      1.761842      1.025351
33991 H      -1.858578      1.295821      1.475489
33992 H      -1.293033      2.678934      0.524347
33993 H      -0.260863      2.003060      1.798372
33994 C      0.959534      1.464487      -0.473406
33995 O      1.848472      1.765774      0.278395
33996 H      1.000657      1.678541      -1.552979
33997 H      0.583304      -0.393522      1.525756
33998 C      0.695485      -1.508674      -0.318156
33999 O      1.892664      -0.942936      -0.799242
34000 H      0.890671      -2.453128      0.190387
34001 H      0.100680      -1.689592      -1.210096
34002 O      2.813720      -0.890292      0.279563
34003 H      2.884858      0.066741      0.435124
34004 Rotational constants (GHz):      1.3305100      0.8539800      0.6564900
34005 Vibrational harmonic frequencies (cm-1):
34006 i3182.9360      70.0933      125.4924
34007      166.6899      175.1531      196.2146
34008      206.8238      228.8561      255.9104
34009      264.4258      304.7313      329.9826
34010      344.1828      352.2807      424.1822
34011      456.3935      462.2194      479.5083
34012      588.1768      614.4331      687.8228
34013      698.5546      773.2584      910.5861
34014      943.9700      961.2631      987.1766
34015      1007.2659      1025.7849      1033.2146
34016      1112.4058      1119.8151      1135.3733
34017      1140.3803      1177.2910      1224.0190
34018      1254.6939      1289.2147      1331.9714
34019      1374.7374      1397.9741      1406.9189
34020      1413.7887      1464.2632      1483.4769
34021      1486.9596      1491.0192      1502.3148
34022      1838.6387      3020.8094      3085.3386
34023      3094.3297      3118.3314      3162.9244
34024      3168.4832      3185.5409      3707.0834
34025 Zero-point correction (Hartree): 0.150958
34026
34027 TS.diHPCARP_I.1600HHshift.a.ttptuu
34028 -----
34029 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14394006
34030 Electronic state : 2-A

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34031 Cartesian coordinates (Angs):
34032 O -2.354949 1.195944 0.165772
34033 H -1.491379 1.986044 -0.058061
34034 O -0.406571 2.344327 -0.262886
34035 O -1.796851 0.352670 1.077027
34036 O 0.151413 1.272303 -0.883511
34037 C -0.853295 -0.536061 0.437075
34038 C 0.419115 0.228006 0.069488
34039 C -0.579908 -1.601019 1.491436
34040 H -1.527366 -1.966453 1.884751
34041 H 0.000770 -1.177460 2.310016
34042 H -0.035574 -2.434893 1.056419
34043 C -1.544686 -1.190458 -0.755713
34044 O -0.937721 -1.818756 -1.573661
34045 H -2.642788 -1.094040 -0.775382
34046 H 0.793186 0.701416 0.979892
34047 C 1.526701 -0.602741 -0.560428
34048 O 2.760930 0.071761 -0.494327
34049 H 1.614780 -1.580373 -0.088299
34050 H 1.337922 -0.739906 -1.623028
34051 O 3.164414 0.030654 0.875300
34052 H 3.497578 0.928080 0.992835
34053 Rotational constants (GHz): 1.2273200 0.7399000 0.6248200
34054 Vibrational harmonic frequencies (cm-1):
34055 i2969.3977 41.5290 63.5948
34056 93.4479 141.9468 171.7706
34057 177.3316 202.5911 212.7601
34058 252.7809 283.9957 292.9628
34059 320.5910 340.9483 368.8678
34060 421.5182 443.7464 517.1795
34061 570.4934 589.9199 651.7133
34062 695.2362 859.1204 885.8809
34063 918.6142 954.9712 977.0398
34064 1002.7577 1053.5195 1083.8338
34065 1104.9478 1127.1228 1144.4299
34066 1157.6102 1161.2753 1208.7217
34067 1276.9339 1292.4741 1327.8341
34068 1373.2264 1400.9590 1416.6342
34069 1423.4317 1428.4673 1462.5111
34070 1491.9420 1495.0757 1502.7489
34071 1868.2857 3008.0985 3076.5806
34072 3091.5043 3106.3304 3151.8579
34073 3165.5583 3176.6163 3841.8296
34074 Zero-point correction (Hartree): 0.150071
34075
34076 TS.diHPCARP_I.16OOHHshift.b.htppuu
34077 -----
34078 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14343885
34079 Electronic state : 2-A
34080 Cartesian coordinates (Angs):
34081 O 1.897438 -1.618367 0.696361
34082 H 1.034567 -2.222080 0.102707
34083 O 0.115933 -2.410662 -0.587984
34084 O 2.047365 -0.487497 -0.031227
34085 O -0.114029 -1.175876 -1.095735
34086 C 0.992873 0.463354 0.242259
34087 C -0.351439 -0.238240 -0.029067
34088 C 1.085305 1.016957 1.647190
34089 H 2.047173 1.503234 1.798963
34090 H 0.974139 0.206251 2.364511
34091 H 0.297715 1.752792 1.802184
34092 C 1.256608 1.542258 -0.803871
34093 O 0.762822 2.631456 -0.734656
34094 H 1.920963 1.246924 -1.633510
34095 H -0.658965 -0.803413 0.850208
34096 C -1.478729 0.684710 -0.452928
34097 O -2.725773 0.037684 -0.359943
34098 H -1.470819 1.601615 0.138875
34099 H -1.379081 0.946160 -1.507294
34100 O -2.983714 -0.152415 1.028478
34101 H -3.793738 0.359708 1.139499
34102 Rotational constants (GHz): 1.0973200 0.8151300 0.6050800

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34103 Vibrational harmonic frequencies (cm-1):
34104 i2789.0607 50.6590 58.6317
34105 79.7628 129.5020 169.5294
34106 184.1788 197.1812 201.3861
34107 246.9371 260.3138 294.0530
34108 316.0040 340.5210 374.2047
34109 440.9882 476.9755 529.4998
34110 546.7733 576.1866 678.3756
34111 682.4732 839.3579 847.2535
34112 871.5144 907.5529 970.0426
34113 988.0661 1008.1796 1098.3620
34114 1103.6317 1142.7477 1157.1406
34115 1162.3009 1173.3886 1210.2759
34116 1257.7319 1315.1183 1343.6489
34117 1378.3202 1396.0427 1400.1959
34118 1416.0833 1436.0114 1459.5230
34119 1483.1417 1498.7744 1706.5770
34120 1866.9519 2999.1286 3078.8874
34121 3081.6864 3120.6411 3138.3675
34122 3159.8681 3166.0987 3831.1105
34123 Zero-point correction (Hartree): 0.150012
34124
34125 TS.diHPCARP_I.1600HHshift.b.ttptuu
34126 -----
34127 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14373600
34128 Electronic state : 2-A
34129 Cartesian coordinates (Angs):
34130 O 1.762247 -1.775295 0.625320
34131 H 0.836534 -2.284437 0.048558
34132 O -0.125016 -2.371452 -0.613199
34133 O 1.993542 -0.648675 -0.086227
34134 O -0.246211 -1.110837 -1.096181
34135 C 1.042210 0.391694 0.240450
34136 C -0.367201 -0.176829 -0.006465
34137 C 1.227481 0.898114 1.654214
34138 H 2.238012 1.279595 1.788646
34139 H 1.053648 0.086142 2.357555
34140 H 0.524142 1.706803 1.846701
34141 C 1.380626 1.469592 -0.785084
34142 O 0.970699 2.590424 -0.686652
34143 H 2.017128 1.144347 -1.625343
34144 H -0.694060 -0.732455 0.871565
34145 C -1.422882 0.847593 -0.372030
34146 O -2.713905 0.289032 -0.352870
34147 H -1.366853 1.710929 0.293746
34148 H -1.290481 1.191323 -1.398017
34149 O -3.031307 0.048585 1.016998
34150 H -3.359854 -0.857487 0.972566
34151 Rotational constants (GHz): 1.1046900 0.8153900 0.6018900
34152 Vibrational harmonic frequencies (cm-1):
34153 i2748.6162 47.4184 57.1158
34154 74.2824 132.5046 168.2920
34155 197.0198 204.4203 212.5815
34156 244.7634 259.7214 296.6887
34157 316.4286 342.5495 372.4192
34158 434.7397 474.0443 526.9572
34159 548.0862 578.2211 677.4638
34160 680.6734 841.6830 854.2340
34161 871.9057 905.5825 970.1208
34162 990.2466 1006.4142 1101.4605
34163 1104.5777 1141.1661 1158.8837
34164 1165.3450 1174.5035 1209.1039
34165 1259.1756 1309.9682 1341.0990
34166 1378.0335 1397.3678 1411.7739
34167 1415.8798 1435.4619 1461.7539
34168 1483.0489 1499.4725 1707.8705
34169 1868.3997 3000.1667 3078.9480
34170 3083.0607 3121.2668 3142.6670
34171 3160.4562 3165.6619 3835.7003
34172 Zero-point correction (Hartree): 0.150129
34173
34174

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34175
34176 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-di-
34177 HPCARP-Ia), forming C (di-HPCARP-Ic)
34178 =====
34179 =====
34180
34181 TS.diHPCARP_I.1700HHshift.BB.ctddd
34182 -----
34183 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15011872
34184 Electronic state : 2-A
34185 Cartesian coordinates (Angs):
34186 O -1.522586 -2.061228 -0.679756
34187 H -0.358021 -2.044665 -0.897616
34188 O 0.792726 -1.748128 -0.891227
34189 O -1.596849 -1.546972 0.572031
34190 O 0.965058 -1.275898 0.367149
34191 C -1.739423 -0.138351 0.507738
34192 C 0.816301 0.134784 0.414707
34193 C -0.550927 0.542829 -0.174660
34194 C 1.935596 0.812952 -0.383743
34195 C 0.981648 0.508068 1.880219
34196 O 2.889589 0.238218 -0.808867
34197 H 1.805078 1.903877 -0.503333
34198 H 1.972912 0.209136 2.216291
34199 H 0.239843 -0.010390 2.484354
34200 H 0.863463 1.582065 2.010814
34201 H -0.556876 0.322192 -1.243125
34202 O -0.649736 1.943978 0.015991
34203 O -1.737103 2.408778 -0.772423
34204 H -1.281727 2.901778 -1.466890
34205 H -2.651558 0.115396 -0.031944
34206 H -1.821066 0.188942 1.542698
34207 Rotational constants (GHz): 1.0342200 0.9429200 0.6431800
34208 Vibrational harmonic frequencies (cm-1):
34209 i2230.1425 48.3805 80.3521
34210 95.1178 121.9290 176.5022
34211 193.9199 224.3756 237.1278
34212 257.2089 279.0974 296.6393
34213 313.4081 348.3400 407.0290
34214 439.4680 449.4775 463.9848
34215 561.0522 607.6104 638.3815
34216 712.5548 820.5664 892.5294
34217 906.8423 926.8071 984.4632
34218 1000.8104 1022.7854 1043.2052
34219 1105.0428 1132.0056 1169.8038
34220 1177.5967 1182.1138 1231.0657
34221 1256.8788 1293.1576 1344.6411
34222 1376.5537 1402.0999 1406.1477
34223 1415.5709 1421.7326 1486.3990
34224 1487.7716 1511.2473 1690.6651
34225 1883.1490 2975.7085 3080.8125
34226 3095.2292 3096.8584 3155.8708
34227 3161.9487 3167.3270 3813.4678
34228 Zero-point correction (Hartree): 0.150520
34229
34230 TS.diHPCARP_I.1700HHshift.BB.hmddd
34231 -----
34232 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15190153
34233 Electronic state : 2-A
34234 Cartesian coordinates (Angs):
34235 O 2.546121 -0.497106 -0.712740
34236 H 2.232090 0.609350 -0.504259
34237 O 1.622541 1.574388 -0.115210
34238 O 1.990049 -1.147215 0.336785
34239 O 0.900019 1.075296 0.920284
34240 C 0.700112 -1.633627 0.003336
34241 C -0.390869 0.654957 0.462626
34242 C -0.238710 -0.537605 -0.504156
34243 C -0.995485 1.862516 -0.262719
34244 C -1.187796 0.375598 1.722798
34245 O -1.538175 1.813166 -1.323569
34246 H -0.887297 2.805980 0.305057

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34247      H      -1.198746      1.269931      2.345047
34248      H      -0.733837      -0.435923      2.288809
34249      H      -2.206012      0.097608      1.464605
34250      H      0.141549      -0.146735      -1.448351
34251      O      -1.483069      -1.081772      -0.883451
34252      O      -1.979527      -1.908076      0.177148
34253      H      -2.258870      -2.681516      -0.326858
34254      H      0.786296      -2.396752      -0.772937
34255      H      0.337654      -2.082431      0.923593
34256      Rotational constants (GHz):      1.1291900      0.9407800      0.6847500
34257      Vibrational harmonic frequencies (cm-1):
34258      i2180.7045      63.5745      85.7246
34259      137.8972      146.8713      177.1944
34260      194.5044      220.2131      244.0688
34261      251.6561      288.5004      304.0060
34262      306.9132      337.1837      383.3833
34263      409.2568      493.7654      537.1014
34264      590.8676      640.8912      647.4357
34265      666.0779      757.8426      882.9277
34266      919.5604      943.0681      956.6180
34267      979.6816      1018.0621      1044.4809
34268      1122.2644      1131.7118      1162.8313
34269      1167.0183      1181.1754      1224.6194
34270      1260.6663      1292.1870      1332.0814
34271      1386.2455      1395.6437      1407.2721
34272      1415.1030      1428.4418      1485.5205
34273      1490.1019      1504.1106      1698.4952
34274      1882.8013      2967.8467      3078.3858
34275      3079.8298      3120.8211      3151.7238
34276      3173.0465      3177.9016      3839.5106
34277      Zero-point correction (Hartree): 0.150784
34278
34279      TS.diHPCARP_I.1700HHshift.BB.hpddd
34280      -----
34281      IRC pathway available
34282      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18492426
34283      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.06141295
34284      T1 diagnostic: 0.025549
34285      E(MP2/Aug-CC-pVTZ) (Hartree): -721.01834784
34286      E(MP3/Aug-CC-pVTZ) (Hartree): -721.03307861
34287      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.02770547
34288      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03843054
34289      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48463575
34290      E(UHF/Aug-CC-pVTZ) (Hartree): -718.47134504
34291      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15973097
34292      Electronic state : 2-A
34293      Cartesian coordinates (Angs):
34294      O      -2.515917      0.491135      -0.930008
34295      H      -1.994117      -0.525371      -1.136285
34296      O      -1.244694      -1.480541      -1.052760
34297      O      -2.270318      0.694719      0.386471
34298      O      -0.912658      -1.453531      0.263053
34299      C      -1.072471      1.437242      0.548216
34300      C      0.300530      -0.725758      0.445713
34301      C      0.149328      0.733122      -0.044479
34302      C      1.378496      -1.462687      -0.341179
34303      C      0.614389      -0.835643      1.929135
34304      O      2.356209      -0.943618      -0.802576
34305      H      1.203366      -2.549114      -0.428004
34306      H      0.812210      -1.872556      2.198004
34307      H      -0.241258      -0.492166      2.508649
34308      H      1.484236      -0.226673      2.162358
34309      H      0.087709      0.745224      -1.130745
34310      O      1.267367      1.491757      0.363578
34311      O      2.070270      1.832449      -0.752701
34312      H      2.562468      1.004646      -0.888251
34313      H      -1.173339      2.409511      0.065880
34314      H      -0.964976      1.569879      1.623503
34315      Rotational constants (GHz):      1.2428900      0.8488400      0.6821100
34316      Vibrational harmonic frequencies (cm-1):
34317      i2130.4540      62.1016      89.3596
34318      116.8203      158.3966      201.8631

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34319	226.9752	231.3857	254.4777			
34320	277.8480	296.7656	331.6461			
34321	337.7665	389.8987	443.2117			
34322	452.9337	533.3062	549.8750			
34323	568.4972	614.5383	647.6614			
34324	690.9091	757.6452	881.9928			
34325	923.5366	956.8721	978.2257			
34326	990.4969	1034.3150	1041.9494			
34327	1118.0955	1147.2212	1168.6274			
34328	1178.0228	1184.5371	1224.9174			
34329	1254.8405	1288.9389	1336.8172			
34330	1373.8419	1395.0374	1402.7472			
34331	1413.1799	1477.8308	1482.4657			
34332	1490.2938	1507.8564	1697.7300			
34333	1858.6807	2996.2005	3077.6929			
34334	3092.6091	3131.5464	3149.6386			
34335	3157.8008	3175.8285	3704.2494			
34336	Zero-point correction (Hartree): 0.151563					
34337						
34338	TS.diHPCARP_I.1700HHshift.BB.hpudd					
34339	-----					
34340	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15265231					
34341	Electronic state : 2-A					
34342	Cartesian coordinates (Angs):					
34343	O	2.548816	-0.162019	-0.926241		
34344	H	2.047985	0.873846	-0.748882		
34345	O	1.316356	1.734292	-0.320438		
34346	O	2.286824	-0.795450	0.241052		
34347	O	0.829278	1.176746	0.817479		
34348	C	1.101539	-1.563981	0.133159		
34349	C	-0.402255	0.489566	0.540648		
34350	C	-0.129749	-0.769425	-0.309892		
34351	C	-1.246420	1.523837	-0.217322		
34352	C	-1.002737	0.189252	1.899797		
34353	O	-1.797788	1.336358	-1.260962		
34354	H	-1.285774	2.501317	0.295523		
34355	H	-1.165403	1.119831	2.441778		
34356	H	-0.314980	-0.426951	2.477293		
34357	H	-1.944690	-0.338418	1.782510		
34358	H	-0.030607	-0.468332	-1.356464		
34359	O	-1.142400	-1.752108	-0.184391		
34360	O	-2.424422	-1.198478	-0.417449		
34361	H	-2.368166	-0.840062	-1.316916		
34362	H	1.259589	-2.377642	-0.575307		
34363	H	0.946463	-1.973807	1.129710		
34364	Rotational constants (GHz):			1.2836300	0.8634300	0.6942800
34365	Vibrational harmonic frequencies (cm-1):					
34366	i2202.5944		70.3811			109.7869
34367	131.4609		158.5915			190.4819
34368	213.7986		233.7887			239.9899
34369	252.1750		305.0943			307.4451
34370	335.1069		346.0444			379.5805
34371	443.2165		496.1410			517.7038
34372	587.6514		612.3275			651.0356
34373	679.9621		735.7805			861.2469
34374	917.6040		945.2493			978.6093
34375	989.0624		1022.3815			1057.4431
34376	1116.4690		1153.6114			1164.1907
34377	1176.7616		1188.8201			1224.7735
34378	1257.6314		1293.5946			1340.8636
34379	1399.7441		1405.1744			1412.5769
34380	1422.0669		1463.0987			1486.3971
34381	1493.7248		1502.2273			1700.0899
34382	1872.6456		2985.3923			3074.6387
34383	3080.9154		3088.8393			3150.5201
34384	3155.0726		3185.3068			3756.0960
34385	Zero-point correction (Hartree): 0.151089					
34386						
34387	TS.diHPCARP_I.1700HHshift.BB.lmduu					
34388	-----					
34389	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15163394					
34390	Electronic state : 2-A					

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34391 Cartesian coordinates (Angs):
34392 O 2.528901 -0.318742 0.076744
34393 H 1.879262 -0.265386 1.060250
34394 O 0.980765 -0.358284 1.839261
34395 O 1.782088 -1.113176 -0.724438
34396 O 0.090507 -1.116584 1.161601
34397 C 0.900482 -0.326124 -1.510579
34398 C -0.813651 -0.309063 0.394487
34399 C -0.116199 0.490912 -0.718903
34400 C -1.745895 -1.350082 -0.211516
34401 C -1.630930 0.582308 1.321778
34402 O -2.300340 -1.205727 -1.263240
34403 H -1.902539 -2.242693 0.419264
34404 H -0.960515 1.275309 1.823702
34405 H -2.139927 -0.032253 2.063458
34406 H -2.361696 1.146353 0.746275
34407 H -0.897911 0.779683 -1.424776
34408 O 0.507928 1.669081 -0.242579
34409 O -0.466144 2.712375 -0.254352
34410 H -0.028472 3.362268 -0.817674
34411 H 1.484982 0.348841 -2.136036
34412 H 0.374345 -1.051386 -2.130042
34413 Rotational constants (GHz): 1.0729500 0.9046200 0.7768200
34414 Vibrational harmonic frequencies (cm-1):
34415 i2250.4696 60.7411 92.2914
34416 114.2819 126.3558 179.0509
34417 187.2263 217.3944 243.2003
34418 282.8662 297.0443 306.7557
34419 324.6312 366.2976 403.7272
34420 417.3373 460.6368 477.7325
34421 535.6321 664.0658 679.5596
34422 691.2964 791.6446 858.7216
34423 881.4491 925.1196 961.3828
34424 974.8161 1004.7112 1054.0281
34425 1074.9167 1137.0189 1164.5231
34426 1177.9207 1188.2636 1211.9462
34427 1261.0919 1301.2667 1352.4540
34428 1376.5526 1394.8527 1397.6553
34429 1404.9099 1411.6367 1472.6239
34430 1487.0445 1502.2565 1702.8110
34431 1866.8700 2989.7251 3078.5621
34432 3086.7520 3093.7808 3150.6992
34433 3160.3830 3178.9496 3828.9478
34434 Zero-point correction (Hartree): 0.150437
34435
34436 TS.diHPCARP_I.1700HHshift.BB.lmuuu
34437 -----
34438 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15122218
34439 Electronic state : 2-A
34440 Cartesian coordinates (Angs):
34441 O 2.535497 -0.311608 0.083799
34442 H 1.891863 -0.200432 1.057846
34443 O 0.986516 -0.239025 1.844940
34444 O 1.780412 -1.138154 -0.675044
34445 O 0.101232 -1.046826 1.218895
34446 C 0.902523 -0.383604 -1.498462
34447 C -0.809463 -0.296224 0.403868
34448 C -0.117172 0.462608 -0.741750
34449 C -1.715199 -1.383259 -0.162540
34450 C -1.655952 0.613382 1.286414
34451 O -2.293159 -1.278727 -1.205750
34452 H -1.827452 -2.268248 0.488334
34453 H -0.996796 1.304045 1.807526
34454 H -2.189135 0.014998 2.024595
34455 H -2.367537 1.168125 0.679322
34456 H -0.899823 0.714614 -1.460900
34457 O 0.504357 1.665097 -0.333652
34458 O -0.459061 2.708872 -0.487742
34459 H -0.356724 3.176549 0.349950
34460 H 1.488313 0.270415 -2.143772
34461 H 0.382508 -1.134506 -2.091661
34462 Rotational constants (GHz): 1.0709100 0.9039900 0.7764300

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34463 Vibrational harmonic frequencies (cm-1):
34464 i2246.7143 57.3135 87.2366
34465 109.5580 133.1146 145.9022
34466 185.6756 213.8512 242.7363
34467 279.2578 298.5331 307.0741
34468 322.6084 362.7400 402.6171
34469 418.5958 460.2953 478.5274
34470 535.0135 663.6074 678.4685
34471 689.7781 805.9252 858.3828
34472 881.9759 924.6092 962.1369
34473 971.2665 1003.4823 1057.1728
34474 1078.3169 1137.7164 1162.8966
34475 1177.9162 1186.6331 1212.9787
34476 1257.9953 1301.5105 1348.5075
34477 1379.5026 1391.7526 1394.1321
34478 1409.8460 1411.9251 1473.0634
34479 1484.4731 1505.1187 1703.1373
34480 1868.3946 2987.7054 3076.5433
34481 3088.6544 3095.5749 3155.1822
34482 3155.5518 3175.4053 3832.9178
34483 Zero-point correction (Hartree): 0.150338
34484
34485 TS.diHPCARP_I.1700HHshift.BB.lpudd
34486 -----
34487 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15350514
34488 Electronic state : 2-A
34489 Cartesian coordinates (Angs):
34490 O -2.740691 0.020408 -0.691913
34491 H -1.985215 -0.846433 -1.032879
34492 O -1.044379 -1.545417 -1.120091
34493 O -2.340547 0.275575 0.575955
34494 O -0.561754 -1.542675 0.149447
34495 C -1.340139 1.277409 0.574853
34496 C 0.452858 -0.539552 0.338640
34497 C -0.073410 0.822915 -0.156532
34498 C 1.649531 -0.988500 -0.520046
34499 C 0.783836 -0.566765 1.810560
34500 O 2.731978 -1.201479 -0.066483
34501 H 1.409020 -1.143561 -1.585749
34502 H 1.240428 -1.519120 2.067296
34503 H -0.119434 -0.433616 2.402692
34504 H 1.495192 0.225474 2.033285
34505 H -0.269276 0.770864 -1.227894
34506 O 0.857665 1.852608 0.098140
34507 O 1.906272 1.732022 -0.854361
34508 H 1.781324 2.529941 -1.383978
34509 H -1.724800 2.176001 0.093021
34510 H -1.131637 1.479057 1.623796
34511 Rotational constants (GHz): 1.3083900 0.8172000 0.6564600
34512 Vibrational harmonic frequencies (cm-1):
34513 i2174.6575 53.3181 85.3079
34514 109.1977 136.7562 188.0498
34515 209.8863 223.1300 229.2776
34516 240.5410 278.2819 285.7920
34517 332.2358 367.6197 391.8171
34518 433.8055 471.4240 513.7273
34519 582.6239 593.8730 647.6260
34520 664.4644 771.5756 903.2778
34521 906.8388 932.8890 983.6045
34522 1010.8942 1028.8323 1048.0558
34523 1108.9495 1148.3026 1159.1387
34524 1164.3984 1184.7536 1208.6285
34525 1263.3966 1308.4985 1341.9336
34526 1378.8005 1395.8881 1400.4169
34527 1406.7860 1435.4347 1482.3421
34528 1486.4054 1506.3067 1697.3015
34529 1876.8088 2995.0256 3088.8184
34530 3093.2766 3104.6193 3159.0646
34531 3171.3442 3175.8061 3816.7472
34532 Zero-point correction (Hartree): 0.150778
34533
34534 TS.diHPCARP_I.1700HHshift.BB.lpuuu

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34535 -----
34536 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15037937
34537 Electronic state : 2-A
34538 Cartesian coordinates (Angs):
34539   O      2.276334      -0.753383      0.430375
34540   H      1.680225      -0.098144      1.231716
34541   O      0.807734      0.405172      1.849183
34542   O      1.339360      -1.662363      0.072318
34543   O     -0.263816      -0.313319      1.462739
34544   C      0.650144      -1.257537     -1.101932
34545   C     -0.925927      0.230211      0.308724
34546   C     -0.174525      0.034353     -1.023311
34547   C     -2.206806     -0.610603      0.297772
34548   C     -1.326835      1.681250      0.537971
34549   O     -2.776930     -0.947030     -0.698283
34550   H     -2.589206     -0.849932      1.304852
34551   H     -0.432588      2.279291      0.684777
34552   H     -1.964066      1.751855      1.418982
34553   H     -1.865832      2.048347     -0.333326
34554   H     -0.966488     -0.095071     -1.767186
34555   O      0.473565      1.173089     -1.541260
34556   O      1.459352      1.687963     -0.664595
34557   H      2.173348      1.034101     -0.718950
34558   H      1.362971     -1.162672     -1.923534
34559   H     -0.019470     -2.094857     -1.296491
34560 Rotational constants (GHz):      1.2332200      0.8490400      0.8105700
34561 Vibrational harmonic frequencies (cm-1):
34562   i2211.9329      66.7976      111.7962
34563      145.9610      175.0826      193.5871
34564      232.6938      245.4769      259.6009
34565      274.2083      301.5359      318.0019
34566      335.9263      354.8721      407.4015
34567      453.8051      464.3453      513.9794
34568      597.8041      659.7782      666.7077
34569      682.5085      793.0363      878.5562
34570      883.0208      939.9106      970.5933
34571      975.2347      990.9047     1049.1161
34572     1071.5442     1138.0974     1172.2803
34573     1189.3116     1189.6233     1214.3255
34574     1242.2581     1298.2830     1354.6217
34575     1387.6288     1395.9152     1406.0585
34576     1415.1611     1460.9159     1478.5022
34577     1482.0791     1505.5999     1710.2461
34578     1871.6889     2997.5716     3074.6372
34579     3079.2059     3080.7660     3141.9773
34580     3158.0486     3190.6025     3745.9526
34581 Zero-point correction (Hartree): 0.151259
34582
34583 TS.diHPCARP_I.1700HHshift.BB.ltddd
34584 -----
34585 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15408195
34586 Electronic state : 2-A
34587 Cartesian coordinates (Angs):
34588   O      -2.655064      0.052533     -0.653262
34589   H     -1.984421     -0.852178     -0.976603
34590   O     -1.084112     -1.644219     -1.061134
34591   O     -2.253857      0.272038      0.622290
34592   O     -0.569504     -1.641928      0.194856
34593   C     -1.175005      1.188961      0.641423
34594   C      0.518383     -0.720249      0.312810
34595   C      0.054595      0.686903     -0.123610
34596   C      1.620690     -1.178354     -0.649779
34597   C      0.978180     -0.793117      1.752121
34598   O      2.777457     -0.937360     -0.475488
34599   H      1.253983     -1.747245     -1.521854
34600   H      1.295003     -1.808035      1.983550
34601   H      0.169902     -0.516848      2.425624
34602   H      1.822570     -0.122274      1.889606
34603   H     -0.150059      0.682725     -1.194874
34604   O      1.134932      1.554791      0.143759
34605   O      0.939453      2.729710     -0.633846
34606   H      1.721490      2.709813     -1.200107

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34607      H      -1.489093      2.138062      0.205716
34608      H      -0.934866      1.326592      1.693750
34609      Rotational constants (GHz):      1.1309900      0.8890400      0.6398100
34610      Vibrational harmonic frequencies (cm-1):
34611      i2206.3248      32.5111      68.9823
34612      103.7015      118.6945      179.8499
34613      195.8058      226.7277      238.3784
34614      250.2278      270.1442      284.5489
34615      324.0305      330.0993      422.8499
34616      428.5523      447.8564      508.1995
34617      547.0112      603.6000      650.9676
34618      681.1266      775.4664      886.4091
34619      911.9848      940.1458      991.5180
34620      1010.0367      1023.1361      1045.1297
34621      1107.9101      1138.3839      1160.8156
34622      1175.3220      1183.2491      1201.7620
34623      1258.9032      1304.2241      1343.8886
34624      1372.6272      1395.2960      1400.9869
34625      1416.8383      1422.2021      1481.1055
34626      1485.6907      1506.8313      1694.1461
34627      1872.1103      2993.5153      3087.0987
34628      3090.9122      3099.7799      3158.3209
34629      3165.8271      3179.6571      3818.2563
34630      Zero-point correction (Hartree): 0.150389
34631
34632      TS.diHPCARP_I.1700HHshift.BB.ltduu
34633      -----
34634      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15422223
34635      Electronic state : 2-A
34636      Cartesian coordinates (Angs):
34637      O      -2.076882      1.052655      -0.452401
34638      H      -1.359737      1.486082      0.380884
34639      O      -0.387383      1.797658      1.005177
34640      O      -1.207284      0.811096      -1.464525
34641      O      0.619737      1.481661      0.163156
34642      C      -0.723906      -0.524468      -1.393731
34643      C      1.047845      0.117512      0.318380
34644      C      -0.037479      -0.886672      -0.083321
34645      C      2.232535      0.038850      -0.638040
34646      C      1.572359      -0.114971      1.731657
34647      O      2.540714      -0.953153      -1.231553
34648      H      2.816128      0.973834      -0.705798
34649      H      0.783754      0.104772      2.445360
34650      H      2.424011      0.537973      1.920586
34651      H      1.879546      -1.153497      1.841073
34652      H      0.451768      -1.852278      -0.249787
34653      O      -0.905209      -0.986345      1.034533
34654      O      -1.998241      -1.817552      0.699246
34655      H      -2.679445      -1.153337      0.513658
34656      H      -1.545378      -1.214945      -1.578689
34657      H      -0.002399      -0.598262      -2.206029
34658      Rotational constants (GHz):      1.2252600      0.8283700      0.7862800
34659      Vibrational harmonic frequencies (cm-1):
34660      i2285.2441      56.5119      71.7198
34661      106.4974      172.5893      198.6797
34662      227.7322      233.1259      255.9821
34663      267.3644      309.5627      325.3243
34664      354.8101      402.4566      421.5467
34665      441.0748      458.3398      487.6072
34666      546.9637      663.4218      674.5770
34667      722.0795      827.8942      842.4444
34668      878.7582      921.7336      965.8516
34669      980.9621      1014.0148      1039.5181
34670      1065.5636      1141.3320      1165.3818
34671      1180.7997      1185.1604      1214.1937
34672      1264.1187      1292.7845      1373.6012
34673      1377.0435      1394.3223      1398.0785
34674      1412.9786      1427.7158      1484.7525
34675      1489.2838      1498.8030      1706.9621
34676      1871.5771      2991.7362      3059.1805
34677      3076.7969      3104.2579      3154.7333
34678      3157.4176      3183.0823      3757.9979

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34679 Zero-point correction (Hartree): 0.151040
34680
34681 TS.diHPCARP_I.1700HHshift.BB.tmudd
34682 -----
34683 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15676008
34684 Electronic state : 2-A
34685 Cartesian coordinates (Angs):
34686 O -2.770971 0.257801 -0.486202
34687 H -2.236880 -0.772439 -0.688827
34688 O -1.423710 -1.658369 -0.730380
34689 O -2.131474 0.749346 0.602660
34690 O -0.770953 -1.476679 0.442125
34691 C -1.005304 1.518310 0.201589
34692 C 0.383030 -0.630510 0.321782
34693 C 0.012027 0.627469 -0.511716
34694 C 1.473500 -1.382984 -0.431897
34695 C 0.789510 -0.411996 1.771482
34696 O 2.612653 -1.008146 -0.440054
34697 H 1.145325 -2.289331 -0.968908
34698 H 0.855539 -1.383160 2.260580
34699 H 0.038759 0.178162 2.290860
34700 H 1.751351 0.082541 1.834527
34701 H -0.443582 0.273247 -1.436163
34702 O 1.105905 1.358310 -0.991008
34703 O 1.912227 1.800883 0.092525
34704 H 2.629114 1.147044 0.049332
34705 H -1.322047 2.306532 -0.480918
34706 H -0.603570 1.950498 1.114750
34707 Rotational constants (GHz): 1.3633700 0.8489900 0.6660400
34708 Vibrational harmonic frequencies (cm-1):
34709 i2255.7967 76.5218 111.7876
34710 133.9105 155.5333 183.4459
34711 213.2791 238.0611 267.4765
34712 269.4627 303.6179 322.4643
34713 341.0519 403.3742 432.1417
34714 478.7160 506.9198 536.7616
34715 589.4952 636.9200 640.6820
34716 653.9119 780.3369 917.6915
34717 920.5786 950.1566 981.5031
34718 989.7768 998.1240 1031.1757
34719 1103.1959 1156.3676 1164.7760
34720 1171.8691 1175.8355 1214.6204
34721 1244.0395 1285.9814 1343.3780
34722 1369.2296 1395.9485 1414.4357
34723 1425.3545 1453.7712 1483.2978
34724 1486.6800 1512.4653 1687.0177
34725 1851.6102 3001.6688 3092.4319
34726 3098.1385 3120.1469 3161.3768
34727 3172.0088 3215.4643 3731.8277
34728 Zero-point correction (Hartree): 0.151721
34729
34730 TS.diHPCARP_I.1700HHshift.BB.tpduu
34731 -----
34732 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15054839
34733 Electronic state : 2-A
34734 Cartesian coordinates (Angs):
34735 O 2.166852 -1.175473 0.482242
34736 H 1.702476 -0.385953 1.192065
34737 O 0.901555 0.361681 1.724216
34738 O 1.085969 -1.712862 -0.118362
34739 O -0.252047 -0.298472 1.472810
34740 C 0.697133 -0.969802 -1.270022
34741 C -0.952057 0.226289 0.338486
34742 C -0.165075 0.273785 -0.989353
34743 C -2.101155 -0.772146 0.201890
34744 C -1.533211 1.593468 0.681454
34745 O -2.697390 -0.947278 -0.820737
34746 H -2.362118 -1.299883 1.135101
34747 H -0.725063 2.284078 0.912380
34748 H -2.189811 1.510885 1.546405
34749 H -2.093611 1.981622 -0.166693
34750 H -0.953805 0.289603 -1.745718

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34751	O	0.484571	1.498325	-1.243813		
34752	O	1.770206	1.549785	-0.655607		
34753	H	1.575530	1.662407	0.287842		
34754	H	1.585956	-0.671415	-1.821911		
34755	H	0.108905	-1.686557	-1.840189		
34756	Rotational constants (GHz):		1.2210900	0.8668000	0.7986200	
34757	Vibrational harmonic frequencies (cm-1):					
34758	i2146.4099		63.3480		93.5132	
34759	121.0751		173.4103		190.5030	
34760	227.2009		234.3138		253.8392	
34761	272.2026		297.1603		314.4980	
34762	330.3710		402.1852		412.3551	
34763	454.9398		473.2228		515.3685	
34764	582.5337		649.6565		670.4081	
34765	680.1322		785.4556		884.2230	
34766	902.6669		938.9474		957.9038	
34767	979.6903		993.0141		1050.5115	
34768	1081.2187		1137.6341		1160.2083	
34769	1187.7349		1197.9864		1209.9577	
34770	1251.7013		1312.0240		1348.0937	
34771	1378.4192		1400.2031		1408.5530	
34772	1414.2385		1462.6400		1466.6680	
34773	1482.9021		1496.1743		1704.2725	
34774	1869.6432		3001.1571		3077.5622	
34775	3084.7762		3105.2204		3159.3375	
34776	3168.5755		3169.4072		3738.9375	
34777	Zero-point correction (Hartree): 0.151225					
34778						
34779	TS.diHPCARP_I.1700HHshift.BC.tmuuu					
34780	-----					
34781	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15109821					
34782	Electronic state : 2-A					
34783	Cartesian coordinates (Angs):					
34784	O	2.899279	0.057529	-0.354164		
34785	H	2.186106	-0.727903	-0.737077		
34786	O	1.249620	-1.520553	-0.927845		
34787	O	2.231958	1.238474	-0.310521		
34788	O	0.712997	-1.597945	0.319239		
34789	C	1.197703	1.210578	0.659640		
34790	C	-0.440371	-0.775434	0.398934		
34791	C	-0.115282	0.699587	0.036088		
34792	C	-1.473658	-1.345171	-0.567306		
34793	C	-0.955889	-0.941038	1.821349		
34794	O	-2.384807	-0.711648	-1.021932		
34795	H	-1.338284	-2.416152	-0.798141		
34796	H	-0.211477	-0.581592	2.530448		
34797	H	-1.145942	-1.993631	2.026552		
34798	H	-1.873024	-0.372595	1.945121		
34799	H	-0.025112	0.797804	-1.045198		
34800	O	-1.185579	1.509292	0.477086		
34801	O	-1.896915	2.032577	-0.631558		
34802	H	-2.453732	1.273315	-0.873364		
34803	H	1.532019	0.618871	1.512081		
34804	H	1.042000	2.248942	0.944903		
34805	Rotational constants (GHz):		1.2279300	0.8243500	0.6391200	
34806	Vibrational harmonic frequencies (cm-1):					
34807	i2440.4756		35.0433		81.8063	
34808	108.0216		132.0103		185.5660	
34809	203.0294		218.1312		245.7085	
34810	268.6978		283.7628		301.6728	
34811	336.2494		344.6718		428.4048	
34812	475.9480		530.5630		544.1394	
34813	548.0570		576.5674		662.9738	
34814	683.2938		789.2323		924.4884	
34815	943.7604		968.7066		990.9022	
34816	1032.7454		1052.8293		1076.6323	
34817	1135.9717		1151.0283		1161.4757	
34818	1182.3705		1195.4631		1222.6907	
34819	1243.0802		1303.4948		1332.2515	
34820	1355.7536		1395.2209		1399.0626	
34821	1410.8483		1413.5734		1467.4678	
34822	1474.3965		1491.4305		1499.3214	

34823 1856.9297 2995.5508 3079.3422
 34824 3089.5222 3116.3454 3150.9801
 34825 3160.6922 3183.1354 3709.1658
 34826 Zero-point correction (Hartree): 0.150701
 34827

34828 TS.diHPCARP_I.1700HHshift.CR.hmddd
 34829 -----
 34830 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15292205
 34831 Electronic state : 2-A

34832 Cartesian coordinates (Angs):
 34833 O 2.224304 -1.497229 -0.175775
 34834 H 1.236237 -1.717152 -0.773302
 34835 O 0.131401 -1.695711 -1.207866
 34836 O 2.028176 -0.223228 0.234169
 34837 O -0.169319 -0.378761 -1.355240
 34838 C 1.071754 -0.155475 1.294122
 34839 C -0.962373 0.101779 -0.257182
 34840 C -0.117159 0.699650 0.876912
 34841 C -1.804291 -1.064155 0.259444
 34842 C -1.919238 1.131683 -0.847361
 34843 O -2.015035 -1.264827 1.420276
 34844 H -2.259579 -1.674355 -0.537828
 34845 H -2.612260 0.642796 -1.530556
 34846 H -1.352936 1.885002 -1.386707
 34847 H -2.478181 1.611624 -0.045797
 34848 H -0.771414 0.770788 1.749358
 34849 O 0.265345 2.040252 0.647647
 34850 O 0.857307 2.181948 -0.636564
 34851 H 1.714229 1.738728 -0.548569
 34852 H 0.768698 -1.164677 1.566277
 34853 H 1.565610 0.326789 2.138343

34854 Rotational constants (GHz): 1.0985600 0.9812700 0.7584400

34855 Vibrational harmonic frequencies (cm-1):
 34856 i2427.2254 67.4018 103.3988
 34857 126.8806 176.6310 191.7900
 34858 212.3842 232.2030 263.8565
 34859 287.2965 303.0157 313.3952
 34860 330.0530 360.7834 379.4784
 34861 434.7532 489.4041 515.6189
 34862 581.9814 628.2136 657.7294
 34863 695.0957 852.4621 875.4248
 34864 916.5001 927.6450 947.0044
 34865 983.0161 994.2979 1008.7900
 34866 1099.6537 1130.1400 1149.1772
 34867 1166.3605 1183.1373 1226.8316
 34868 1242.1510 1289.1543 1352.8163
 34869 1369.4605 1380.4359 1401.6737
 34870 1414.2939 1449.8389 1478.6622
 34871 1484.6310 1507.2502 1659.9918
 34872 1866.1450 3005.3442 3080.0014
 34873 3085.9807 3095.2933 3156.3101
 34874 3157.6009 3185.7950 3767.5256

34875 Zero-point correction (Hartree): 0.150911
 34876
 34877
 34878

34879 1,7-hydroperoxide-H-shift in (2R,3R)-2-Me-2,4-diOOH-butanal-3-peroxyl (B, R,R-di-
 34880 HPCARP-Ib), forming C (di-HPCARP-Ic)

34881 =====
 34882 =====

34883
 34884 TS.diHPCARP_Ib.1600HHshift.a.cmpuu
 34885 -----
 34886 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14309573
 34887 Electronic state : 2-A

34888 Cartesian coordinates (Angs):
 34889 O 3.106418 -0.036409 0.412337
 34890 H 2.597124 0.972663 0.197536
 34891 O 1.722692 1.740667 -0.126952
 34892 O 2.536284 -0.885728 -0.484596
 34893 O 0.591267 1.145786 0.338805
 34894 C 1.185741 -1.164403 -0.084056

34895	C	0.280809	-0.010368	-0.473444	
34896	H	1.165332	-1.350038	0.986621	
34897	H	0.919830	-2.069409	-0.626795	
34898	H	0.488219	0.281408	-1.506695	
34899	C	-1.231337	-0.256436	-0.368295	
34900	C	-1.672833	-1.290417	-1.403307	
34901	H	-1.205201	-2.253807	-1.213833	
34902	H	-1.409026	-0.946283	-2.402364	
34903	H	-2.753791	-1.408236	-1.352296	
34904	C	-1.733559	-0.742679	0.986142	
34905	O	-1.933527	0.925581	-0.723759	
34906	O	-1.093566	-1.441285	1.717973	
34907	H	-2.777537	-0.460215	1.198525	
34908	O	-2.032490	1.775774	0.411756	
34909	H	-1.174500	2.224648	0.412542	
34910	Rotational constants (GHz):		1.3879500	0.7107900	0.6058300
34911	Vibrational harmonic frequencies (cm-1):				
34912	i3000.1014		32.9659		75.7498
34913	107.9530		159.7479		179.0794
34914	205.4197		219.6275		250.1899
34915	276.3632		317.4399		318.0055
34916	330.4097		369.0404		417.1533
34917	425.3534		456.3784		513.8440
34918	559.6061		567.0118		638.7264
34919	687.5114		878.7538		920.3085
34920	926.6469		961.6220		973.4390
34921	1016.7764		1037.4227		1052.7058
34922	1099.9753		1106.7222		1133.7520
34923	1147.0344		1185.9906		1204.9170
34924	1282.9652		1301.0237		1325.6304
34925	1377.4471		1402.7083		1417.5743
34926	1421.5860		1438.9318		1463.7319
34927	1489.4335		1493.6842		1503.7898
34928	1869.7799		3011.7485		3074.0200
34929	3079.3161		3114.6761		3156.3569
34930	3169.3986		3181.3442		3777.9689
34931	Zero-point correction (Hartree): 0.150602				
34932					
34933	TS.diHPCARP_Ib.16OOHHshift.a.cpmmuu				
34934	-----				
34935	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14243405				
34936	Electronic state : 2-A				
34937	Cartesian coordinates (Angs):				
34938	O	-3.148277	0.256393	0.174343	
34939	H	-2.723614	-0.785609	-0.152842	
34940	O	-1.907292	-1.593579	-0.439698	
34941	O	-2.342299	1.146695	-0.464440	
34942	O	-0.847986	-1.245050	0.335836	
34943	C	-1.057044	1.177366	0.167146	
34944	C	-0.239175	-0.048967	-0.185330	
34945	H	-1.204955	1.271611	1.244505	
34946	H	-0.575858	2.069055	-0.227669	
34947	H	-0.176258	-0.165600	-1.268013	
34948	C	1.167607	-0.005839	0.427429	
34949	C	1.208105	-0.374265	1.904269	
34950	H	0.827750	-1.381973	2.047774	
34951	H	0.601003	0.320092	2.482140	
34952	H	2.235557	-0.317964	2.261799	
34953	C	2.130846	-0.916218	-0.331919	
34954	O	1.698827	1.311093	0.383524	
34955	O	1.805338	-1.731170	-1.139989	
34956	H	3.190927	-0.754311	-0.050261	
34957	O	1.732747	1.696079	-0.993707	
34958	H	2.634958	2.028543	-1.073962	
34959	Rotational constants (GHz):		1.3803100	0.7092000	0.5958400
34960	Vibrational harmonic frequencies (cm-1):				
34961	i3028.8022		62.1333		78.6470
34962	93.8711		123.4223		146.1921
34963	187.6990		208.0886		229.9862
34964	245.6762		259.8908		281.3482
34965	324.2600		350.1242		386.2636
34966	409.5355		443.5841		518.1813

34967	563.1957	570.8446	635.9157			
34968	690.5758	874.8402	898.8536			
34969	927.1388	960.8558	997.3873			
34970	1016.8750	1043.7327	1060.5899			
34971	1100.3695	1110.7482	1143.5505			
34972	1148.3728	1196.4242	1219.8959			
34973	1266.6620	1307.7604	1347.6430			
34974	1371.8257	1391.1097	1409.2086			
34975	1414.2221	1430.9493	1460.7825			
34976	1490.5371	1491.6049	1501.1428			
34977	1887.5630	2938.1652	3080.1709			
34978	3084.9034	3111.2108	3154.6491			
34979	3166.4247	3179.0287	3837.4298			
34980	Zero-point correction (Hartree): 0.149976					
34981						
34982	TS.diHPCARP_Ib.1600HHshift.a.ctmmuu					
34983	-----					
34984	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14386032					
34985	Electronic state : 2-A					
34986	Cartesian coordinates (Angs):					
34987	O	-3.056253	-0.556090	-0.270625		
34988	H	-2.817786	0.566026	-0.071390		
34989	O	-2.162674	1.531736	0.174551		
34990	O	-2.185640	-1.218878	0.537077		
34991	O	-0.977380	1.267058	-0.436096		
34992	C	-0.858577	-1.116814	-0.000044		
34993	C	-0.271750	0.248353	0.297755		
34994	H	-0.901010	-1.312537	-1.070044		
34995	H	-0.290106	-1.893052	0.508624		
34996	H	-0.393218	0.463112	1.362109		
34997	C	1.209751	0.415297	-0.043001		
34998	C	1.645575	1.872913	0.085776		
34999	H	1.322639	2.268341	1.046901		
35000	H	1.191171	2.459008	-0.708861		
35001	H	2.729492	1.944820	0.008786		
35002	C	2.083181	-0.406106	0.897434		
35003	O	1.536108	0.069371	-1.379417		
35004	O	1.735851	-0.793949	1.973621		
35005	H	3.107249	-0.569131	0.512478		
35006	O	1.477217	-1.358357	-1.475609		
35007	H	2.264654	-1.535576	-2.004140		
35008	Rotational constants (GHz):			1.351590	0.6831600	0.6313500
35009	Vibrational harmonic frequencies (cm-1):					
35010	i3041.6227		53.2155			95.4685
35011	103.4524		152.0852			178.3613
35012	185.0237		199.1022			220.0823
35013	241.6773		273.9601			296.4784
35014	318.4562		348.7043			358.0588
35015	417.8707		447.5367			536.9873
35016	568.5291		572.6358			639.7264
35017	689.4782		882.6037			907.4745
35018	937.6534		974.3648			982.6108
35019	991.2190		1045.2555			1051.0841
35020	1102.9661		1117.9644			1140.0408
35021	1148.5644		1170.5820			1239.8958
35022	1259.4500		1307.3699			1335.9787
35023	1370.7867		1394.2145			1410.8394
35024	1411.2165		1431.4191			1456.2480
35025	1486.6650		1490.1073			1499.8908
35026	1876.0492		2968.2680			3079.5675
35027	3091.2996		3105.5513			3158.8379
35028	3171.2041		3173.8312			3837.7509
35029	Zero-point correction (Hartree): 0.150144					
35030						
35031	TS.diHPCARP_Ib.1600HHshift.a.ctmpdd					
35032	-----					
35033	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14364546					
35034	Electronic state : 2-A					
35035	Cartesian coordinates (Angs):					
35036	O	2.812243	-0.415652	-0.234301		
35037	H	2.350875	0.202929	0.675186		
35038	O	1.512408	0.644159	1.348195		

35039	O	1.773128	-0.468870	-1.113744			
35040	O	0.706305	-0.417880	1.626179			
35041	C	0.781807	-1.385782	-0.619509			
35042	C	-0.077319	-0.799348	0.484075			
35043	H	1.304609	-2.274652	-0.268492			
35044	H	0.163473	-1.627560	-1.482526			
35045	H	-0.676266	-1.617740	0.889136			
35046	C	-1.076045	0.273260	0.008650			
35047	C	-1.452773	1.268592	1.098227			
35048	H	-0.591934	1.877652	1.356287			
35049	H	-1.791450	0.732436	1.983595			
35050	H	-2.249941	1.917701	0.737206			
35051	C	-2.380616	-0.420772	-0.410825			
35052	O	-0.715987	0.904543	-1.212252			
35053	O	-2.720138	-1.505982	-0.039580			
35054	H	-3.008536	0.201739	-1.070555			
35055	O	0.216220	1.946187	-1.004572			
35056	H	1.055413	1.479771	-1.142947			
35057	Rotational constants (GHz):				1.3765700	0.7688800	0.7322800
35058	Vibrational harmonic frequencies (cm-1):						
35059	i3029.3048			63.5202		103.0629	
35060	126.8105			170.2308		179.9521	
35061	211.9953			236.0279		252.8758	
35062	277.2214			307.4234		329.5664	
35063	343.7942			357.5033		425.9668	
35064	455.3771			470.2597		514.7789	
35065	551.4012			657.3667		684.8303	
35066	695.0722			852.9874		888.6204	
35067	926.5171			955.1260		977.1997	
35068	988.1322			1051.1105		1066.8510	
35069	1083.3316			1090.4628		1137.6980	
35070	1145.1489			1179.7523		1216.7743	
35071	1251.4604			1313.0026		1367.3059	
35072	1392.5321			1395.8071		1401.4581	
35073	1413.2504			1445.1090		1465.9853	
35074	1477.5079			1480.4808		1505.5336	
35075	1868.1666			3005.0210		3077.6542	
35076	3093.9865			3102.7570		3153.0661	
35077	3157.8735			3185.4653		3749.5659	
35078	Zero-point correction (Hartree):				0.150992		
35079	TS.diHPCARP_Ib.1600HHshift.a.ctmpuu						
35081	-----						
35082	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.14359436		
35083	Electronic state : 2-A						
35084	Cartesian coordinates (Angs):						
35085	O	3.058717	-0.519437	0.266348			
35086	H	2.801799	0.597614	0.043573			
35087	O	2.133857	1.547864	-0.212479			
35088	O	2.193428	-1.213340	-0.520970			
35089	O	0.953012	1.276921	0.404706			
35090	C	0.868808	-1.116495	0.023625			
35091	C	0.262130	0.232482	-0.306474			
35092	H	0.937553	-1.280945	1.097319			
35093	H	0.306221	-1.916076	-0.453589			
35094	H	0.391566	0.417064	-1.375468			
35095	C	-1.224191	0.400742	0.012160			
35096	C	-1.683990	1.832269	-0.257806			
35097	H	-1.387520	2.128833	-1.262037			
35098	H	-1.223838	2.503547	0.462896			
35099	H	-2.766823	1.896467	-0.164748			
35100	C	-2.076477	-0.516630	-0.858009			
35101	O	-1.566236	0.181402	1.369727			
35102	O	-1.713865	-0.965142	-1.906316			
35103	H	-3.088795	-0.693408	-0.452552			
35104	O	-1.531844	-1.230419	1.596910			
35105	H	-1.064396	-1.270089	2.440230			
35106	Rotational constants (GHz):				1.3471800	0.6814200	0.6331800
35107	Vibrational harmonic frequencies (cm-1):						
35108	i3052.1195			45.7502		95.3496	
35109	103.7595			151.6889		166.0215	
35110	193.3428			212.1005		218.7448	

35111	239.3897	277.5279	295.5369			
35112	312.6261	340.5743	359.8345			
35113	421.8155	446.1773	533.7221			
35114	563.4247	572.8752	640.6905			
35115	688.9580	885.4148	908.5136			
35116	939.0638	974.3516	981.8565			
35117	990.1568	1049.5595	1051.2423			
35118	1102.6170	1119.2641	1138.7383			
35119	1145.1109	1171.6470	1239.5524			
35120	1259.0153	1309.5131	1336.8686			
35121	1367.9415	1390.7952	1408.6885			
35122	1410.9754	1428.8566	1453.7117			
35123	1486.6385	1491.6489	1502.3981			
35124	1871.3650	2989.5998	3080.9664			
35125	3091.8262	3107.2528	3161.5664			
35126	3173.2081	3173.5338	3833.0847			
35127	Zero-point correction (Hartree): 0.150146					
35128						
35129	TS.diHPCARP_Ib.1600HHshift.a.ctpddd					
35130	-----					
35131	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14743268					
35132	Electronic state : 2-A					
35133	Cartesian coordinates (Angs):					
35134	O	-2.814905	-0.421063	-0.005528		
35135	H	-2.360045	0.621902	0.353214		
35136	O	-1.577399	1.472546	0.479954		
35137	O	-1.733621	-1.246127	-0.009231		
35138	O	-0.931972	1.509048	-0.719714		
35139	C	-0.855366	-0.894899	-1.091132		
35140	C	-0.059915	0.375611	-0.853858		
35141	H	-1.470749	-0.780847	-1.983415		
35142	H	-0.181269	-1.741946	-1.204246		
35143	H	0.458876	0.577307	-1.793166		
35144	C	1.037161	0.351653	0.222828		
35145	C	1.557449	1.758479	0.501183		
35146	H	0.796928	2.322096	1.037021		
35147	H	1.785780	2.266532	-0.433988		
35148	H	2.454893	1.703514	1.115053		
35149	C	2.213215	-0.489740	-0.269533		
35150	O	0.664311	-0.143337	1.495806		
35151	O	2.420563	-0.746764	-1.420858		
35152	H	2.888129	-0.812409	0.542179		
35153	O	0.557632	-1.559774	1.419759		
35154	H	-0.404678	-1.679007	1.388907		
35155	Rotational constants (GHz):			1.350900	0.8101600	0.7306200
35156	Vibrational harmonic frequencies (cm-1):					
35157	i3049.9122		62.1921			95.2254
35158	138.0733		166.9059			200.3758
35159	224.5497		236.6681			256.8059
35160	282.9650		308.3904			318.6104
35161	340.4279		357.7344			430.4516
35162	459.5097		531.6477			545.7922
35163	579.7969		631.2811			683.0346
35164	694.0297		858.6288			913.6907
35165	939.0351		955.1182			971.5083
35166	991.4279		1053.2901			1055.1819
35167	1063.8125		1076.8124			1141.4619
35168	1147.2539		1180.5737			1236.2182
35169	1257.7820		1315.5911			1369.9027
35170	1376.4392		1398.2036			1404.8197
35171	1414.6931		1437.7718			1466.8930
35172	1474.7411		1483.2233			1504.3225
35173	1864.6633		2993.5801			3078.6087
35174	3092.5794		3104.0671			3159.5637
35175	3160.0483		3167.8810			3733.5534
35176	Zero-point correction (Hartree): 0.151242					
35177						
35178	TS.diHPCARP_Ib.1600HHshift.a.ctpmuu					
35179	-----					
35180	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14324797					
35181	Electronic state : 2-A					
35182	Cartesian coordinates (Angs):					

35183	O	3.032802	0.060449	-0.482675		
35184	H	2.705658	-0.556654	0.436988		
35185	O	1.957550	-0.994642	1.267944		
35186	O	2.308044	1.206459	-0.374376		
35187	O	0.776030	-1.090661	0.603465		
35188	C	0.942405	0.946319	-0.715640		
35189	C	0.211058	0.222768	0.397986		
35190	H	0.916057	0.375117	-1.644544		
35191	H	0.504815	1.931760	-0.863659		
35192	H	0.300332	0.776646	1.334389		
35193	C	-1.266517	-0.011307	0.072473		
35194	C	-1.991116	-0.771417	1.180529		
35195	H	-1.955475	-0.185904	2.098252		
35196	H	-1.522089	-1.735100	1.349943		
35197	H	-3.029383	-0.932430	0.893434		
35198	C	-2.004390	1.316118	-0.077130		
35199	O	-1.424555	-0.618161	-1.204780		
35200	O	-1.647224	2.334074	0.440383		
35201	H	-2.933849	1.241661	-0.668009		
35202	O	-1.257649	-2.022765	-1.123413		
35203	H	-0.294703	-2.128001	-1.098497		
35204	Rotational constants (GHz):			1.2826700	0.7363800	0.6056200
35205	Vibrational harmonic frequencies (cm-1):					
35206	i2962.5365		48.6379			89.8143
35207	99.2023		147.3685			159.1543
35208	204.1588		211.6409			249.9366
35209	267.0634		282.5849			334.0491
35210	347.0713		357.3856			383.1397
35211	411.2723		449.6443			472.2633
35212	543.2458		580.6039			676.8359
35213	691.5297		872.5790			899.6024
35214	929.5507		972.2493			981.0215
35215	996.6452		1057.2357			1059.8419
35216	1101.7934		1110.3811			1138.1279
35217	1152.3360		1166.6395			1222.9215
35218	1269.7743		1298.0435			1333.6756
35219	1365.3847		1396.2770			1407.5789
35220	1429.4999		1448.9111			1466.3680
35221	1485.7481		1488.7859			1499.9712
35222	1868.1400		2996.6196			3081.0404
35223	3089.0809		3106.0449			3155.4350
35224	3163.2886		3188.7597			3765.6088
35225	Zero-point correction (Hartree):			0.150294		
35226	TS.diHPCARP_Ib.16OOHHshift.a.ctppuu					
35227	-----					
35228	-----					
35229	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14178835		
35230	Electronic state : 2-A					
35231	Cartesian coordinates (Angs):					
35232	O	3.049656	-0.009424	-0.405251		
35233	H	2.694280	-0.237434	0.684350		
35234	O	1.945632	-0.359632	1.600257		
35235	O	2.243967	1.011694	-0.803061		
35236	O	0.805619	-0.808015	1.009575		
35237	C	0.919424	0.513759	-1.027772		
35238	C	0.197420	0.275152	0.281543		
35239	H	0.980386	-0.399728	-1.618973		
35240	H	0.418722	1.299030	-1.594105		
35241	H	0.263055	1.164430	0.912818		
35242	C	-1.281389	-0.046958	0.073914		
35243	C	-1.908452	-0.729639	1.283932		
35244	H	-1.721503	-0.136675	2.177840		
35245	H	-1.467701	-1.712890	1.424966		
35246	H	-2.984514	-0.825993	1.137298		
35247	C	-2.064398	1.244097	-0.173456		
35248	O	-1.526069	-0.767227	-1.131114		
35249	O	-1.769915	2.300445	0.302077		
35250	H	-2.964249	1.109417	-0.799494		
35251	O	-0.850064	-2.013001	-1.064742		
35252	H	-1.584719	-2.637341	-1.015601		
35253	Rotational constants (GHz):			1.2884900	0.7033100	0.6394900
35254	Vibrational harmonic frequencies (cm-1):					

35255	i3043.3309	57.5214	82.5709			
35256	96.4753	124.3172	156.0616			
35257	191.2729	203.2921	225.1181			
35258	255.5750	266.7414	290.0300			
35259	309.0611	350.4133	405.1654			
35260	416.9847	450.2502	466.0043			
35261	536.8963	572.7118	678.0073			
35262	691.4412	877.0640	898.6142			
35263	926.9633	962.9826	992.9027			
35264	993.5942	1056.9055	1060.2485			
35265	1105.3650	1117.3506	1140.1668			
35266	1148.9515	1168.2593	1223.0398			
35267	1268.0714	1307.4044	1332.3990			
35268	1383.0519	1395.5776	1404.8777			
35269	1411.0501	1430.8194	1458.9499			
35270	1486.4179	1491.4959	1502.0574			
35271	1875.1634	2985.3958	3073.3487			
35272	3088.3829	3093.7860	3151.0171			
35273	3153.8955	3173.9199	3821.0396			
35274	Zero-point correction (Hartree): 0.149873					
35275						
35276	TS.diHPCARP_Ib.1600HHshift.a.hpmmuu					
35277	-----					
35278	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14737747					
35279	Electronic state : 2-A					
35280	Cartesian coordinates (Angs):					
35281	O	-3.232679	0.200873	0.138283		
35282	H	-2.819201	-0.748663	-0.374897		
35283	O	-1.993104	-1.504699	-0.810373		
35284	O	-2.411229	1.193071	-0.300312		
35285	O	-0.944019	-1.327574	0.036288		
35286	C	-1.140309	1.091019	0.352551		
35287	C	-0.325402	-0.051570	-0.216720		
35288	H	-1.311212	0.977427	1.423820		
35289	H	-0.639425	2.033739	0.144721		
35290	H	-0.252848	0.064119	-1.300080		
35291	C	1.077211	-0.144621	0.420664		
35292	C	1.061431	-0.702914	1.839287		
35293	H	0.671305	-1.717913	1.844648		
35294	H	0.440171	-0.084185	2.482884		
35295	H	2.077963	-0.701427	2.228908		
35296	C	1.945065	-1.048344	-0.444740		
35297	O	1.654223	1.136659	0.537690		
35298	O	2.992460	-0.695853	-0.911283		
35299	H	1.546519	-2.063732	-0.615855		
35300	O	1.690092	1.744146	-0.746834		
35301	H	2.532801	1.406221	-1.088070		
35302	Rotational constants (GHz):			1.5780200	0.6392400	0.5624300
35303	Vibrational harmonic frequencies (cm-1):					
35304	i2997.9434		60.3339			80.1451
35305	122.0055		143.9177			195.9291
35306	214.6746		235.0300			256.7331
35307	274.3934		290.0769			314.5378
35308	343.0326		371.1557			417.8898
35309	453.8242		459.9626			500.2329
35310	527.0700		574.1020			687.9522
35311	761.3713		861.6070			893.6985
35312	923.8960		972.0525			991.3213
35313	998.4141		1050.7197			1058.6512
35314	1094.6101		1115.2479			1142.4715
35315	1150.0087		1178.0399			1240.1140
35316	1284.7786		1310.6226			1332.2197
35317	1370.1942		1406.4316			1417.1656
35318	1427.1351		1435.1834			1460.7194
35319	1484.3554		1492.1900			1504.7867
35320	1859.4895		2993.5407			3083.1346
35321	3087.6262		3096.3909			3162.3377
35322	3170.0845		3174.1575			3754.5300
35323	Zero-point correction (Hartree): 0.150957					
35324						
35325	TS.diHPCARP_Ib.1600HHshift.a.hptpuu					
35326	-----					

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35327 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14453878
35328 Electronic state : 2-A
35329 Cartesian coordinates (Angs):
35330 O 3.327026 -0.339802 0.119527
35331 H 2.931944 0.739032 -0.024486
35332 O 2.130098 1.616064 -0.191400
35333 O 2.521570 -1.093290 -0.677502
35334 O 1.034032 1.164141 0.474270
35335 C 1.224514 -1.201216 -0.079826
35336 C 0.437034 0.079982 -0.261104
35337 H 1.353632 -1.448326 0.974408
35338 H 0.730952 -2.015640 -0.605861
35339 H 0.428286 0.360278 -1.317546
35340 C -1.010077 -0.025834 0.253956
35341 C -1.102900 -0.298412 1.751580
35342 H -0.543246 0.452044 2.307557
35343 H -0.699082 -1.283636 1.974709
35344 H -2.143075 -0.278857 2.067931
35345 C -1.719106 1.288403 -0.063917
35346 O -1.544433 -1.073684 -0.530394
35347 O -2.609315 1.367390 -0.864276
35348 H -1.370942 2.168708 0.501493
35349 O -2.899652 -1.281268 -0.173173
35350 H -3.339868 -0.627537 -0.738743
35351 Rotational constants (GHz): 1.7080600 0.5967700 0.5190200
35352 Vibrational harmonic frequencies (cm-1):
35353 i3009.3341 42.8634 69.0542
35354 110.2300 154.6520 171.5891
35355 213.3133 222.8528 252.3069
35356 268.5464 293.0236 327.1038
35357 348.6521 373.4451 396.8778
35358 434.4913 463.1005 497.9531
35359 534.3620 567.6079 687.2536
35360 771.1903 836.8770 897.4003
35361 927.2944 976.5672 983.8649
35362 1004.7884 1041.7925 1051.5486
35363 1100.6356 1119.2527 1142.9454
35364 1148.7792 1172.1814 1243.9630
35365 1278.3199 1305.6386 1322.6172
35366 1366.9394 1403.6932 1414.7656
35367 1431.6167 1443.9846 1465.2092
35368 1483.4484 1489.0301 1506.4748
35369 1857.6455 3003.7690 3080.1012
35370 3083.4803 3093.8936 3162.0561
35371 3166.2039 3168.9282 3754.2678
35372 Zero-point correction (Hartree): 0.150656
35373
35374 TS.diHPCARP_Ib.1600HHshift.a.httpuu
35375 -----
35376 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14397857
35377 Electronic state : 2-A
35378 Cartesian coordinates (Angs):
35379 O 3.163497 -0.590150 0.544675
35380 H 2.978380 0.477097 0.116080
35381 O 2.381705 1.390834 -0.367000
35382 O 2.330182 -1.384904 -0.179836
35383 O 1.142636 1.284483 0.183187
35384 C 0.975545 -1.136795 0.214725
35385 C 0.468544 0.155622 -0.395498
35386 H 0.922623 -1.105203 1.301765
35387 H 0.406775 -1.987392 -0.161168
35388 H 0.689652 0.171848 -1.467788
35389 C -1.039408 0.350189 -0.195237
35390 C -1.472338 1.781365 -0.498267
35391 H -1.138088 2.072333 -1.494041
35392 H -1.025223 2.453089 0.228725
35393 H -2.554945 1.862222 -0.443661
35394 C -1.744003 -0.594445 -1.164181
35395 O -1.297724 -0.035212 1.139265
35396 O -2.381542 -1.547324 -0.815710
35397 H -1.640268 -0.331224 -2.233857
35398 O -2.683052 0.108901 1.401758

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35399      H      -3.014564      -0.761410      1.133981
35400 Rotational constants (GHz):      1.5933700      0.6181900      0.5469800
35401 Vibrational harmonic frequencies (cm-1):
35402      i3023.6752      58.6285      76.4407
35403      106.6328      159.8953      185.8095
35404      210.7662      222.1386      243.8209
35405      270.1109      304.9916      337.7685
35406      357.3791      374.6817      386.1302
35407      426.8197      465.1996      489.2484
35408      544.2589      576.4304      687.7203
35409      780.4329      845.2874      902.9137
35410      929.1370      955.7337      985.0454
35411      1008.1585      1045.6741      1057.5693
35412      1099.7128      1115.8735      1139.1297
35413      1146.2336      1189.5304      1221.0343
35414      1257.1725      1301.7797      1332.0455
35415      1384.4268      1401.8491      1413.8870
35416      1423.9620      1437.7367      1464.7486
35417      1483.3297      1487.8811      1504.3484
35418      1862.0807      2964.3559      3058.8305
35419      3083.9765      3096.0406      3158.3933
35420      3160.9081      3184.1800      3768.3420
35421 Zero-point correction (Hartree): 0.150670
35422
35423 TS.diHPCARP_Ib.16OOHHshift.a.lmppdd
35424 -----
35425 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14571010
35426 Electronic state : 2-A
35427 Cartesian coordinates (Angs):
35428      O      -3.104845      0.072259      0.043028
35429      H      -2.437080      1.014961      -0.011551
35430      O      -1.428430      1.651246      -0.145399
35431      O      -2.270439      -0.878856      0.543278
35432      O      -0.790753      1.018473      -1.169222
35433      C      -1.329848      -1.266991      -0.464808
35434      C      -0.247453      -0.240253      -0.732827
35435      H      -1.884670      -1.475399      -1.380320
35436      H      -0.870137      -2.181930      -0.091267
35437      H      0.298109      -0.577659      -1.614503
35438      C      0.809644      -0.080864      0.381609
35439      C      0.289805      -0.083693      1.817377
35440      H      -0.225786      -1.018424      2.025030
35441      H      -0.402159      0.737948      1.977982
35442      H      1.137748      0.006571      2.495062
35443      C      1.604085      1.209867      0.202179
35444      O      1.665687      -1.211058      0.335360
35445      O      2.794511      1.223421      0.046736
35446      H      1.021873      2.142060      0.278031
35447      O      2.327662      -1.278173      -0.919314
35448      H      3.057565      -0.655028      -0.775383
35449 Rotational constants (GHz):      1.6219100      0.6904400      0.6175500
35450 Vibrational harmonic frequencies (cm-1):
35451      i3074.7644      52.9379      91.0018
35452      120.8301      177.3818      200.3594
35453      247.2955      247.4279      261.1817
35454      293.9558      306.5570      319.8375
35455      344.8425      367.7805      386.3990
35456      471.7595      501.1437      523.9561
35457      551.2090      617.4250      692.0910
35458      810.0041      840.3617      872.3671
35459      928.7944      945.5071      963.0464
35460      996.3334      1049.8153      1055.4951
35461      1065.8383      1077.7433      1147.5713
35462      1149.5276      1165.4066      1240.8569
35463      1263.3476      1312.6594      1364.5897
35464      1391.8254      1402.7323      1405.3609
35465      1420.1576      1438.4606      1463.0082
35466      1473.5625      1488.0055      1506.6080
35467      1852.1792      3019.1796      3082.8598
35468      3083.9999      3118.9105      3145.2377
35469      3161.4398      3183.4800      3740.0501
35470 Zero-point correction (Hartree): 0.151274

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35471
35472 TS.diHPCARP_Ib.16OOHshift.a.lmtmdd
35473 -----
35474 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14292643
35475 Electronic state : 2-A
35476 Cartesian coordinates (Angs):
35477 O -3.123046 -0.124331 0.273016
35478 H -2.493888 0.816502 0.502571
35479 O -1.524228 1.526717 0.505036
35480 O -2.208632 -1.131483 0.301093
35481 O -1.003709 1.352038 -0.741142
35482 C -1.390474 -1.065887 -0.870953
35483 C -0.377537 0.063420 -0.858187
35484 H -2.047496 -0.967956 -1.736125
35485 H -0.863024 -2.018760 -0.907357
35486 H 0.060274 0.106939 -1.857769
35487 C 0.812647 -0.108282 0.113269
35488 C 0.486061 -0.660827 1.496138
35489 H 0.026661 -1.642498 1.404771
35490 H -0.200852 -0.002299 2.020520
35491 H 1.405800 -0.761158 2.067867
35492 C 1.518801 1.237341 0.272306
35493 O 1.629318 -1.000390 -0.633446
35494 O 2.605582 1.454646 -0.187093
35495 H 0.980762 1.991384 0.870342
35496 O 2.807412 -1.297454 0.093575
35497 H 3.373196 -0.554683 -0.168576
35498 Rotational constants (GHz): 1.6737500 0.6822800 0.5820200
35499 Vibrational harmonic frequencies (cm-1):
35500 i3051.3862 53.7156 78.2832
35501 117.1621 173.8607 189.2607
35502 211.3698 247.8840 256.4576
35503 282.6385 308.2148 340.2596
35504 345.6288 364.1608 380.4232
35505 463.5497 482.2553 506.4013
35506 567.1303 614.1030 691.1986
35507 829.2076 838.7442 853.3330
35508 930.7502 943.1997 960.0547
35509 1006.7395 1048.6632 1059.2187
35510 1064.2795 1079.1191 1148.2788
35511 1150.5575 1169.3156 1231.5238
35512 1269.5783 1314.3302 1366.0113
35513 1384.0631 1402.0382 1406.1471
35514 1416.9809 1440.5869 1464.6157
35515 1476.6687 1487.3749 1503.5667
35516 1856.1141 3007.1318 3081.2492
35517 3092.7165 3097.7775 3147.5282
35518 3168.5587 3183.7184 3752.9108
35519 Zero-point correction (Hartree): 0.151058
35520
35521 TS.diHPCARP_Ib.16OOHshift.a.mmpmuu
35522 -----
35523 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14267110
35524 Electronic state : 2-A
35525 Cartesian coordinates (Angs):
35526 O -3.105063 -0.214679 -0.117409
35527 H -2.619031 0.760223 -0.523623
35528 O -1.756986 1.554972 -0.749827
35529 O -2.421357 -0.463837 1.031335
35530 O -0.661296 0.778738 -0.957162
35531 C -1.103482 -0.932832 0.714762
35532 C -0.214598 0.219903 0.293328
35533 H -1.178107 -1.696545 -0.058691
35534 H -0.741428 -1.372738 1.642118
35535 H -0.260466 1.012617 1.043264
35536 C 1.255026 -0.160361 0.071115
35537 C 1.877258 -0.753150 1.325670
35538 H 1.504097 -1.762226 1.486995
35539 H 1.656047 -0.132780 2.192342
35540 H 2.956666 -0.798793 1.194514
35541 C 1.372015 -1.133390 -1.104673
35542 O 1.982277 0.967223 -0.396982

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35543	O	1.068889	-2.287246	-1.005649	
35544	H	1.747547	-0.697653	-2.044679	
35545	O	1.939668	1.986249	0.588686	
35546	H	1.448299	2.675515	0.122616	
35547	Rotational constants (GHz): 1.2944500 0.7249000 0.6027900				
35548	Vibrational harmonic frequencies (cm-1):				
35549	i3006.5019		31.6525		91.8805
35550	97.4051		116.9508		171.6496
35551	203.5124		217.4396		231.2951
35552	254.2666		287.1925		311.3792
35553	320.6979		349.7094		392.1628
35554	450.6971		453.8285		463.7457
35555	532.0845		578.4138		665.6365
35556	689.0587		854.1967		896.0245
35557	916.7245		977.1865		1001.0302
35558	1018.0136		1052.4690		1055.3329
35559	1102.0838		1116.4115		1145.4190
35560	1152.1421		1173.8190		1214.7339
35561	1269.9070		1306.2637		1321.2361
35562	1376.8442		1398.2854		1415.4876
35563	1416.7205		1427.8660		1464.9605
35564	1492.3274		1493.3344		1504.0070
35565	1868.3042		3009.6979		3080.7221
35566	3091.1961		3102.1976		3161.1959
35567	3162.7222		3170.4421		3806.0547
35568	Zero-point correction (Hartree): 0.150191				
35569					
35570	TS.diHPCARP_Ib.1600HHshift.a.mttmuu				
35571	-----				
35572	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14257450				
35573	Electronic state : 2-A				
35574	Cartesian coordinates (Angs):				
35575	O	-3.175453	0.080748	0.637935	
35576	H	-2.880368	-0.630504	-0.241326	
35577	O	-2.184765	-1.152151	-1.051961	
35578	O	-2.404955	1.183061	0.434500	
35579	O	-0.982573	-1.241014	-0.422816	
35580	C	-1.044079	0.877668	0.759155	
35581	C	-0.391036	0.067399	-0.343951	
35582	H	-1.018608	0.348131	1.710673	
35583	H	-0.557180	1.848890	0.856038	
35584	H	-0.535629	0.556602	-1.310281	
35585	C	1.114610	-0.120958	-0.135322	
35586	C	1.699342	-1.105172	-1.137316	
35587	H	1.483830	-0.755126	-2.145106	
35588	H	1.254943	-2.087583	-0.997323	
35589	H	2.778986	-1.164160	-1.020298	
35590	C	1.779146	1.249310	-0.288583	
35591	O	1.255166	-0.547599	1.216042	
35592	O	1.790811	1.841804	-1.328393	
35593	H	2.235213	1.656075	0.630789	
35594	O	2.642967	-0.660316	1.497297	
35595	H	2.761330	-1.618074	1.532103	
35596	Rotational constants (GHz): 1.4400700 0.6106100 0.5846700				
35597	Vibrational harmonic frequencies (cm-1):				
35598	i3025.0592		55.3763		60.0857
35599	96.4448		120.1502		176.8357
35600	199.1196		217.5931		226.7811
35601	253.7087		276.6948		301.7725
35602	322.8974		341.0251		366.8818
35603	417.5610		452.7992		475.3276
35604	542.0894		630.3609		650.0442
35605	688.5928		837.2700		901.5702
35606	954.3280		971.0061		990.7074
35607	1004.9372		1048.2462		1055.9803
35608	1103.6903		1117.5523		1140.8087
35609	1147.5304		1180.1037		1233.3951
35610	1247.0911		1301.0792		1331.1163
35611	1376.6203		1392.4883		1403.2477
35612	1408.9248		1426.9832		1461.1944
35613	1488.8739		1490.9850		1504.5773
35614	1868.6660		2991.8113		3086.5755

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35615          3087.6311          3092.0409          3151.3190
35616          3165.9173          3174.5489          3816.0329
35617 Zero-point correction (Hartree): 0.149965
35618
35619 TS.diHPCARP_Ib.1600HHshift.b.cpmuu
35620 -----
35621 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14283615
35622 Electronic state : 2-A
35623 Cartesian coordinates (Angs):
35624 O          2.985100          -0.325693          -0.621504
35625 H          2.552292          0.779910          -0.573678
35626 O          1.826676          1.675514          -0.306547
35627 O          2.390482          -0.940681          0.430230
35628 O          0.945376          1.084424          0.536288
35629 C          1.035999          -1.266081          0.104257
35630 C          0.255590          0.025380          -0.153101
35631 H          0.674096          -1.787746          0.987927
35632 H          1.006189          -1.937300          -0.753333
35633 H          0.237426          0.291738          -1.207128
35634 C          -1.174316          -0.036981          0.396488
35635 C          -1.254633          0.181189          1.900406
35636 H          -0.885763          1.172869          2.149217
35637 H          -0.654032          -0.560679          2.424058
35638 H          -2.289521          0.084028          2.225975
35639 C          -2.085224          0.971908          -0.295812
35640 O          -1.720553          -1.332033          0.193988
35641 O          -1.699291          1.892089          -0.950551
35642 H          -3.163010          0.782516          -0.119344
35643 O          -1.674850          -1.574864          -1.215566
35644 H          -2.565702          -1.907881          -1.377820
35645 Rotational constants (GHz): 1.3629100          0.7284200          0.6147200
35646 Vibrational harmonic frequencies (cm-1):
35647 i2731.3130          49.6510          74.6897
35648 83.7517          119.2017          132.0393
35649 178.0615          202.9559          234.2036
35650 247.0596          261.0674          317.2981
35651 325.5326          347.2735          392.5647
35652 423.6097          443.6582          537.3985
35653 559.2996          627.6557          658.1753
35654 683.3223          813.8100          839.6154
35655 924.7080          944.6353          960.5181
35656 989.3763          1024.1542          1043.1505
35657 1074.9144          1124.6038          1144.7322
35658 1168.9150          1198.1126          1230.7129
35659 1271.1329          1283.6160          1352.5108
35660 1375.7796          1391.3068          1408.9340
35661 1412.4790          1417.0239          1485.4951
35662 1493.9706          1503.8183          1703.8167
35663 1885.7934          2944.2315          3079.0575
35664 3098.8254          3140.3687          3152.7204
35665 3161.5855          3175.3316          3837.0266
35666 Zero-point correction (Hartree): 0.150257
35667
35668 TS.diHPCARP_Ib.1600HHshift.b.cptpuu
35669 -----
35670 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14581985
35671 Electronic state : 2-A
35672 Cartesian coordinates (Angs):
35673 O          3.299481          -0.450946          0.084203
35674 H          2.955048          0.634858          -0.127943
35675 O          2.211463          1.579871          -0.300565
35676 O          2.132141          -1.081095          0.367402
35677 O          1.060876          1.176814          0.289428
35678 C          1.250607          -0.987470          -0.762058
35679 C          0.371123          0.247269          -0.560363
35680 H          0.652677          -1.896257          -0.782889
35681 H          1.856302          -0.922507          -1.662388
35682 H          0.142438          0.732239          -1.511928
35683 C          -0.947750          -0.060378          0.171143
35684 C          -0.744551          -0.722128          1.527878
35685 H          -0.159870          -0.074613          2.178770
35686 H          -0.212502          -1.664220          1.410232

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35687	H	-1.709766	-0.924452	1.985727	
35688	C	-1.716337	1.245638	0.350602	
35689	O	-1.609639	-0.894632	-0.759933	
35690	O	-2.734184	1.484824	-0.238332	
35691	H	-1.285519	1.959218	1.072338	
35692	O	-2.872677	-1.272477	-0.242344	
35693	H	-3.417039	-0.520735	-0.523994	
35694	Rotational constants (GHz):		1.7854300	0.6215700	0.5336200
35695	Vibrational harmonic frequencies (cm-1):				
35696	i2713.4066		54.1320		71.0229
35697	96.6447		163.2494		172.6174
35698	215.2804		244.7156		247.8725
35699	292.7068		307.1127		323.1529
35700	347.5663		369.1738		415.8833
35701	433.9379		486.3694		512.4998
35702	551.2070		679.0410		700.9122
35703	730.9166		818.6761		837.6356
35704	888.2842		932.0581		943.9957
35705	1000.3218		1009.1970		1041.9866
35706	1061.4988		1120.7444		1151.3830
35707	1168.0269		1183.4308		1243.5194
35708	1269.5898		1289.9659		1349.0010
35709	1380.1819		1388.7148		1411.3724
35710	1418.7320		1442.2003		1481.9947
35711	1495.2230		1507.3247		1703.4123
35712	1856.1588		3006.4428		3085.0382
35713	3085.2537		3113.1597		3163.2274
35714	3170.4192		3171.8590		3749.7302
35715	Zero-point correction (Hartree): 0.151170				
35716	TS.diHPCARP_Ib.16OOHHshift.b.ctmmuu				
35717	-----				
35718	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14234660				
35719	Electronic state : 2-A				
35720	Cartesian coordinates (Angs):				
35721	O	-2.902834	-0.526813	0.629863	
35722	H	-2.699104	0.601267	0.338989	
35723	O	-2.130389	1.552720	-0.111681	
35724	O	-2.218556	-1.224120	-0.308028	
35725	O	-1.107628	0.954457	-0.773903	
35726	C	-0.814880	-1.256862	-0.007359	
35727	C	-0.329476	0.175900	0.158573	
35728	H	-0.385768	-1.730987	-0.884303	
35729	H	-0.626779	-1.856483	0.884301	
35730	H	-0.561432	0.542766	1.157056	
35731	C	1.155875	0.436856	-0.077439	
35732	C	1.426204	1.933080	-0.210971	
35733	H	0.945166	2.468043	0.605965	
35734	H	1.016654	2.289617	-1.153014	
35735	H	2.498190	2.123136	-0.191478	
35736	C	1.986951	-0.084172	1.089690	
35737	O	1.661496	-0.124044	-1.280330	
35738	O	1.544218	-0.333633	2.171595	
35739	H	3.066067	-0.162541	0.861290	
35740	O	1.838608	-1.529057	-1.064742	
35741	H	2.719638	-1.659702	-1.435956	
35742	Rotational constants (GHz):		1.3531500	0.6898600	0.6431200
35743	Vibrational harmonic frequencies (cm-1):				
35744	i2784.3816		38.7017		86.9220
35745	93.4988		148.7503		177.7063
35746	191.5378		221.9597		228.1481
35747	249.2757		277.0457		312.2470
35748	328.0332		355.4002		369.4238
35749	430.6304		442.1196		552.9291
35750	563.6196		611.0080		657.2880
35751	679.0516		860.9387		875.3967
35752	924.4060		939.9510		970.1677
35753	990.8982		1010.7017		1042.1741
35754	1081.8812		1115.4299		1145.1441
35755	1163.0902		1189.1302		1237.8248
35756	1263.4672		1289.1015		1346.1617
35757	1382.5862		1394.1796		1406.6898

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35759      1411.3453      1428.9891      1486.5995
35760      1491.0473      1499.3814      1709.2877
35761      1875.3648      2968.2863      3078.2999
35762      3092.4703      3127.2454      3158.8404
35763      3170.1493      3187.4694      3833.5913
35764 Zero-point correction (Hartree): 0.150730
35765
35766 TS.diHPCARP_Ib.1600HHshift.b.ctmpuu
35767 -----
35768 IRC pathway available
35769 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17410582
35770 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05124181
35771 T1 diagnostic: 0.026314
35772 E(MP2/Aug-CC-pVTZ) (Hartree): -721.00693352
35773 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02339975
35774 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01692166
35775 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02909117
35776 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47822259
35777 E(UHF/Aug-CC-pVTZ) (Hartree): -718.46416604
35778 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14793026
35779 Electronic state : 2-A
35780 Cartesian coordinates (Angs):
35781 O -2.957723 -0.615950 0.043411
35782 H -2.741040 0.540369 0.147681
35783 O -2.127619 1.558067 0.229527
35784 O -1.715810 -1.119783 -0.161968
35785 O -0.942363 1.261581 -0.354835
35786 C -0.853437 -0.766144 0.937480
35787 C -0.110229 0.513592 0.548748
35788 H -0.181425 -1.601784 1.105218
35789 H -1.481922 -0.616224 1.811112
35790 H 0.083839 1.112161 1.440485
35791 C 1.218285 0.347726 -0.200029
35792 C 1.870203 1.703289 -0.463678
35793 H 2.000287 2.241040 0.473613
35794 H 1.237409 2.284906 -1.130173
35795 H 2.841382 1.559527 -0.934244
35796 C 2.190228 -0.485139 0.621801
35797 O 1.094145 -0.228008 -1.485447
35798 O 2.104407 -0.619972 1.809421
35799 H 3.010896 -0.927508 0.029416
35800 O 0.738460 -1.597403 -1.337716
35801 H -0.207702 -1.580696 -1.548186
35802 Rotational constants (GHz): 1.4011800 0.7385800 0.6834600
35803 Vibrational harmonic frequencies (cm-1):
35804 i2801.4260 53.4554 104.4611
35805 115.5478 154.3504 183.3853
35806 208.7136 234.2809 250.6498
35807 281.3538 303.9326 309.8606
35808 336.6736 365.9242 407.6262
35809 476.4493 513.5066 537.1908
35810 567.0210 627.4932 684.0817
35811 729.6372 781.1643 831.0229
35812 927.4084 935.6122 961.1983
35813 980.8914 1028.3928 1049.0352
35814 1057.9260 1110.5563 1152.2659
35815 1167.7344 1179.9890 1248.4595
35816 1264.1891 1289.8994 1345.0084
35817 1387.2299 1394.2264 1399.7055
35818 1414.8769 1428.6459 1489.2908
35819 1494.2305 1502.1754 1700.0288
35820 1864.3957 2989.3826 3079.0303
35821 3095.9506 3127.6246 3159.6612
35822 3169.2639 3190.8343 3758.2856
35823 Zero-point correction (Hartree): 0.151273
35824
35825 TS.diHPCARP_Ib.1600HHshift.b.ctmpuu
35826 -----
35827 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14432800
35828 Electronic state : 2-A
35829 Cartesian coordinates (Angs):
35830 O 3.039052 0.517789 -0.022104

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35831	H	2.656948	-0.283274	0.734457			
35832	O	1.910821	-1.059878	1.272624			
35833	O	2.141156	0.445785	-1.034823			
35834	O	0.849726	-1.063565	0.429938			
35835	C	0.920558	1.084397	-0.645898			
35836	C	0.218006	0.232848	0.423574			
35837	H	0.339597	1.113820	-1.566183			
35838	H	1.127473	2.094044	-0.298691			
35839	H	0.326317	0.657201	1.420251			
35840	C	-1.261951	-0.006091	0.123099			
35841	C	-1.960026	-0.802208	1.218674			
35842	H	-1.951214	-0.228579	2.144832			
35843	H	-1.450579	-1.747739	1.378915			
35844	H	-2.989519	-1.004728	0.927610			
35845	C	-1.978845	1.335044	0.008099			
35846	O	-1.439155	-0.574930	-1.168589			
35847	O	-1.519609	2.361259	0.420175			
35848	H	-2.976449	1.275380	-0.460143			
35849	O	-1.280683	-1.982550	-1.130073			
35850	H	-0.319491	-2.091350	-1.183515			
35851	Rotational constants (GHz):				1.2914200	0.7508400	0.6285800
35852	Vibrational harmonic frequencies (cm-1):						
35853	i2604.1195			13.6535		72.0416	
35854	96.1291			139.7276		144.3795	
35855	205.1615			216.3958		240.8323	
35856	270.4577			331.7132		335.6618	
35857	350.7551			373.6173		380.2734	
35858	420.2675			448.1573		475.5163	
35859	573.4852			646.0807		684.0853	
35860	695.7922			785.7600		828.5242	
35861	921.5695			933.3619		961.8253	
35862	990.8841			1005.9364		1059.4072	
35863	1077.9803			1115.3095		1155.4806	
35864	1165.9299			1187.4355		1225.6623	
35865	1274.5175			1295.7303		1348.0503	
35866	1356.3399			1395.9348		1406.5207	
35867	1416.1543			1447.9920		1483.9650	
35868	1486.2664			1498.9900		1702.7450	
35869	1864.3222			2997.0139		3079.8913	
35870	3105.7525			3124.8398		3155.3541	
35871	3167.5598			3180.9195		3767.1010	
35872	Zero-point correction (Hartree):				0.150553		
35873							
35874	TS.diHPCARP_Ib.1600HHshift.b.cttmuu						
35875	-----						
35876	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14204303						
35877	Electronic state : 2-A						
35878	Cartesian coordinates (Angs):						
35879	O	-3.115573	0.584212	-0.021547			
35880	H	-2.786826	-0.372683	-0.638948			
35881	O	-2.100425	-1.266408	-1.023052			
35882	O	-2.366327	0.507080	1.105061			
35883	O	-1.065945	-1.211553	-0.146425			
35884	C	-1.031493	0.949455	0.843451			
35885	C	-0.426010	0.072536	-0.252971			
35886	H	-0.520718	0.807340	1.792926			
35887	H	-1.035454	2.004795	0.563927			
35888	H	-0.641081	0.465833	-1.245669			
35889	C	1.090905	-0.109223	-0.156223			
35890	C	1.595523	-1.058285	-1.230422			
35891	H	1.374721	-0.637958	-2.209678			
35892	H	1.102812	-2.023071	-1.131564			
35893	H	2.673116	-1.180833	-1.148827			
35894	C	1.719733	1.278081	-0.306568			
35895	O	1.331954	-0.581334	1.163410			
35896	O	1.714614	1.873944	-1.344611			
35897	H	2.155084	1.699248	0.616570			
35898	O	2.738601	-0.650232	1.349946			
35899	H	2.891221	-1.603724	1.355410			
35900	Rotational constants (GHz):				1.4524100	0.6190100	0.5973600
35901	Vibrational harmonic frequencies (cm-1):						
35902	i2750.0840			51.3479		57.7382	

35903	68.9438	107.9551	174.6525		
35904	188.4146	218.8819	235.7284		
35905	265.2025	285.8599	315.7378		
35906	336.9485	344.9586	368.3055		
35907	430.7158	443.3146	476.6784		
35908	613.9762	635.2602	662.1849		
35909	677.2821	827.4714	848.9410		
35910	894.0684	967.9090	975.2635		
35911	994.7434	1006.7034	1049.2702		
35912	1088.2446	1119.2124	1143.1443		
35913	1166.1789	1203.5823	1233.9732		
35914	1247.6809	1288.3369	1350.2682		
35915	1373.7229	1391.9157	1403.3361		
35916	1409.3509	1420.4408	1491.6645		
35917	1492.7734	1505.3324	1704.5285		
35918	1867.5600	2989.4936	3079.4356		
35919	3085.5154	3121.6345	3163.4818		
35920	3165.8494	3171.8787	3816.0928		
35921	Zero-point correction (Hartree): 0.150403				
35922					
35923	TS.diHPCARP_Ib.1600HHshift.b.hpmmuu				
35924	-----				
35925	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14765579				
35926	Electronic state : 2-A				
35927	Cartesian coordinates (Angs):				
35928	O	-3.058434	0.396605	-0.645843	
35929	H	-2.639052	-0.685156	-0.790245	
35930	O	-1.905252	-1.632784	-0.682127	
35931	O	-2.482269	0.813766	0.508730	
35932	O	-1.049829	-1.210518	0.281903	
35933	C	-1.122285	1.189992	0.267324	
35934	C	-0.339365	-0.046093	-0.180193	
35935	H	-0.775754	1.562947	1.228381	
35936	H	-1.075851	1.987846	-0.472261	
35937	H	-0.294902	-0.109748	-1.265878	
35938	C	1.075883	-0.098788	0.426934	
35939	C	1.077916	-0.508616	1.893494	
35940	H	0.734925	-1.535246	1.999783	
35941	H	0.422188	0.137750	2.473328	
35942	H	2.091035	-0.421350	2.281879	
35943	C	1.908749	-1.094048	-0.366189	
35944	O	1.660147	1.184325	0.393918	
35945	O	2.937445	-0.803285	-0.910024	
35946	H	1.496065	-2.118048	-0.414963	
35947	O	1.643727	1.657335	-0.946835	
35948	H	2.471686	1.282772	-1.286033	
35949	Rotational constants (GHz): 1.5553000			0.6492500	0.5836300
35950	Vibrational harmonic frequencies (cm-1):				
35951	i2703.3470	49.5519		76.2671	
35952	99.6217	134.6088		188.5704	
35953	198.5686	243.0967		254.1133	
35954	282.7966	315.4145		320.0495	
35955	363.5443	368.3798		414.5090	
35956	457.8655	469.4419		482.0837	
35957	557.4464	646.9860		678.4941	
35958	750.6520	813.1538		848.6480	
35959	905.4131	928.9111		969.1658	
35960	988.6970	1024.0576		1046.7747	
35961	1072.4051	1124.9423		1146.8319	
35962	1165.4356	1189.4120		1238.7974	
35963	1278.1261	1293.6804		1356.7647	
35964	1361.6326	1403.6668		1415.5856	
35965	1417.4861	1427.0943		1484.7307	
35966	1494.8908	1505.3531		1698.1619	
35967	1860.6288	2982.8669		3083.4493	
35968	3105.0941	3120.1615		3161.4761	
35969	3167.6552	3170.7213		3754.1558	
35970	Zero-point correction (Hartree): 0.151175				
35971					
35972	TS.diHPCARP_Ib.1600HHshift.b.hptpuu				
35973	-----				
35974	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14453395				


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35975 Electronic state : 2-A
35976 Cartesian coordinates (Angs):
35977 O 3.206216 -0.288355 -0.656671
35978 H 2.820984 0.790376 -0.421631
35979 O 2.092575 1.664018 -0.029583
35980 O 2.514666 -1.070132 0.208565
35981 O 1.154959 0.959692 0.651846
35982 C 1.179275 -1.259719 -0.269017
35983 C 0.453734 0.091460 -0.255617
35984 H 0.741737 -1.963648 0.434031
35985 H 1.199016 -1.702242 -1.263413
35986 H 0.477706 0.560736 -1.239089
35987 C -0.998781 -0.008694 0.240878
35988 C -1.101969 -0.288719 1.734844
35989 H -0.706691 0.550311 2.304450
35990 H -0.539147 -1.181546 1.998784
35991 H -2.144590 -0.445791 1.999200
35992 C -1.689460 1.309883 -0.079326
35993 O -1.517536 -1.050740 -0.562350
35994 O -2.612422 1.399137 -0.840902
35995 H -1.280286 2.195325 0.438468
35996 O -2.877855 -1.273143 -0.234319
35997 H -3.310348 -0.592597 -0.774059
35998 Rotational constants (GHz): 1.7021000 0.6077500 0.5303300
35999 Vibrational harmonic frequencies (cm-1):
36000 i2679.0693 41.8397 70.4996
36001 92.7467 139.7259 161.2205
36002 208.2266 237.7827 255.6135
36003 292.4552 311.2769 327.5649
36004 360.1200 373.6457 418.9045
36005 440.7095 469.9511 498.3118
36006 546.8696 647.5822 676.0602
36007 761.4552 807.7475 837.1595
36008 897.2922 926.2240 968.2397
36009 1004.1737 1018.3350 1036.6434
36010 1088.2851 1121.9990 1146.9020
36011 1165.3915 1188.2482 1251.6200
36012 1274.2376 1286.3607 1353.8695
36013 1365.8872 1405.0533 1414.8925
36014 1416.6669 1446.1804 1484.9941
36015 1493.5193 1508.8309 1698.0935
36016 1858.4712 2987.2222 3088.0361
36017 3106.0865 3110.2092 3163.3967
36018 3173.1199 3176.2339 3746.6624
36019 Zero-point correction (Hartree): 0.151154
36020
36021 TS.diHPCARP_Ib.16OOHHshift.b.htpmuu
36022 -----
36023 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14715237
36024 Electronic state : 2-A
36025 Cartesian coordinates (Angs):
36026 O -2.919211 -0.265675 -0.568569
36027 H -2.670774 -0.269442 0.587462
36028 O -2.021408 -0.236597 1.585222
36029 O -1.696933 -0.060873 -1.122378
36030 O -0.874743 0.366835 1.189477
36031 C -0.797540 -1.107830 -0.707601
36032 C -0.029308 -0.576064 0.500980
36033 H -0.139711 -1.310910 -1.549066
36034 H -1.390974 -1.987700 -0.476344
36035 H 0.243688 -1.377495 1.188395
36036 C 1.228467 0.193173 0.098078
36037 C 1.830300 0.997673 1.243835
36038 H 2.006888 0.346734 2.099396
36039 H 1.151662 1.793747 1.533454
36040 H 2.774521 1.437508 0.924411
36041 C 2.292459 -0.797134 -0.373344
36042 O 1.024710 0.978653 -1.068649
36043 O 2.264996 -1.970103 -0.136232
36044 H 3.116255 -0.326048 -0.937126
36045 O 0.272494 2.139151 -0.761086
36046 H -0.637057 1.823571 -0.884552

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36047 Rotational constants (GHz): 1.3697700 0.7428700 0.6902500
36048 Vibrational harmonic frequencies (cm-1):
36049 i2748.0039 63.0001 92.7107
36050 101.1698 159.7371 161.0972
36051 212.3399 243.6934 250.0186
36052 269.1606 318.3312 331.1942
36053 365.3860 395.1259 403.4717
36054 447.9665 455.6648 510.1413
36055 567.0205 658.1488 686.4754
36056 735.6190 794.6567 841.5047
36057 915.4296 931.0607 962.7378
36058 979.4786 1021.4144 1042.2387
36059 1062.5346 1107.7512 1141.8312
36060 1162.4931 1180.6365 1225.8392
36061 1267.5410 1283.7201 1348.6239
36062 1378.1239 1388.3635 1401.9493
36063 1412.6048 1464.6686 1485.2245
36064 1493.0381 1503.0573 1703.3818
36065 1867.2754 2993.1565 3077.0858
36066 3106.7772 3120.3074 3149.9893
36067 3180.4208 3186.1562 3738.5730
36068 Zero-point correction (Hartree): 0.151150
36069
36070 TS.diHPCARP_Ib.1600HHshift.b.lmppdd
36071 -----
36072 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14703738
36073 Electronic state : 2-A
36074 Cartesian coordinates (Angs):
36075 O 3.263198 0.241081 0.191878
36076 H 2.668949 -0.748533 0.191498
36077 O 1.756368 -1.538319 0.042369
36078 O 2.422661 1.085257 -0.457130
36079 O 1.005916 -1.001939 -0.954091
36080 C 1.155767 1.124199 0.216699
36081 C 0.250667 0.135339 -0.505328
36082 H 0.763469 2.133505 0.119910
36083 H 1.310305 0.888425 1.267008
36084 H -0.060608 0.582401 -1.448925
36085 C -0.997619 -0.260972 0.310848
36086 C -0.733711 -1.220277 1.463582
36087 H 0.031290 -0.826014 2.127716
36088 H -0.399882 -2.185190 1.089371
36089 H -1.659706 -1.346752 2.022890
36090 C -2.011453 -0.904700 -0.621685
36091 O -1.537793 0.897983 0.916501
36092 O -3.124529 -0.483914 -0.775778
36093 H -1.652576 -1.801379 -1.158416
36094 O -1.819900 1.859252 -0.092737
36095 H -2.710514 1.586790 -0.363834
36096 Rotational constants (GHz): 1.6800100 0.6523300 0.5664900
36097 Vibrational harmonic frequencies (cm-1):
36098 i2882.6230 56.8364 84.1106
36099 112.7194 144.1780 195.5535
36100 244.3116 249.2814 268.5593
36101 282.3300 298.9292 314.1875
36102 332.2410 369.2419 387.9837
36103 472.8501 493.1415 516.5434
36104 540.7053 681.1687 689.3367
36105 732.0806 825.4777 835.3946
36106 882.4680 927.6087 968.3684
36107 988.5973 1008.9078 1046.2649
36108 1063.2392 1113.3572 1143.1927
36109 1167.7906 1191.3381 1237.8089
36110 1279.2650 1291.6203 1348.0752
36111 1373.7276 1403.7924 1413.2537
36112 1419.0328 1426.1881 1484.5349
36113 1488.7536 1501.8106 1694.3719
36114 1857.7506 2980.8835 3082.5479
36115 3113.9006 3118.3191 3161.1582
36116 3173.6515 3178.9229 3753.6918
36117 Zero-point correction (Hartree): 0.151296
36118

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36119 TS.diHPCARP_Ib.16OOHHshift.b.mmpmuu
36120 -----
36121 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14311819
36122 Electronic state : 2-A
36123 Cartesian coordinates (Angs):
36124 O -3.004631 0.136558 0.541950
36125 H -2.534237 0.955552 -0.165771
36126 O -1.729930 1.495230 -0.867391
36127 O -2.365928 -1.001426 0.177880
36128 O -0.805770 0.514873 -1.021537
36129 C -1.059011 -1.045564 0.761858
36130 C -0.263952 0.162216 0.265987
36131 H -0.641978 -1.982353 0.396608
36132 H -1.140061 -1.065143 1.849167
36133 H -0.397154 1.022268 0.919675
36134 C 1.235815 -0.085551 0.100515
36135 C 1.846331 -0.570785 1.404271
36136 H 1.471152 -1.564451 1.643240
36137 H 1.607698 0.118278 2.212147
36138 H 2.927712 -0.626874 1.296331
36139 C 1.477853 -1.086152 -1.032530
36140 O 1.875534 1.083590 -0.393700
36141 O 1.365461 -2.268060 -0.877818
36142 H 1.752538 -0.640089 -2.001980
36143 O 1.710113 2.136709 0.542730
36144 H 1.173334 2.758035 0.033070
36145 Rotational constants (GHz): 1.2778600 0.7583900 0.6080700
36146 Vibrational harmonic frequencies (cm-1):
36147 i2720.5182 49.1992 67.0180
36148 96.0858 130.9733 162.6045
36149 210.2727 217.9097 232.3658
36150 278.9623 295.4953 308.7643
36151 323.8195 335.0077 402.6888
36152 447.4882 461.4322 470.8511
36153 556.4577 617.5856 674.7312
36154 691.8068 840.3012 846.8074
36155 910.4318 920.0077 982.3175
36156 997.8154 1021.6803 1053.2999
36157 1083.2701 1126.9467 1150.6389
36158 1168.1466 1193.5435 1219.3045
36159 1272.7436 1296.7908 1341.5174
36160 1378.6890 1398.2707 1416.6052
36161 1417.6066 1420.1287 1488.6683
36162 1497.8184 1502.6512 1704.6303
36163 1867.0373 3011.8764 3080.8376
36164 3086.9755 3124.5317 3158.6128
36165 3163.0944 3164.5965 3807.9378
36166 Zero-point correction (Hartree): 0.150695

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36167
36168 TS.diHPCARP_Ib.16OOHHshift.b.pptpdd
36169 -----
36170 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14402391
36171 Electronic state : 2-A
36172 Cartesian coordinates (Angs):
36173 O 3.080038 0.015618 0.481711
36174 H 2.246171 -0.708314 0.852411
36175 O 1.206715 -1.325790 0.859754
36176 O 2.635375 0.359713 -0.752093
36177 O 0.855981 -1.377100 -0.448243
36178 C 1.346734 0.977933 -0.638689
36179 C 0.308508 -0.121001 -0.872237
36180 H 1.293043 1.742444 -1.410849
36181 H 1.263620 1.437936 0.344832
36182 H 0.157076 -0.286435 -1.939956
36183 C -1.055027 0.184812 -0.243792
36184 C -1.563270 1.525395 -0.752796
36185 H -1.530284 1.553439 -1.841992
36186 H -0.962994 2.335532 -0.343900
36187 H -2.586845 1.678289 -0.418014
36188 C -0.980810 0.174484 1.286954
36189 O -1.869127 -0.898278 -0.670993
36190 O -0.698303 1.153343 1.917708

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36191	H	-1.218670	-0.792016	1.756199	
36192	O	-3.120726	-0.780636	-0.005038	
36193	H	-3.717546	-0.585582	-0.737816	
36194	Rotational constants (GHz):		1.6241800	0.6529700	0.6367700
36195	Vibrational harmonic frequencies (cm-1):				
36196	i2734.4520		61.3088		93.4151
36197	119.5443		140.3348		164.7144
36198	214.9609		232.9790		261.8103
36199	280.6985		290.1050		311.4754
36200	347.4428		350.8809		389.4695
36201	416.2448		455.3377		517.3599
36202	602.4865		645.0194		685.7355
36203	707.2745		790.5161		836.8151
36204	881.0352		956.4551		982.5937
36205	999.2294		1011.1914		1042.9721
36206	1065.6814		1113.3764		1152.3440
36207	1165.3253		1200.4800		1216.1378
36208	1262.6264		1301.1573		1329.2985
36209	1384.3594		1393.4949		1400.1734
36210	1405.8832		1416.4347		1484.6142
36211	1497.0838		1509.8599		1700.1499
36212	1858.9597		3028.2316		3075.6013
36213	3102.8007		3103.9353		3156.7321
36214	3163.8727		3166.1894		3823.9633
36215	Zero-point correction (Hartree): 0.150970				
36216	TS.diHPCARP_Ib.1600HHshift.b.pttpdd				
36217	-----				
36218	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14196055				
36219	Electronic state : 2-A				
36220	Cartesian coordinates (Angs):				
36221	O	-3.141754	-0.186313	-0.583683	
36222	H	-2.478868	-0.950216	-0.003730	
36223	O	-1.570547	-1.393406	0.656864	
36224	O	-2.507461	0.988689	-0.341754	
36225	O	-1.096925	-0.306422	1.316535	
36226	C	-1.145049	0.892020	-0.777084	
36227	C	-0.318795	0.532972	0.454576	
36228	H	-0.857326	1.869573	-1.162614	
36229	H	-1.083393	0.146909	-1.565072	
36230	H	-0.165614	1.419515	1.070381	
36231	C	1.075768	-0.033777	0.153316	
36232	C	1.693946	-0.647165	1.401919	
36233	H	1.104123	-1.506289	1.715490	
36234	H	1.697098	0.091903	2.201109	
36235	H	2.719746	-0.951667	1.208831	
36236	C	1.942377	1.120818	-0.351700	
36237	O	0.911684	-0.973670	-0.903315	
36238	O	2.091677	2.131475	0.274664	
36239	H	2.413426	0.961372	-1.336392	
36240	O	2.192606	-1.494386	-1.233607	
36241	H	2.127078	-2.398043	-0.899793	
36242	Rotational constants (GHz):		1.4271100	0.6735200	0.6017400
36243	Vibrational harmonic frequencies (cm-1):				
36244	i2788.0047		46.7909		50.1772
36245	76.6853		116.3788		168.2713
36246	199.3539		221.6505		234.1632
36247	261.8661		274.4386		307.4164
36248	319.8323		361.9691		384.5562
36249	398.3485		463.1253		512.7093
36250	600.2206		634.4920		685.0346
36251	710.6430		781.3145		844.9679
36252	888.0562		953.8329		972.0200
36253	993.9582		1005.8238		1042.9888
36254	1070.7308		1113.0882		1147.8957
36255	1162.3026		1204.5075		1219.8032
36256	1244.0259		1295.1893		1336.1039
36257	1388.6022		1395.5991		1407.8455
36258	1409.2019		1412.3805		1487.0768
36259	1495.1038		1505.1585		1701.8397
36260	1860.8235		3003.6637		3083.0649
36261	3102.6705		3119.0211		3164.4435
36262					

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36263          3169.3676          3174.1834          3818.7973
36264 Zero-point correction (Hartree): 0.150367
36265
36266
36267
36268 1,4-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-
36269 di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde
36270 =====
36271 =====
36272
36273 TS.diHPCARP_I.14HPHshift.mmmmmmtu
36274 -----
36275 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13090445
36276 Electronic state : 2-A
36277 Cartesian coordinates (Angs):
36278 C -0.057038 0.006780 -0.817354
36279 C -0.749506 -0.442537 0.501879
36280 O -2.136828 -0.239864 0.234361
36281 O -2.327055 -0.691590 -1.067431
36282 H -1.132846 -0.346189 -1.457162
36283 C -0.470969 -1.899726 0.846996
36284 C -0.397215 0.460457 1.666986
36285 H 0.582708 -2.049612 1.064629
36286 H -0.775315 -2.533443 0.015748
36287 H -1.066506 -2.170175 1.717726
36288 O 0.739878 0.707661 1.962802
36289 H -1.251232 0.852922 2.241818
36290 O 0.164333 1.351917 -0.956611
36291 O -0.880625 2.107028 -0.378100
36292 H -1.660344 1.866731 -0.906204
36293 C 1.161765 -0.732338 -1.323104
36294 O 2.151600 -0.911930 -0.335814
36295 H 0.880655 -1.742365 -1.619677
36296 H 1.573232 -0.200132 -2.181979
36297 O 2.747347 0.345201 -0.066327
36298 H 2.258231 0.619059 0.729650
36299 Rotational constants (GHz): 1.252900 0.8241300 0.8025700
36300 Vibrational harmonic frequencies (cm-1):
36301 i2059.6381 101.4178 114.8649
36302 129.6978 156.2149 174.7404
36303 201.3135 221.9456 228.2900
36304 258.4473 259.8273 287.9813
36305 325.3766 342.8900 359.8927
36306 429.9216 439.7325 464.9919
36307 492.0457 570.5918 620.1203
36308 673.9404 701.4260 823.8126
36309 913.9744 924.4282 971.1942
36310 981.1492 993.2655 1042.6418
36311 1060.8016 1115.3645 1132.7053
36312 1170.1512 1177.1432 1226.3537
36313 1250.4607 1313.9838 1348.0059
36314 1389.3118 1395.7374 1408.2879
36315 1449.6160 1465.5374 1480.3630
36316 1497.0819 1503.0011 1733.5766
36317 1851.4865 3016.6178 3079.7570
36318 3083.9780 3142.3493 3153.7203
36319 3183.9738 3685.6318 3725.2874
36320 Zero-point correction (Hartree): 0.150920
36321
36322 TS.diHPCARP_I.14HPHshift.mmmmmptu
36323 -----
36324 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12864494
36325 Electronic state : 2-A
36326 Cartesian coordinates (Angs):
36327 C 0.071735 -0.757316 -0.339217
36328 C 0.662302 0.680955 -0.198489
36329 O 2.067915 0.462709 -0.327585
36330 O 2.203363 -0.438124 -1.376951
36331 H 1.078240 -1.038142 -1.116867
36332 C 0.165668 1.630573 -1.279004
36333 C 0.452572 1.262873 1.187067
36334 H -0.902095 1.805398 -1.184746

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36335	H	0.385587	1.208546	-2.258316	
36336	H	0.701208	2.574028	-1.184428	
36337	O	-0.640639	1.406619	1.663223	
36338	H	1.367279	1.567110	1.719120	
36339	O	0.099077	-1.535265	0.786878	
36340	O	1.213054	-1.243844	1.603660	
36341	H	1.974145	-1.505041	1.059311	
36342	C	-1.236270	-1.052817	-1.045726	
36343	O	-2.372564	-0.858889	-0.237970	
36344	H	-1.310044	-0.472718	-1.965474	
36345	H	-1.257361	-2.115942	-1.288398	
36346	O	-2.640239	0.531679	-0.159131	
36347	H	-2.172734	0.792076	0.655025	
36348	Rotational constants (GHz):			1.2163200	0.8151200 0.7928700
36349	Vibrational harmonic frequencies (cm-1):				
36350	i2082.2806		87.1301		119.7583
36351	135.5539		146.8397		162.0385
36352	218.3483		229.9158		235.3658
36353	258.8317		268.2631		296.7532
36354	344.2826		357.9615		361.3552
36355	414.9847		438.7728		468.3852
36356	502.2899		591.2440		615.0344
36357	678.2995		708.5789		788.1133
36358	919.6909		936.1954		967.8758
36359	989.2886		1005.0547		1042.6153
36360	1060.4548		1107.7848		1134.4907
36361	1167.4649		1172.0551		1220.8136
36362	1243.9723		1308.2205		1345.5207
36363	1391.6231		1400.2989		1411.6399
36364	1449.3270		1463.5690		1486.7666
36365	1497.5583		1505.5091		1733.2917
36366	1849.8223		3026.8101		3080.5948
36367	3087.8417		3140.0164		3153.8077
36368	3188.5774		3659.5590		3731.5083
36369	Zero-point correction (Hartree):			0.151060	
36370	TS.diHPCARP_I.14HPHshift.mmtmtu				
36371	-----				
36372	-----				
36373	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.12961510	
36374	Electronic state : 2-A				
36375	Cartesian coordinates (Angs):				
36376	C	-0.052635	-0.055276	-0.819371	
36377	C	-0.783803	-0.384878	0.518509	
36378	O	-2.160428	-0.220199	0.201512	
36379	O	-2.305695	-0.799091	-1.049333	
36380	H	-1.146041	-0.418351	-1.453009	
36381	C	-0.510976	-1.802292	1.013127	
36382	C	-0.462214	0.620405	1.601090	
36383	H	0.535844	-1.932493	1.270938	
36384	H	-0.797187	-2.512949	0.240064	
36385	H	-1.130586	-1.986117	1.889817	
36386	O	0.667741	0.906512	1.897363	
36387	H	-1.330951	1.059337	2.117795	
36388	O	0.253694	1.259169	-1.032229	
36389	O	-0.854113	2.058460	-0.638328	
36390	H	-0.428014	2.925258	-0.607919	
36391	C	1.144602	-0.876956	-1.240665	
36392	O	2.121999	-1.008701	-0.230689	
36393	H	0.830499	-1.898530	-1.451816	
36394	H	1.583712	-0.437696	-2.137583	
36395	O	2.733245	0.254140	-0.027393	
36396	H	2.221339	0.593203	0.728347	
36397	Rotational constants (GHz):			1.2330900	0.8337900 0.8007700
36398	Vibrational harmonic frequencies (cm-1):				
36399	i2225.4768		96.5391		110.2530
36400	135.8624		151.7360		173.6191
36401	199.2638		219.4642		228.2562
36402	232.1447		255.7113		265.2491
36403	288.2041		329.9518		357.0001
36404	427.9664		443.1302		464.1246
36405	485.8548		571.9481		615.4679
36406	675.3565		701.2291		815.8672

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36407          911.5975          927.3508          972.4514
36408          978.7983          997.5371         1045.0018
36409         1062.1531         1109.6650         1134.5109
36410         1163.9628         1169.8235         1216.5729
36411         1245.3692         1312.5554         1333.4039
36412         1388.1953         1395.8114         1409.0613
36413         1463.4247         1469.3262         1488.2514
36414         1498.0835         1505.6477         1739.3242
36415         1844.0682          3013.5482         3080.7938
36416         3085.0088          3143.1595         3154.6489
36417         3187.7879          3674.0849         3824.3504
36418 Zero-point correction (Hartree): 0.150791
36419
36420 TS.diHPCARP_I.14HPHshift.mmtmptu
36421 -----
36422 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12734186
36423 Electronic state : 2-A
36424 Cartesian coordinates (Angs):
36425 C      -0.042780      0.464932      -0.683954
36426 C      -0.719864     -0.663593      0.162326
36427 O     -2.105609     -0.499854     -0.118470
36428 O     -2.168242     -0.277406     -1.482966
36429 H     -1.071819      0.385977     -1.504132
36430 C     -0.256771     -2.061987     -0.229348
36431 C     -0.565139     -0.438693      1.651099
36432 H      0.801754     -2.198657     -0.028836
36433 H     -0.457292     -2.219420     -1.287715
36434 H     -0.834832     -2.789177      0.339214
36435 O      0.507667     -0.302205      2.177540
36436 H     -1.504285     -0.425557      2.227084
36437 O      0.061284      1.685929     -0.084074
36438 O     -1.130702      1.960808      0.637444
36439 H     -0.807157      2.652992      1.229401
36440 C      1.251987      0.255365     -1.443415
36441 O      2.407396      0.475015     -0.666284
36442 H      1.269506     -0.735908     -1.895319
36443 H      1.314999      1.009593     -2.228607
36444 O      2.577790     -0.625657      0.212007
36445 H      2.087853     -0.349030      1.007100
36446 Rotational constants (GHz): 1.1970200      0.8134300      0.8062200
36447 Vibrational harmonic frequencies (cm-1):
36448 i2237.1827          80.4587          117.9043
36449          135.6791          147.3978          162.9357
36450          204.5143          222.6393          230.7862
36451          245.9268          258.3553          266.9806
36452          289.8392          344.7895          353.3192
36453          419.6661          436.2964          466.6811
36454          494.7445          573.4826          610.5166
36455          677.9652          709.9560          775.2322
36456          921.4301          938.3908          967.5850
36457          988.5597         1004.9278         1042.0405
36458         1063.7994         1099.2924         1136.9417
36459         1159.5856         1163.8076         1209.1198
36460         1240.8753         1307.7947         1334.4875
36461         1386.8707         1395.9957         1407.8402
36462         1461.2520         1473.6611         1480.9008
36463         1496.7920         1504.9499         1740.4967
36464         1843.5513         3014.4506         3079.8847
36465         3090.2208         3142.2401         3153.3628
36466         3187.5400         3665.9813         3820.4875
36467 Zero-point correction (Hartree): 0.150703
36468
36469 TS.diHPCARP_I.14HPHshift.mtmmtu
36470 -----
36471 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.15903610
36472 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.03764431
36473 T1 diagnostic: 0.023133
36474 E(MP2/Aug-CC-pVTZ) (Hartree): -720.99481796
36475 E(MP3/Aug-CC-pVTZ) (Hartree): -721.01271484
36476 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.00319930
36477 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.01781574
36478 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.46662690

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36479 E(UHF/Aug-CC-pVTZ) (Hartree): -718.45511364
36480 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13181197
36481 Electronic state : 2-A
36482 Cartesian coordinates (Angs):
36483 C -0.031985 -0.694737 0.225079
36484 C -1.122201 0.372127 -0.038746
36485 O -2.225889 -0.415003 -0.474853
36486 O -2.268455 -1.466341 0.432185
36487 H -0.975644 -1.541246 0.538056
36488 C -1.471007 1.196193 1.195653
36489 C -0.786651 1.308836 -1.183251
36490 H -0.611015 1.776080 1.523457
36491 H -1.804345 0.532055 1.990582
36492 H -2.288864 1.871893 0.948629
36493 O 0.268021 1.876359 -1.276742
36494 H -1.597233 1.468591 -1.913319
36495 O 0.498781 -1.019455 -1.001422
36496 O 1.605802 -1.887305 -0.891945
36497 H 2.327128 -1.243232 -0.776192
36498 C 0.934492 -0.507113 1.365890
36499 O 1.661690 0.705580 1.264810
36500 H 0.380999 -0.410983 2.298556
36501 H 1.609974 -1.357436 1.441359
36502 O 2.449179 0.660450 0.081929
36503 H 1.910085 1.218155 -0.510579
36504 Rotational constants (GHz): 1.2334600 0.8488500 0.7450400
36505 Vibrational harmonic frequencies (cm-1):
36506 i2169.3637 92.1431 123.7076
36507 146.3281 159.8384 178.4332
36508 204.6434 223.9154 241.1041
36509 270.8954 281.1459 287.4919
36510 332.3000 347.8811 383.4876
36511 448.7193 474.0700 530.7006
36512 547.9169 568.8958 656.2126
36513 698.2433 731.3739 828.8801
36514 915.1477 919.9682 959.7425
36515 985.3282 991.6548 1033.6418
36516 1049.9230 1099.2042 1147.8118
36517 1160.6812 1206.2664 1214.7878
36518 1252.2064 1323.6660 1329.4398
36519 1388.1125 1394.1240 1410.4964
36520 1465.9793 1478.6423 1481.8446
36521 1497.1978 1506.5335 1744.4510
36522 1852.6529 3007.6948 3077.7474
36523 3106.1297 3153.4390 3157.4495
36524 3174.4548 3636.7253 3691.1154
36525 Zero-point correction (Hartree): 0.151664
36526
36527 TS.diHPCARP_I.14HPHshift.mtmmptu
36528 -----
36529 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12885758
36530 Electronic state : 2-A
36531 Cartesian coordinates (Angs):
36532 C 0.010342 -0.696504 -0.238054
36533 C 1.092966 0.390639 -0.002768
36534 O 2.261905 -0.393230 0.218939
36535 O 2.230410 -1.347856 -0.786843
36536 H 0.945536 -1.459011 -0.750160
36537 C 1.259012 1.337068 -1.182776
36538 C 0.874656 1.169166 1.283145
36539 H 0.362597 1.936986 -1.322853
36540 H 1.463750 0.760785 -2.083249
36541 H 2.107406 1.992456 -0.991888
36542 O -0.114858 1.818773 1.489442
36543 H 1.695715 1.113444 2.015905
36544 O -0.354133 -1.145643 1.009651
36545 O -1.375066 -2.119856 0.929839
36546 H -2.171271 -1.566452 0.980249
36547 C -1.137712 -0.533331 -1.207585
36548 O -2.253641 0.086159 -0.596115
36549 H -0.827410 0.022323 -2.090968
36550 H -1.495579 -1.515818 -1.511015

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36551      O      -2.033753      1.487301      -0.568921
36552      H      -1.563240      1.627887      0.274271
36553      Rotational constants (GHz):      1.1446700      0.8684500      0.7209400
36554      Vibrational harmonic frequencies (cm-1):
36555      i2189.7022      88.8550      99.3974
36556      115.5456      127.4620      160.3383
36557      203.0423      223.4002      247.3478
36558      259.8374      279.2860      285.7003
36559      341.3113      361.2283      372.0064
36560      422.2433      463.3068      479.4788
36561      519.9656      554.2104      609.6289
36562      695.6218      743.4542      799.1278
36563      917.0945      940.6570      958.9969
36564      984.0772      1000.2025      1035.4991
36565      1045.8997      1101.8262      1146.5636
36566      1156.2199      1188.4190      1216.6637
36567      1242.6256      1319.1519      1328.0616
36568      1388.8972      1397.1766      1409.3648
36569      1445.9231      1468.6888      1493.6520
36570      1499.5553      1503.6642      1746.5710
36571      1851.7351      3015.4915      3078.2102
36572      3104.9941      3154.6490      3157.2458
36573      3173.7803      3627.3475      3743.3625
36574      Zero-point correction (Hartree): 0.151029
36575
36576
36577
36578      1,5-alpha-hydroperoxide-H-shift in (2R,3R)-2-Me-3,4-diOOH-butanal-2-peroxyl (A, R,R-
36579      di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde
36580      =====
36581      =====
36582
36583      TS.diHPCARP_I.15HPHshift.dcmdpddd
36584      -----
36585      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13693901
36586      Electronic state : 2-A
36587      Cartesian coordinates (Angs):
36588      O      -1.092450      0.523504      1.322983
36589      O      -0.220170      -0.366588      1.945396
36590      H      0.757208      -0.405801      1.127203
36591      C      1.095169      -0.586229      -0.111756
36592      C      0.006113      0.206600      -0.797734
36593      C      -1.312029      0.067647      -0.006078
36594      C      -2.419333      0.932414      -0.584217
36595      H      -2.609720      0.638814      -1.614994
36596      H      -2.120332      1.978360      -0.566719
36597      H      -3.331063      0.809268      -0.001725
36598      C      -1.795198      -1.375056      0.041718
36599      O      -1.618012      -2.152911      -0.851796
36600      H      -2.366373      -1.629981      0.951746
36601      H      -0.162803      -0.174155      -1.808449
36602      O      0.347480      1.563313      -0.984645
36603      O      0.894186      2.100044      0.214060
36604      H      0.116831      2.202779      0.783285
36605      H      0.982701      -1.666564      -0.203208
36606      O      2.340066      -0.147635      -0.459137
36607      O      3.279721      -1.103781      0.002595
36608      H      3.838645      -0.552546      0.565623
36609      Rotational constants (GHz):      1.2493100      0.7589500      0.6408800
36610      Vibrational harmonic frequencies (cm-1):
36611      i1789.7801      62.8435      92.8482
36612      98.4569      126.9578      171.6251
36613      175.0618      203.1200      205.3339
36614      238.2172      256.3937      295.0948
36615      311.0919      330.0237      340.3445
36616      386.3039      400.3141      448.1929
36617      491.7130      550.4239      600.9992
36618      633.8374      783.3223      822.7039
36619      914.8418      938.4010      965.8881
36620      975.4062      993.4958      1032.3936
36621      1064.1759      1103.9788      1147.6507
36622      1183.1163      1220.1572      1235.1655

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36623      1249.6711      1289.6035      1333.8006
36624      1347.2843      1394.4505      1396.3660
36625      1408.6895      1430.2071      1450.5982
36626      1490.1347      1496.0163      1596.9279
36627      1864.3258      2990.8991      3078.5377
36628      3086.5108      3119.5202      3159.0860
36629      3165.8348      3764.4050      3816.3567
36630      Zero-point correction (Hartree): 0.149742
36631
36632      TS.diHPCARP_I.15HPHshift.dcmumddd
36633      -----
36634      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13688071
36635      Electronic state : 2-A
36636      Cartesian coordinates (Angs):
36637      O      -0.894867      0.401898      1.440475
36638      O      -0.525274      -0.870018      1.855528
36639      H      0.441900      -1.086186      1.136173
36640      C      0.829908      -1.160706      -0.132269
36641      C      0.112463      0.040022      -0.745496
36642      C      -1.169712      0.346673      0.047379
36643      C      -1.793496      1.677488      -0.335997
36644      H      -1.957622      1.707465      -1.411762
36645      H      -1.125905      2.485337      -0.049748
36646      H      -2.746967      1.798788      0.176481
36647      C      -2.200351      -0.757173      -0.178620
36648      O      -2.244497      -1.436630      -1.163952
36649      H      -2.936821      -0.845895      0.639302
36650      H      -0.199237      -0.237814      -1.757514
36651      O      0.943914      1.159446      -0.959532
36652      O      1.176554      1.853376      0.257675
36653      H      1.828260      1.284847      0.700626
36654      H      0.351086      -2.099362      -0.408391
36655      O      2.167669      -1.346568      -0.371864
36656      O      2.939794      -0.273438      0.154021
36657      H      3.166089      0.210465      -0.653956
36658      Rotational constants (GHz):      1.3375500      0.7782800      0.6852700
36659      Vibrational harmonic frequencies (cm-1):
36660      i2004.0665      68.8906      84.6595
36661      129.3029      158.6128      190.2791
36662      208.5212      222.4274      243.6435
36663      263.9149      274.4623      289.6374
36664      332.3293      369.0059      395.3486
36665      430.7177      442.0526      457.2431
36666      562.6764      581.1776      597.0277
36667      650.5493      794.0125      817.6332
36668      901.1424      935.3981      959.1006
36669      979.5079      987.2119      1010.3766
36670      1062.2914      1081.0383      1146.5256
36671      1188.6672      1194.4827      1241.1630
36672      1245.1152      1290.8337      1313.7902
36673      1363.4937      1387.5979      1395.5484
36674      1407.5874      1425.9469      1452.0379
36675      1483.6857      1506.1911      1575.4098
36676      1864.1747      2992.3690      3066.5694
36677      3080.2589      3137.5619      3156.1118
36678      3181.4520      3698.9737      3781.5043
36679      Zero-point correction (Hartree): 0.150489
36680
36681      TS.diHPCARP_I.15HPHshift.dcmumudd
36682      -----
36683      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13587523
36684      Electronic state : 2-A
36685      Cartesian coordinates (Angs):
36686      O      -0.799243      0.268862      1.480575
36687      O      -0.430990      -1.039560      1.761703
36688      H      0.459387      -1.206797      0.955703
36689      C      0.836198      -1.130097      -0.320219
36690      C      0.067159      0.106293      -0.790853
36691      C      -1.163422      0.333495      0.107894
36692      C      -1.812979      1.687022      -0.119959
36693      H      -2.033900      1.811113      -1.178676
36694      H      -1.132879      2.471949      0.198732

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36695	H	-2.737882	1.754539	0.451531	
36696	C	-2.204166	-0.755989	-0.140807	
36697	O	-2.295457	-1.374095	-1.162626	
36698	H	-2.901932	-0.897943	0.703368	
36699	H	-0.319888	-0.117197	-1.790382	
36700	O	0.850535	1.251522	-1.003346	
36701	O	1.168297	1.881844	0.227884	
36702	H	1.991075	1.426630	0.462570	
36703	H	0.402857	-2.048116	-0.715653	
36704	O	2.187630	-1.224971	-0.549091	
36705	O	2.900254	-0.245221	0.194927	
36706	H	3.288214	-0.785564	0.896252	
36707	Rotational constants (GHz):		1.3290300	0.7806700	0.6865600
36708	Vibrational harmonic frequencies (cm-1):				
36709	i1967.7751		49.8767		78.1264
36710	124.2293		158.4921		172.4188
36711	205.9607		223.6857		236.5595
36712	260.1714		270.3605		274.6845
36713	300.6672		335.5177		391.6854
36714	429.6220		450.8963		454.4801
36715	471.6590		578.8771		595.0667
36716	643.8642		794.2263		802.2430
36717	900.1439		934.5428		954.7634
36718	974.9777		987.2355		1012.2097
36719	1057.7240		1081.1205		1148.2032
36720	1181.4776		1196.2084		1237.6184
36721	1242.8167		1273.6504		1292.2207
36722	1369.3113		1380.7891		1396.2121
36723	1408.4653		1413.1784		1459.4849
36724	1482.7625		1506.2282		1573.0695
36725	1864.3715		2988.1126		3063.3571
36726	3079.9157		3132.2071		3155.9197
36727	3182.0927		3753.2749		3804.7460
36728	Zero-point correction (Hartree):		0.149885		
36729					
36730	TS.diHPCARP_I.15HPHshift.dcmupddd				
36731	-----				
36732	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13736498				
36733	Electronic state : 2-A				
36734	Cartesian coordinates (Angs):				
36735	O	-0.939722	0.070175	1.492049	
36736	O	-0.247276	-1.113377	1.707140	
36737	H	0.683757	-0.969058	0.922301	
36738	C	1.089255	-0.664514	-0.293397	
36739	C	-0.007760	0.281271	-0.759052	
36740	C	-1.274095	0.127331	0.117282	
36741	C	-2.226953	1.297106	-0.054161	
36742	H	-2.444760	1.443112	-1.110469	
36743	H	-1.762583	2.197090	0.341912	
36744	H	-3.153875	1.102152	0.483340	
36745	C	-1.999453	-1.167225	-0.241137	
36746	O	-1.940007	-1.688419	-1.317881	
36747	H	-2.625117	-1.563859	0.577731	
36748	H	-0.304908	0.012890	-1.776551	
36749	O	0.422291	1.613050	-0.889583	
36750	O	0.785173	2.117865	0.388957	
36751	H	1.744226	1.991911	0.377860	
36752	H	1.084652	-1.643473	-0.771718	
36753	O	2.326840	-0.060030	-0.329607	
36754	O	3.314619	-1.049485	-0.112084	
36755	H	3.517299	-0.932809	0.826441	
36756	Rotational constants (GHz):		1.2582400	0.7449000	0.6367900
36757	Vibrational harmonic frequencies (cm-1):				
36758	i1911.2977		38.4684		80.8783
36759	92.9040		143.4990		157.2924
36760	169.8200		211.9688		221.2556
36761	236.1172		257.0241		295.6381
36762	306.8053		322.9677		356.4284
36763	371.3456		404.0303		456.7667
36764	507.6214		551.6480		616.4141
36765	620.0566		783.4895		809.5037
36766	925.3738		942.8453		973.5205

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36767      983.6084      1005.1343      1036.4063
36768      1079.4622      1096.6779      1153.1177
36769      1192.0528      1199.0839      1235.8336
36770      1239.7762      1296.6702      1300.9069
36771      1364.5299      1376.2136      1396.6519
36772      1408.1200      1423.0154      1427.0194
36773      1483.0473      1500.1256      1575.3583
36774      1864.1293      2994.7678      3078.9757
36775      3082.6144      3120.3148      3158.4245
36776      3172.7369      3794.2459      3796.8238
36777      Zero-point correction (Hartree): 0.149652
36778
36779      TS.diHPCARP_I.15HPHshift.dcmupudd
36780      -----
36781      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13729439
36782      Electronic state : 2-A
36783      Cartesian coordinates (Angs):
36784      O      -0.978833      0.120404      1.481201
36785      O      -0.259173      -1.034539      1.749329
36786      H      0.694362      -0.888994      0.993832
36787      C      1.086708      -0.665411      -0.247534
36788      C      -0.001358      0.265653      -0.755080
36789      C      -1.283198      0.126314      0.099207
36790      C      -2.243995      1.279316      -0.131638
36791      H      -2.446041      1.383944      -1.195974
36792      H      -1.793741      2.197251      0.238779
36793      H      -3.177827      1.095808      0.397832
36794      C      -1.984694      -1.188344      -0.231720
36795      O      -1.905233      -1.737341      -1.293604
36796      H      -2.612655      -1.573245      0.590946
36797      H      -0.278947      -0.019763      -1.773639
36798      O      0.438055      1.594038      -0.897415
36799      O      0.778428      2.116653      0.379490
36800      H      1.721241      1.902745      0.434152
36801      H      1.054440      -1.677663      -0.650865
36802      O      2.325677      -0.076857      -0.358368
36803      O      3.288283      -1.019670      0.091934
36804      H      3.900760      -1.026772      -0.655021
36805      Rotational constants (GHz):      1.2633800      0.7444300      0.6388800
36806      Vibrational harmonic frequencies (cm-1):
36807      i1964.0771      46.3038      85.4482
36808      97.3125      140.1680      153.3982
36809      174.2346      183.1080      217.6548
36810      233.3072      255.0600      296.4078
36811      309.1299      321.7880      363.1736
36812      389.7387      414.0222      452.9791
36813      495.3200      552.6972      612.0351
36814      621.3738      784.6148      810.4750
36815      925.6727      941.8560      974.6027
36816      982.5586      1002.3992      1038.0593
36817      1080.0908      1099.2020      1151.9198
36818      1190.4786      1196.6362      1238.0447
36819      1239.7052      1299.2942      1310.1652
36820      1364.5314      1380.1119      1396.0654
36821      1407.5644      1424.2091      1432.3391
36822      1483.0324      1499.8753      1570.4458
36823      1862.7412      2995.1386      3078.8755
36824      3080.8375      3113.2285      3158.6617
36825      3173.0734      3781.8631      3819.6364
36826      Zero-point correction (Hartree): 0.149682
36827
36828      TS.diHPCARP_I.15HPHshift.dcmutudd
36829      -----
36830      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13711440
36831      Electronic state : 2-A
36832      Cartesian coordinates (Angs):
36833      O      -1.151745      0.441699      1.367991
36834      O      -0.812204      -0.788065      1.901499
36835      H      0.230522      -0.985069      1.380734
36836      C      0.953218      -1.012365      0.233432
36837      C      0.195115      -0.001783      -0.613244
36838      C      -1.208609      0.300336      -0.041517

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36839	C	-1.797847	1.586107	-0.593387		
36840	H	-1.780436	1.557407	-1.681256		
36841	H	-1.207245	2.430307	-0.246788		
36842	H	-2.825992	1.699512	-0.252434		
36843	C	-2.151448	-0.859197	-0.359677		
36844	O	-2.035330	-1.564108	-1.319905		
36845	H	-2.983620	-0.962751	0.358637		
36846	H	0.030983	-0.408009	-1.615802		
36847	O	0.977440	1.153297	-0.843278		
36848	O	1.129126	1.882244	0.367431		
36849	H	1.840947	1.393930	0.810948		
36850	H	0.842509	-2.054980	-0.061682		
36851	O	2.250582	-0.651800	0.532700		
36852	O	3.025176	-0.819309	-0.671408		
36853	H	2.845394	0.019403	-1.126252		
36854	Rotational constants (GHz):			1.3266900	0.7435300	0.6846400
36855	Vibrational harmonic frequencies (cm-1):					
36856	i1979.5181		55.0214			85.9226
36857	124.0236		146.4916			174.8037
36858	190.3905		225.2119			232.2208
36859	274.9019		309.4886			310.5579
36860	327.6992		371.0445			411.7342
36861	432.3803		457.0153			502.2554
36862	531.2374		565.8173			597.2296
36863	626.7035		767.1331			822.6150
36864	919.1379		927.8837			938.5048
36865	969.6796		984.3007			997.6491
36866	1049.5693		1096.6244			1132.3774
36867	1155.3493		1193.3545			1207.2283
36868	1235.9754		1240.7873			1293.7443
36869	1353.5507		1364.2274			1395.4395
36870	1408.2734		1411.3674			1441.3806
36871	1483.7394		1502.9917			1558.5380
36872	1867.0586		2991.5590			3075.2611
36873	3080.6375		3124.4544			3158.8168
36874	3177.4354		3736.9862			3746.7593
36875	Zero-point correction (Hartree):			0.149818		
36876	TS.diHPCARP_I.15HPHshift.dcpdmudd					
36877	-----					
36879	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.13716142		
36880	Electronic state : 2-A					
36881	Cartesian coordinates (Angs):					
36882	O	1.024016	-0.451682	-1.458586		
36883	O	0.775980	-1.761983	-1.066036		
36884	H	-0.170339	-1.590478	-0.303534		
36885	C	-0.744490	-0.907693	0.664003		
36886	C	-0.119804	0.472894	0.454535		
36887	C	1.222284	0.320322	-0.284027		
36888	C	1.809392	1.650089	-0.725198		
36889	H	1.851143	2.332872	0.121465		
36890	H	1.181822	2.084541	-1.498643		
36891	H	2.813622	1.498145	-1.118779		
36892	C	2.240662	-0.402694	0.591444		
36893	O	2.186783	-0.441298	1.786965		
36894	H	3.066535	-0.859253	0.017790		
36895	H	0.088573	0.913702	1.435359		
36896	O	-0.889730	1.363549	-0.309450		
36897	O	-1.975907	1.803240	0.489179		
36898	H	-2.698657	1.260311	0.139848		
36899	H	-0.380503	-1.393068	1.568192		
36900	O	-2.109716	-1.061059	0.674065		
36901	O	-2.652785	-0.648089	-0.577159		
36902	H	-3.069590	-1.465699	-0.878066		
36903	Rotational constants (GHz):			1.3231200	0.7486900	0.6664000
36904	Vibrational harmonic frequencies (cm-1):					
36905	i1913.7566		49.6253			81.2956
36906	106.5191		117.2712			157.3647
36907	197.9593		212.2995			221.1865
36908	239.2081		254.3655			290.9011
36909	320.0607		336.6825			360.1262
36910	414.8734		451.9927			478.2506

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36911      492.6091      560.2058      587.5781
36912      638.9419      714.7051      874.9125
36913      890.2814      934.0576      963.0505
36914      974.6286      992.8398     1043.5674
36915     1057.1924     1079.8964     1156.8444
36916     1179.8309     1195.3463     1232.7409
36917     1247.1959     1260.9853     1302.7751
36918     1359.2219     1370.6230     1396.7354
36919     1410.2697     1420.6849     1445.7276
36920     1485.5314     1498.0451     1583.4666
36921     1866.4403     2988.5172     3051.6719
36922     3079.2267     3139.1261     3156.7879
36923     3175.9127     3767.8193     3822.2722
36924 Zero-point correction (Hartree): 0.149649
36925
36926 TS.diHPCARP_I.15HPHshift.dcpdpddd
36927 -----
36928 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13848922
36929 Electronic state : 2-A
36930 Cartesian coordinates (Angs):
36931 O      1.123490      -0.519731      -1.447069
36932 O      0.543503      -1.753112      -1.171981
36933 H     -0.443343      -1.392673      -0.516521
36934 C     -0.995390      -0.610480       0.373460
36935 C     -0.029745       0.566603       0.377126
36936 C      1.330070       0.138994      -0.209703
36937 C      2.247033       1.319192      -0.479789
36938 H      2.323227       1.937367       0.412956
36939 H      1.839368       1.917750      -1.289984
36940 H      3.237432       0.961791      -0.758333
36941 C      2.031368      -0.831610       0.735571
36942 O      1.812321      -0.892038       1.910984
36943 H      2.797955      -1.452284       0.239178
36944 H      0.143776       0.908887       1.400646
36945 O     -0.497522       1.637728      -0.409228
36946 O     -1.440068       2.368296       0.358373
36947 H     -2.270226       1.926087       0.129481
36948 H     -0.998623      -1.221534       1.275280
36949 O     -2.257421      -0.218055      -0.018305
36950 O     -3.142805      -1.306373       0.161560
36951 H     -3.261573      -1.615301      -0.747361
36952 Rotational constants (GHz):      1.1903700      0.7418800      0.6107200
36953 Vibrational harmonic frequencies (cm-1):
36954 i1863.4927      39.8588      80.8319
36955      87.8305      130.9144      154.1508
36956      179.8782      207.8774      227.1449
36957      252.7071      264.0221      287.9113
36958      310.9912      324.5567      359.4578
36959      399.7866      409.0607      451.5047
36960      510.5585      551.0625      603.3091
36961      625.7430      709.9441      865.0808
36962      931.7463      936.0590      972.5992
36963      990.7896     1038.4196     1048.2297
36964     1073.0572     1094.9476     1161.1517
36965     1179.1345     1198.6652     1235.4987
36966     1250.6479     1277.9704     1307.7897
36967     1353.1300     1365.6274     1396.0754
36968     1410.5577     1425.8326     1438.1514
36969     1485.4603     1498.1317     1577.8858
36970     1866.7366     2989.8600     3076.3466
36971     3080.0419     3125.0687     3157.7028
36972     3174.9548     3781.4565     3797.2305
36973 Zero-point correction (Hartree): 0.149747
36974
36975 TS.diHPCARP_I.15HPHshift.dcpdpudd
36976 -----
36977 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13674039
36978 Electronic state : 2-A
36979 Cartesian coordinates (Angs):
36980 O      1.186525      -0.401189      -1.466607
36981 O      0.537292      -1.622995      -1.336901
36982 H     -0.481503      -1.282403      -0.723719

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36983	C	-0.994258	-0.621283	0.287930			
36984	C	-0.033915	0.551635	0.383475			
36985	C	1.345184	0.139119	-0.167620			
36986	C	2.299833	1.314691	-0.290389			
36987	H	2.357440	1.842792	0.659736			
36988	H	1.937877	1.996662	-1.055019			
36989	H	3.291363	0.958019	-0.565876			
36990	C	1.980587	-0.922920	0.722930			
36991	O	1.726243	-1.055735	1.885657			
36992	H	2.737555	-1.536979	0.204035			
36993	H	0.097843	0.854628	1.426013			
36994	O	-0.456782	1.654726	-0.384251			
36995	O	-1.435510	2.363192	0.358496			
36996	H	-2.255221	1.978430	0.018277			
36997	H	-0.912955	-1.350958	1.094154			
36998	O	-2.285254	-0.203726	0.058916			
36999	O	-3.103796	-1.359066	-0.037977			
37000	H	-3.706720	-1.229287	0.705766			
37001	Rotational constants (GHz):				1.1854700	0.7410800	0.6114200
37002	Vibrational harmonic frequencies (cm-1):						
37003	i1932.8293		52.7047			91.4960	
37004	92.2500		135.2294			150.1755	
37005	168.0760		188.1439			198.2490	
37006	231.0804		249.7853			282.5247	
37007	307.1732		322.2171			355.2134	
37008	393.3652		400.8053			448.0818	
37009	491.1477		550.9390			596.4057	
37010	627.7033		702.4722			870.5767	
37011	926.9245		935.2016			971.0443	
37012	988.3122		1037.3749			1049.6168	
37013	1072.2348		1096.2615			1161.3338	
37014	1178.9255		1203.6675			1237.4688	
37015	1252.3252		1298.7948			1305.1941	
37016	1349.3283		1376.7681			1396.3473	
37017	1408.9588		1424.1350			1434.3126	
37018	1486.0130		1498.8132			1573.5188	
37019	1865.1899		2991.2790			3069.6438	
37020	3080.0089		3112.0532			3157.2152	
37021	3176.4074		3797.7679			3815.2915	
37022	Zero-point correction (Hartree):				0.149524		
37023	TS.diHPCARP_I.15HPHshift.dlpdtddd						
37024	-----						
37025	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13830141						
37026	Electronic state : 2-A						
37027	Cartesian coordinates (Angs):						
37028	O	0.773357	-0.988003	-1.210845			
37029	O	0.424852	-2.060616	-0.399334			
37030	H	-0.405082	-1.504082	0.322699			
37031	C	-1.037679	-0.422745	0.689646			
37032	C	0.006853	0.648171	0.407871			
37033	C	1.215706	0.054821	-0.357972			
37034	C	1.937973	1.071542	-1.226365			
37035	H	2.186817	1.949628	-0.634182			
37036	H	1.295835	1.373799	-2.049499			
37037	H	2.850127	0.628757	-1.624453			
37038	C	2.226747	-0.545008	0.619178			
37039	O	2.355146	-0.192889	1.754825			
37040	H	2.874293	-1.310095	0.156073			
37041	H	0.377057	1.049877	1.353511			
37042	O	-0.509502	1.691344	-0.389851			
37043	O	-1.506583	2.355871	0.367827			
37044	H	-2.310662	1.915054	0.056429			
37045	H	-1.346148	-0.574165	1.722452			
37046	O	-2.099085	-0.293842	-0.181011			
37047	O	-3.037092	-1.311826	0.116529			
37048	H	-2.828575	-1.969771	-0.562299			
37049	Rotational constants (GHz):				1.2148900	0.7673800	0.6125600
37050	Vibrational harmonic frequencies (cm-1):						
37051	i1854.2365		20.6444			63.1979	
37052	101.8251		125.8095			175.4205	
37053	187.7744		238.3235			241.0072	
37054							

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37055      251.1689      253.0488      293.5065
37056      314.6791      326.4798      361.7468
37057      405.2093      426.4181      468.5840
37058      540.8015      571.2142      615.5182
37059      649.8611      748.9342      834.2580
37060      927.5734      951.0832      973.3094
37061      993.5403      1040.1257     1047.1289
37062      1066.9627     1086.5697     1149.1041
37063      1180.7023     1185.4976     1195.5563
37064      1232.2513     1244.0393     1327.9105
37065      1357.7210     1378.7982     1396.0780
37066      1409.8956     1424.4026     1433.8457
37067      1484.5595     1499.0394     1608.5833
37068      1871.5960     2989.3339     3079.9979
37069      3088.4424     3127.3563     3159.4968
37070      3175.0197     3775.7416     3785.2371
37071      Zero-point correction (Hartree): 0.150045
37072
37073      TS.diHPCARP_I.15HPHshift.dmpumdud
37074      -----
37075      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13728805
37076      Electronic state : 2-A
37077      Cartesian coordinates (Angs):
37078      O      -0.299751     -1.906848      0.109667
37079      O      0.164610     -1.864268     -1.200993
37080      H      0.948535     -0.895295     -1.132138
37081      C      1.220333      0.295471     -0.690141
37082      C      0.296117      0.362662      0.506072
37083      C     -0.881136     -0.641339      0.388829
37084      C     -1.608992     -0.771126      1.717966
37085      H     -1.946898      0.212510      2.037934
37086      H     -0.922715     -1.177969      2.459422
37087      H     -2.464127     -1.439942      1.628879
37088      C     -1.934416     -0.383404     -0.677989
37089      O     -2.371717      0.694658     -0.980147
37090      H     -2.341748     -1.310813     -1.113006
37091      H      0.856361      0.030527      1.380543
37092      O     -0.106173      1.677163      0.854380
37093      O     -0.425981      2.451235     -0.290182
37094      H     -1.319647      2.131314     -0.510055
37095      H      0.957581      0.962750     -1.505656
37096      O      2.560539      0.461750     -0.468402
37097      O      2.971870     -0.473490      0.524911
37098      H      3.734048     -0.008263      0.891784
37099      Rotational constants (GHz): 1.1775100 0.8262200 0.6498000
37100      Vibrational harmonic frequencies (cm-1):
37101      i1915.7196      26.3691      67.6527
37102      105.3186      155.4183      156.9094
37103      179.9128      221.4031      233.5865
37104      249.5573      265.3337      272.3109
37105      319.8809      322.8551      413.2557
37106      422.4798      458.0346      505.3481
37107      559.9673      587.9125      604.1911
37108      617.2588      691.2407      876.4031
37109      922.1524      933.0003      953.9853
37110      975.8667      1000.3702     1019.3688
37111      1062.3875     1107.6678     1131.6682
37112      1169.2240     1200.0411     1210.8082
37113      1248.5121     1264.0464     1310.8231
37114      1363.3841     1400.1349     1401.3947
37115      1417.7392     1468.4401     1487.9225
37116      1497.4902     1503.2385     1579.2378
37117      1851.5740     3011.3569     3072.6893
37118      3114.3603     3150.0030     3167.0186
37119      3171.6577     3635.4037     3836.3926
37120      Zero-point correction (Hartree): 0.150250
37121
37122      TS.diHPCARP_I.15HPHshift.dmpumuud
37123      -----
37124      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13869336
37125      Electronic state : 2-A
37126      Cartesian coordinates (Angs):

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37127	O	0.307482	-1.738473	-0.116878		
37128	O	0.612372	-1.418483	-1.438500		
37129	H	0.997290	-0.229342	-1.299041		
37130	C	1.171210	0.820319	-0.569055		
37131	C	0.182727	0.553081	0.552281		
37132	C	-0.618562	-0.767131	0.350950		
37133	C	-1.150898	-1.268313	1.685411		
37134	H	-1.744319	-0.479686	2.145149		
37135	H	-0.309865	-1.514753	2.332208		
37136	H	-1.766893	-2.157153	1.555372		
37137	C	-1.794794	-0.784432	-0.619131		
37138	O	-2.598536	0.092298	-0.781317		
37139	H	-1.905122	-1.762053	-1.117848		
37140	H	0.763381	0.394366	1.461954		
37141	O	-0.628892	1.666718	0.864334		
37142	O	-1.115711	2.281941	-0.317579		
37143	H	-1.926127	1.768081	-0.482224		
37144	H	0.950497	1.690328	-1.179083		
37145	O	2.503404	0.867800	-0.233820		
37146	O	2.839534	-0.258020	0.557575		
37147	H	2.845833	-0.981199	-0.089743		
37148	Rotational constants (GHz):			1.2213500	0.8416800	0.6682200
37149	Vibrational harmonic frequencies (cm-1):					
37150	i1769.5216		40.4911			85.5427
37151	106.2661		166.7735			169.2942
37152	228.2946		245.8476			257.6303
37153	268.9937		283.0602			293.2940
37154	322.8887		329.6450			402.3944
37155	424.8568		465.2875			530.6413
37156	576.6787		606.9747			615.8770
37157	641.1000		690.6398			868.3413
37158	921.5442		945.2008			961.3145
37159	975.7255		1001.0682			1021.4728
37160	1067.9434		1095.4589			1140.1050
37161	1160.3383		1198.9076			1200.0330
37162	1222.6911		1258.7383			1305.4087
37163	1358.5701		1400.2593			1412.0087
37164	1422.2654		1440.8741			1484.9849
37165	1488.0758		1502.0521			1581.2785
37166	1856.9702		3007.0011			3070.2163
37167	3107.9973		3150.4004			3161.0399
37168	3182.0869		3654.0096			3744.8376
37169	Zero-point correction (Hartree):			0.150636		
37170	TS.diHPCARP_I.15HPHshift.dmpupuud					
37171	-----					
37172	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13848341					
37174	Electronic state : 2-A					
37175	Cartesian coordinates (Angs):					
37176	O	-0.861013	-1.852689	0.329847		
37177	O	-0.058136	-2.089279	-0.781645		
37178	H	0.889627	-1.291271	-0.561137		
37179	C	1.274850	-0.115669	-0.182710		
37180	C	0.127095	0.278477	0.710264		
37181	C	-1.178302	-0.470247	0.328807		
37182	C	-2.250211	-0.257158	1.385733		
37183	H	-2.422350	0.809523	1.513046		
37184	H	-1.909350	-0.683673	2.328227		
37185	H	-3.179617	-0.746081	1.096836		
37186	C	-1.791341	-0.141817	-1.023178		
37187	O	-1.816496	0.950091	-1.525285		
37188	H	-2.296136	-1.002567	-1.491566		
37189	H	0.361970	-0.069302	1.719978		
37190	O	-0.047700	1.674940	0.875462		
37191	O	0.173473	2.380311	-0.334256		
37192	H	-0.651009	2.210351	-0.824825		
37193	H	1.372134	0.426773	-1.120038		
37194	O	2.432299	-0.153885	0.550093		
37195	O	3.510795	-0.383251	-0.342756		
37196	H	4.076406	0.374811	-0.145690		
37197	Rotational constants (GHz):			1.2008900	0.7577300	0.6091300
37198	Vibrational harmonic frequencies (cm-1):					

37199	i1878.3814	36.3840	72.0573			
37200	98.3744	132.3057	161.4468			
37201	183.3691	205.5539	222.9545			
37202	244.3833	266.3023	273.4223			
37203	304.1677	331.1055	358.7506			
37204	434.9161	456.5707	511.0813			
37205	524.9147	570.9990	594.7175			
37206	633.7793	701.4251	858.7320			
37207	927.4019	946.6765	972.4828			
37208	1003.4572	1025.5712	1041.7948			
37209	1063.6391	1118.3651	1139.0024			
37210	1165.2254	1202.5828	1228.8916			
37211	1262.5513	1280.5563	1332.5539			
37212	1356.2441	1402.1486	1415.1312			
37213	1418.5423	1433.8556	1488.7097			
37214	1496.7357	1502.6894	1571.2993			
37215	1850.9913	3015.3941	3073.6495			
37216	3078.5243	3149.0358	3150.8827			
37217	3168.4043	3643.1439	3816.6047			
37218	Zero-point correction (Hartree): 0.150178					
37219						
37220	TS.diHPCARP_I.15HPHshift.dmtmdud					
37221	-----					
37222	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13828807					
37223	Electronic state : 2-A					
37224	Cartesian coordinates (Angs):					
37225	O	0.331616	-1.736685	0.251405		
37226	O	0.735000	-1.820358	-1.070940		
37227	H	1.296721	-0.733897	-1.174370		
37228	C	1.366825	0.526657	-0.857547		
37229	C	0.184957	0.687939	0.086107		
37230	C	-0.579530	-0.655404	0.370949		
37231	C	-1.078586	-0.717252	1.808318		
37232	H	-1.750743	0.114798	1.999475		
37233	H	-0.221720	-0.649615	2.477447		
37234	H	-1.595285	-1.658045	1.991535		
37235	C	-1.749809	-0.929657	-0.568736		
37236	O	-2.694691	-0.199885	-0.707094		
37237	H	-1.700710	-1.908072	-1.071464		
37238	H	0.553609	1.055968	1.045522		
37239	O	-0.611565	1.675046	-0.531841		
37240	O	-1.638340	2.062549	0.367470		
37241	H	-2.365885	1.492804	0.055964		
37242	H	1.253468	1.073602	-1.790602		
37243	O	2.604041	0.837821	-0.362584		
37244	O	2.788577	0.081202	0.831800		
37245	H	3.550301	0.541245	1.206224		
37246	Rotational constants (GHz):			1.2883500	0.7898800	0.6433300
37247	Vibrational harmonic frequencies (cm-1):					
37248	i1897.6304			43.9965		78.8055
37249	110.6377			120.3015		159.3073
37250	195.8405			226.8874		235.1239
37251	245.4542			278.8469		294.7815
37252	302.7434			333.6096		389.3079
37253	427.3365			500.8948		514.3153
37254	546.0007			574.2969		620.5491
37255	632.6512			679.4573		838.3317
37256	925.2811			946.9006		972.1730
37257	980.2889			998.6928		1043.9324
37258	1075.9990			1084.2192		1157.7181
37259	1165.2637			1203.1181		1208.0909
37260	1220.2044			1240.2129		1296.3003
37261	1363.8977			1387.0723		1401.3335
37262	1418.6292			1472.4184		1478.4943
37263	1487.7718			1501.4699		1581.3417
37264	1847.5239			3024.9056		3076.8875
37265	3090.5886			3152.0997		3155.6589
37266	3181.2811			3647.2882		3836.5307
37267	Zero-point correction (Hartree): 0.150298					
37268						
37269	TS.diHPCARP_I.15HPHshift.dmtdmud					
37270	-----					

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37271 IRC pathway available
37272 E(CCS(D(T)/Aug-CC-pVTZ) (Hartree): -721.16773798
37273 E(CCS(D(Aug-CC-pVTZ) (Hartree): -721.04662858
37274 T1 diagnostic: 0.019659
37275 E(MP2/Aug-CC-pVTZ) (Hartree): -721.00763091
37276 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02449712
37277 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01510962
37278 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02877825
37279 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47327164
37280 E(UHF/Aug-CC-pVTZ) (Hartree): -718.46257972
37281 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14099454
37282 Electronic state : 2-A
37283 Cartesian coordinates (Angs):
37284 O 0.554214 -1.635282 0.088188
37285 O 0.869512 -1.592924 -1.264351
37286 H 1.274270 -0.417365 -1.337058
37287 C 1.333025 0.768323 -0.826015
37288 C 0.112847 0.772587 0.077561
37289 C -0.460945 -0.670702 0.341937
37290 C -0.838780 -0.851193 1.804249
37291 H -1.601229 -0.121668 2.067940
37292 H 0.044522 -0.684897 2.419815
37293 H -1.216735 -1.856276 1.984218
37294 C -1.659304 -1.048844 -0.527147
37295 O -2.696613 -0.444582 -0.557243
37296 H -1.526127 -1.989720 -1.083623
37297 H 0.400387 1.193164 1.043034
37298 O -0.804391 1.631352 -0.557454
37299 O -1.823905 1.951062 0.375996
37300 H -2.502834 1.297432 0.128860
37301 H 1.275116 1.471958 -1.653148
37302 O 2.554856 0.936871 -0.221404
37303 O 2.622361 0.157458 0.959601
37304 H 2.723303 -0.745286 0.619786
37305 Rotational constants (GHz): 1.3072000 0.8059200 0.6644500
37306 Vibrational harmonic frequencies (cm-1):
37307 i1797.7005 37.9894 104.9619
37308 123.7954 154.3671 180.8218
37309 214.0793 244.8640 255.7255
37310 272.6554 293.5346 297.5978
37311 312.0626 332.9538 376.8181
37312 434.0661 500.8078 518.7620
37313 549.9621 599.8501 602.9098
37314 656.3196 691.7828 820.0155
37315 922.2341 951.8938 972.9652
37316 980.7531 1004.7804 1051.5604
37317 1078.1702 1085.5141 1161.0681
37318 1166.6132 1199.2608 1202.2805
37319 1216.7783 1236.2265 1297.3094
37320 1360.3076 1402.4818 1405.7180
37321 1420.9312 1443.3644 1477.6062
37322 1487.8160 1502.5201 1594.6741
37323 1851.5868 3026.2400 3074.3681
37324 3088.2886 3154.0194 3154.1441
37325 3169.6972 3649.0356 3758.8718
37326 Zero-point correction (Hartree): 0.150646
37327
37328 TS.diHPCARP_I.15HPHshift.dmtdpdud
37329 -----
37330 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14045600
37331 Electronic state : 2-A
37332 Cartesian coordinates (Angs):
37333 O 0.388499 -1.640100 0.296088
37334 O 0.882091 -1.615977 -1.000859
37335 H 1.301590 -0.462959 -1.026400
37336 C 1.364682 0.691161 -0.419363
37337 C 0.010742 0.766370 0.242259
37338 C -0.639974 -0.666231 0.387438
37339 C -1.269424 -0.850464 1.760202
37340 H -2.026752 -0.084342 1.911144
37341 H -0.496840 -0.746379 2.520967
37342 H -1.722895 -1.836335 1.848778

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37343	C	-1.683267	-1.006799	-0.674106	
37344	O	-2.658932	-0.347547	-0.910747	
37345	H	-1.511196	-1.975868	-1.167662	
37346	H	0.136150	1.163023	1.254411	
37347	O	-0.744548	1.667207	-0.524399	
37348	O	-1.911381	1.996050	0.212140	
37349	H	-2.546033	1.362906	-0.171920	
37350	H	1.581097	1.446539	-1.173329	
37351	O	2.327818	0.559497	0.551886	
37352	O	3.579759	0.393197	-0.087649	
37353	H	3.681866	-0.569420	-0.066252	
37354	Rotational constants (GHz):		1.3966200	0.7133100	0.5897400
37355	Vibrational harmonic frequencies (cm-1):				
37356	i1808.9510		36.6965		60.4521
37357	112.7706		160.2272		178.0417
37358	195.8868		237.8887		247.5458
37359	263.8351		276.9480		295.1320
37360	306.0853		330.6000		375.9810
37361	437.8468		471.2694		496.4133
37362	558.7791		601.1895		617.8055
37363	634.2720		716.8572		804.6341
37364	924.9705		961.9267		980.4192
37365	1004.1557		1032.7914		1063.3729
37366	1078.7872		1106.8014		1163.7899
37367	1169.8750		1179.9350		1209.5582
37368	1223.9726		1227.8290		1289.4308
37369	1357.3916		1391.5552		1402.3112
37370	1420.2228		1427.3877		1480.0754
37371	1487.5605		1501.4326		1628.5323
37372	1850.1054		3025.9883		3057.5898
37373	3074.6212		3125.2793		3153.3681
37374	3170.3190		3618.7981		3782.4883
37375	Zero-point correction (Hartree):		0.150336		
37376	TS.diHPCARP_I.15HPHshift.dppdmudd				
37377	-----				
37379	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13722840				
37380	Electronic state : 2-A				
37381	Cartesian coordinates (Angs):				
37382	O	0.809069	1.092976	1.020801	
37383	O	0.744500	2.046551	0.009087	
37384	H	-0.069057	1.508534	-0.753414	
37385	C	-0.866112	0.524022	-1.074948	
37386	C	-0.144141	-0.641540	-0.391179	
37387	C	1.080326	-0.163935	0.417481	
37388	C	1.469961	-1.114449	1.536580	
37389	H	1.578181	-2.122043	1.140501	
37390	H	0.694119	-1.118448	2.297960	
37391	H	2.411121	-0.792893	1.980670	
37392	C	2.287596	0.025319	-0.501930	
37393	O	2.435505	-0.540726	-1.544931	
37394	H	3.045589	0.711574	-0.084674	
37395	H	0.232393	-1.305711	-1.174254	
37396	O	-0.981435	-1.362029	0.478050	
37397	O	-1.993756	-1.964623	-0.311214	
37398	H	-2.720978	-1.333752	-0.208729	
37399	H	-0.914164	0.475258	-2.159434	
37400	O	-2.122205	0.863822	-0.631744	
37401	O	-2.095222	1.142457	0.760175	
37402	H	-1.594629	1.973551	0.803551	
37403	Rotational constants (GHz):		1.2704600	0.8163200	0.6900600
37404	Vibrational harmonic frequencies (cm-1):				
37405	i1839.1734		32.3923		92.2390
37406	118.3002		129.1745		173.4986
37407	201.2260		224.8149		233.6102
37408	247.8527		284.6661		297.2693
37409	329.5109		336.3706		355.1391
37410	369.6615		414.0651		471.3876
37411	554.2889		565.6162		625.5379
37412	643.5252		764.9505		824.3302
37413	909.6358		929.8885		961.6305
37414	970.3929		1002.8509		1033.4593

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37415      1052.2884          1077.7714          1151.3494
37416      1181.5051          1189.3205          1213.8508
37417      1240.5848          1249.2502          1324.3354
37418      1370.5298          1382.5225          1396.0540
37419      1409.5215          1429.4260          1454.7453
37420      1484.2655          1498.5618          1579.7610
37421      1871.6954          2988.3385          3068.2338
37422      3079.7303          3158.1186          3159.8172
37423      3174.2186          3736.1882          3782.1096
37424      Zero-point correction (Hartree): 0.149907
37425
37426      TS.diHPCARP_I.15HPHshift.dtpdmdud
37427      -----
37428      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13738405
37429      Electronic state : 2-A
37430      Cartesian coordinates (Angs):
37431      O      -0.352547      -1.415725          0.806599
37432      O      -0.483180      -0.582355          1.911021
37433      H      -1.019949          0.402273          1.357210
37434      C      -1.286762          1.038504          0.266625
37435      C      -0.171451          0.547952         -0.643969
37436      C      0.496382         -0.783444         -0.147509
37437      C      0.641878         -1.761211         -1.300627
37438      H      1.298968         -1.316680         -2.046250
37439      H      -0.335648         -1.956032         -1.739446
37440      H      1.078976         -2.697741         -0.959371
37441      C      1.862898         -0.587110          0.505566
37442      O      2.845175         -0.277001         -0.109102
37443      H      1.888541         -0.814299          1.583465
37444      H      -0.605393          0.351514         -1.625266
37445      O      0.757364          1.574343         -0.898250
37446      O      1.210277          2.067137          0.360454
37447      H      2.161604          1.910655          0.283807
37448      H      -1.241506          2.098016          0.503320
37449      O      -2.573335          0.751859         -0.126990
37450      O      -2.645121         -0.566784         -0.642324
37451      H      -2.552330         -1.117636          0.150751
37452      Rotational constants (GHz):      1.3119000          0.8265300          0.6958600
37453      Vibrational harmonic frequencies (cm-1):
37454      i1818.9208          25.5841          82.2365
37455      131.5120          134.4918          192.7086
37456      195.3972          203.9573          258.7728
37457      276.3213          290.2531          291.0145
37458      313.4890          321.2170          391.4869
37459      424.2559          441.4644          466.7558
37460      515.7510          580.9178          635.8573
37461      650.0616          690.8336          841.1429
37462      919.1363          954.5072          969.6371
37463      977.1715          994.3044          1026.4906
37464      1075.4086          1085.1553          1141.2568
37465      1164.2292          1196.7417          1201.3769
37466      1216.2035          1234.9548          1300.9093
37467      1344.8562          1397.4527          1398.3427
37468      1411.1796          1426.2603          1447.4671
37469      1488.5071          1504.6823          1598.1401
37470      1851.9263          3016.0734          3074.1625
37471      3109.5620          3158.0163          3162.7026
37472      3167.1176          3754.6022          3802.8000
37473      Zero-point correction (Hartree): 0.150192
37474
37475      TS.diHPCARP_I.15HPHshift.umpupdud
37476      -----
37477      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13543278
37478      Electronic state : 2-A
37479      Cartesian coordinates (Angs):
37480      O      0.735055          0.027167          1.511827
37481      O      -0.567465         -0.164721          1.948438
37482      H      -1.219465          0.284814          0.983405
37483      C      -1.380685          0.437265         -0.309036
37484      C      0.058136          0.345646         -0.755179
37485      C      0.891127         -0.537100          0.209505
37486      C      0.537422         -2.009978          0.146013

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37487	H	0.818000	-2.394176	-0.832845	
37488	H	-0.523349	-2.170688	0.308178	
37489	H	1.097928	-2.547124	0.909689	
37490	C	2.365701	-0.323633	-0.123328	
37491	O	2.867750	-0.798492	-1.098596	
37492	H	2.934286	0.296485	0.591858	
37493	H	0.136735	-0.075650	-1.760677	
37494	O	0.640351	1.636619	-0.853090	
37495	O	0.220579	2.444132	0.239270	
37496	H	0.740890	2.098670	0.980935	
37497	H	-1.860442	1.402800	-0.450152	
37498	O	-2.104153	-0.625398	-0.798618	
37499	O	-3.463253	-0.429105	-0.447447	
37500	H	-3.585688	-1.089947	0.247499	
37501	Rotational constants (GHz):		1.2674500	0.7152700	0.6416000
37502	Vibrational harmonic frequencies (cm-1):				
37503	i1880.3994		67.6011		75.3777
37504	87.8583		145.2640		156.0459
37505	176.6308		196.8562		205.8084
37506	225.4632		254.2593		286.8101
37507	300.3422		333.5377		360.1275
37508	389.2064		420.0853		452.9430
37509	502.9419		563.3443		612.1126
37510	672.7533		728.7188		845.2994
37511	904.5049		943.1006		951.5132
37512	993.4614		1007.5860		1034.7194
37513	1075.9525		1097.4772		1129.0057
37514	1151.8818		1199.4227		1207.8256
37515	1244.9007		1263.2367		1274.9463
37516	1316.4335		1391.1720		1400.7354
37517	1414.5929		1422.8537		1445.3758
37518	1486.8627		1499.6648		1592.5140
37519	1876.5066		2983.1760		3085.1115
37520	3087.2215		3147.6206		3160.1286
37521	3191.3232		3751.7982		3803.2221
37522	Zero-point correction (Hartree): 0.149437				
37523					
37524	TS.diHPCARP_I.15HPHshift.umpupuud				
37525	-----				
37526	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13506853				
37527	Electronic state : 2-A				
37528	Cartesian coordinates (Angs):				
37529	O	0.759449	0.068134	1.506486	
37530	O	-0.533706	-0.119231	1.970729	
37531	H	-1.209741	0.273763	0.998313	
37532	C	-1.380093	0.430311	-0.294086	
37533	C	0.053464	0.331463	-0.754196	
37534	C	0.893878	-0.534094	0.219567	
37535	C	0.520982	-2.003985	0.201851	
37536	H	0.779764	-2.417241	-0.771294	
37537	H	-0.538651	-2.146358	0.388688	
37538	H	1.089204	-2.527258	0.969569	
37539	C	2.364344	-0.347086	-0.141532	
37540	O	2.837294	-0.827131	-1.129127	
37541	H	2.959793	0.257264	0.565279	
37542	H	0.124363	-0.110415	-1.751500	
37543	O	0.636730	1.619028	-0.883580	
37544	O	0.227955	2.450923	0.194659	
37545	H	0.740207	2.107318	0.943146	
37546	H	-1.855276	1.400983	-0.416805	
37547	O	-2.107499	-0.623795	-0.790434	
37548	O	-3.427198	-0.502270	-0.273497	
37549	H	-3.949315	-0.622965	-1.076898	
37550	Rotational constants (GHz):		1.2618000	0.7175100	0.6447400
37551	Vibrational harmonic frequencies (cm-1):				
37552	i1911.1504		71.2373		75.3154
37553	89.4492		113.9289		147.3304
37554	159.9423		179.8366		203.7741
37555	211.3544		253.7117		286.5665
37556	300.9999		334.2115		363.1512
37557	391.2767		432.1267		453.9919
37558	505.1788		559.4121		607.6958

37559	673.4019	725.1229	846.4523			
37560	905.3813	944.3364	952.2138			
37561	993.3509	1007.4047	1032.3054			
37562	1075.1292	1099.5672	1128.9903			
37563	1151.4729	1195.7690	1204.4981			
37564	1241.1758	1262.5428	1275.8932			
37565	1315.6308	1392.7255	1400.9036			
37566	1414.3282	1430.5988	1448.2673			
37567	1486.8103	1501.5318	1591.2371			
37568	1875.2150	2982.9344	3083.3171			
37569	3085.5445	3141.1800	3158.6442			
37570	3189.7485	3748.6268	3825.8256			
37571	Zero-point correction (Hartree): 0.149285					
37572						
37573	TS.diHPCARP_I.15HPHshift.umtumddd					
37574	-----					
37575	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13589719					
37576	Electronic state : 2-A					
37577	Cartesian coordinates (Angs):					
37578	O	-0.491780	-1.927286	-0.612895		
37579	O	0.808444	-2.337504	-0.369065		
37580	H	1.418906	-1.311488	-0.715341		
37581	C	1.461075	-0.034237	-0.966898		
37582	C	0.036083	0.400200	-0.595587		
37583	C	-0.751939	-0.733383	0.114306		
37584	C	-0.466472	-0.878666	1.604920		
37585	H	-0.691470	0.057283	2.111596		
37586	H	0.576214	-1.135302	1.760799		
37587	H	-1.092381	-1.671619	2.015144		
37588	C	-2.247122	-0.528781	-0.020155		
37589	O	-2.766208	0.555172	-0.049033		
37590	H	-2.844013	-1.456086	-0.040106		
37591	H	-0.485951	0.631371	-1.523146		
37592	O	0.063515	1.577997	0.195207		
37593	O	-0.795241	2.557440	-0.361850		
37594	H	-1.671515	2.201371	-0.130336		
37595	H	1.685729	0.022434	-2.029600		
37596	O	2.501581	0.574044	-0.322880		
37597	O	2.316260	0.499357	1.080703		
37598	H	1.822155	1.317484	1.249979		
37599	Rotational constants (GHz):			1.1499300	0.9223200	0.6385500
37600	Vibrational harmonic frequencies (cm-1):					
37601	i1907.2492		60.4430			77.2044
37602	104.5233		144.2614			190.0268
37603	213.9610		226.9828			249.0947
37604	258.0556		285.5218			306.2571
37605	339.2805		357.8844			411.0357
37606	425.9436		462.5719			493.1181
37607	528.6183		557.8178			602.6454
37608	694.5683		742.8657			767.5631
37609	907.3078		932.1801			968.2341
37610	988.2166		1020.2003			1027.6520
37611	1058.4643		1077.9109			1127.6081
37612	1181.5650		1197.7593			1204.8958
37613	1241.2496		1255.4609			1346.2619
37614	1353.4188		1388.4811			1396.6364
37615	1409.1194		1440.3237			1487.7389
37616	1494.3712		1499.3276			1619.2091
37617	1850.6135		3004.7280			3078.8066
37618	3108.4111		3147.1573			3156.1970
37619	3193.4373		3686.5849			3747.0378
37620	Zero-point correction (Hartree): 0.150580					
37621						
37622	TS.diHPCARP_I.15HPHshift.uppupuud					
37623	-----					
37624	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13362262					
37625	Electronic state : 2-A					
37626	Cartesian coordinates (Angs):					
37627	O	0.791487	-0.719974	1.196844		
37628	O	-0.478864	-1.016901	1.656852		
37629	H	-1.123011	-0.138558	1.104402		
37630	C	-1.365369	0.595208	0.037004		

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37631      C      -0.066657      0.478391      -0.729371
37632      C      0.781334      -0.732649      -0.220648
37633      C      0.271071      -2.044607      -0.792316
37634      H      0.462549      -2.080717      -1.864992
37635      H      -0.797763      -2.149501      -0.625980
37636      H      0.783147      -2.875761      -0.309886
37637      C      2.224092      -0.467222      -0.635265
37638      O      3.020529      0.083438      0.067589
37639      H      2.485814      -0.799094      -1.656225
37640      H      -0.279874      0.323241      -1.790868
37641      O      0.662302      1.686714      -0.703726
37642      O      0.870107      2.063589      0.649093
37643      H      1.674913      1.570027      0.885345
37644      H      -1.602797      1.592650      0.402620
37645      O      -2.375047      -0.008993      -0.680229
37646      O      -3.553206      0.050672      0.113306
37647      H      -4.168272      0.474634      -0.498676
37648      Rotational constants (GHz):      1.4485500      0.7087200      0.6150700
37649      Vibrational harmonic frequencies (cm-1):
37650      i1955.2434      57.6411      81.3175
37651      85.9241      132.0597      160.8797
37652      178.2995      185.6737      193.3151
37653      228.9308      242.6115      291.9010
37654      294.5787      329.5511      356.0730
37655      377.7061      471.8710      482.7684
37656      502.6117      558.0448      620.9302
37657      685.6706      726.6433      851.6162
37658      885.4337      943.5870      958.8584
37659      998.9034      1011.3177      1028.8112
37660      1086.4072      1096.4488      1134.4648
37661      1157.7328      1186.2011      1202.8511
37662      1229.7603      1260.2450      1290.2712
37663      1319.2468      1393.2952      1410.0287
37664      1423.1992      1426.3572      1471.7666
37665      1485.8634      1502.4994      1587.1235
37666      1867.1857      2974.5856      3073.5849
37667      3077.0384      3130.6799      3148.5755
37668      3174.0791      3701.0151      3821.8647
37669      Zero-point correction (Hartree): 0.149347
37670
37671
37672
37673      (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-Ia)
37674      =====
37675
37676      diHPCARP_I.mmmmpmpu
37677      -----
37678      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18108459
37679      Electronic state : 2-A
37680      Cartesian coordinates (Angs):
37681      O      -2.259636      -1.612496      -0.459200
37682      O      -1.547845      -1.166806      0.529196
37683      C      -0.941218      0.123920      0.231281
37684      C      0.009715      -0.057869      -0.991763
37685      C      0.780643      -1.368369      -0.878669
37686      O      1.355084      -1.486759      0.411055
37687      O      2.631395      -0.867048      0.420234
37688      H      2.416184      0.079318      0.425743
37689      C      -2.068063      1.124553      0.021604
37690      H      -2.757029      1.077550      0.864407
37691      H      -2.605874      0.871458      -0.889404
37692      H      -1.673781      2.130408      -0.066322
37693      C      -0.155471      0.445203      1.490121
37694      O      0.477651      1.462440      1.602701
37695      H      -0.221475      -0.294286      2.301927
37696      H      -0.590014      -0.025482      -1.905039
37697      O      1.033984      0.913986      -1.042078
37698      O      0.490171      2.219748      -1.107589
37699      H      0.558883      2.480070      -0.172570
37700      H      0.111312      -2.217790      -0.992412
37701      H      1.561742      -1.410395      -1.636320
37702      Rotational constants (GHz):      1.1223900      0.9431400      0.7456200

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37703 Vibrational harmonic frequencies (cm-1):
37704         62.6533          89.2639          128.6108
37705         137.7148         172.1499          187.9679
37706         199.2184         228.6514          240.0530
37707         257.2740         291.3004          337.7974
37708         350.0778         357.1204          371.1203
37709         422.5238         469.1668          502.5241
37710         513.9092         593.6674          652.2598
37711         698.9977         835.1802          885.0236
37712         910.7645         949.2978          982.6975
37713         997.9026        1028.9981         1077.1486
37714        1119.1803        1138.2854         1162.9262
37715        1189.2228        1239.4958         1289.1736
37716        1303.7842        1336.8793         1366.5541
37717        1385.3840        1404.3114         1423.2295
37718        1463.7471        1469.5655         1479.9800
37719        1486.2175        1499.9095         1839.1621
37720        3036.2034        3077.0395         3084.4457
37721        3105.6659        3159.2912         3165.6795
37722        3207.1807        3693.9572         3742.0304
37723 Zero-point correction (Hartree): 0.156737
37724
37725 diHPCARP_I.mmmmpmpmu
37726 -----
37727 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18134610
37728 Electronic state : 2-A
37729 Cartesian coordinates (Angs):
37730 O      2.554111      -1.412049      0.247871
37731 O      1.778797      -0.901001     -0.656231
37732 C      1.018967      0.243537     -0.166106
37733 C      0.133136     -0.265091      0.998517
37734 C     -0.747074     -1.438063      0.580996
37735 O     -1.325122     -1.253791     -0.698757
37736 O     -2.685570     -0.880477     -0.578082
37737 H     -2.621820      0.002147     -0.173211
37738 C      1.961691      1.344808      0.282605
37739 H      2.626143      1.629412     -0.531786
37740 H      2.552933      0.999640      1.127716
37741 H      1.376300      2.211277      0.580764
37742 C      0.255876      0.695630     -1.406473
37743 O     -0.384253      1.713369     -1.430491
37744 H      0.389728      0.070636     -2.301069
37745 H      0.827790     -0.617384      1.765034
37746 O     -0.529129      0.789830      1.661543
37747 O     -1.655958      1.233126      0.916675
37748 H     -1.263505      1.847171      0.270352
37749 H     -0.119927     -2.326831      0.503266
37750 H     -1.526239     -1.613048      1.321468
37751 Rotational constants (GHz): 1.2557700 0.8314600 0.7424300
37752 Vibrational harmonic frequencies (cm-1):
37753         52.9092          63.8413          119.4269
37754        140.6052         184.6352          203.3784
37755        208.5537         225.2822          235.6603
37756        260.5042         282.2869          313.8732
37757        323.0564         369.2185          435.4469
37758        474.1100         486.9556          496.3806
37759        520.0848         637.8098          655.5479
37760        697.5215         809.3377          881.9356
37761        894.8472         957.2150          984.1931
37762       1008.7615        1028.0084         1060.9375
37763       1132.2978        1135.5721         1169.2917
37764       1182.5721        1244.0806         1290.5629
37765       1308.6990        1347.3395         1381.0257
37766       1394.1534        1400.1405         1421.0984
37767       1470.9450        1481.5300         1482.2338
37768       1486.0479        1500.8060         1842.5079
37769       3040.3768        3081.9455         3084.6974
37770       3092.9046        3144.8336         3162.6375
37771       3176.4589        3655.3153         3678.8835
37772 Zero-point correction (Hartree): 0.156741
37773
37774 diHPCARP_I.mmmmpptmu

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37775 -----
37776 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18316002
37777 Electronic state : 2-A
37778 Cartesian coordinates (Angs):
37779 O 2.642876 -0.943217 -1.010153
37780 O 1.997980 0.175493 -0.891029
37781 C 1.067778 0.175818 0.230654
37782 C -0.016375 -0.875990 -0.073136
37783 C -0.785968 -0.567320 -1.347997
37784 O -1.340343 0.733553 -1.367287
37785 O -2.412749 0.779624 -0.435767
37786 H -2.001823 1.236734 0.319966
37787 C 1.798380 -0.098857 1.530902
37788 H 2.630901 0.594446 1.642687
37789 H 2.174627 -1.119148 1.534381
37790 H 1.102301 0.037516 2.354356
37791 C 0.516368 1.599292 0.220833
37792 O -0.233505 2.006004 1.065125
37793 H 0.886656 2.242125 -0.594693
37794 H 0.482880 -1.843609 -0.193399
37795 O -0.823513 -0.891534 1.090644
37796 O -1.894629 -1.792822 0.887253
37797 H -2.585087 -1.189190 0.568837
37798 H -0.098050 -0.580953 -2.193972
37799 H -1.562438 -1.312386 -1.515984
37800 Rotational constants (GHz): 1.2568000 0.7915500 0.7451400
37801 Vibrational harmonic frequencies (cm-1):
37802 68.5211 111.2545 136.5977
37803 139.4354 165.5754 198.0724
37804 208.4706 227.0040 246.4942
37805 258.6584 287.7751 311.5047
37806 338.7218 354.9409 414.2703
37807 470.4049 474.4846 494.8209
37808 517.5572 554.1205 659.9786
37809 719.9979 830.4039 875.2863
37810 895.1492 960.7959 971.0840
37811 1001.8835 1045.9012 1062.7884
37812 1122.8262 1139.1612 1184.2232
37813 1193.2719 1260.9857 1287.5274
37814 1308.3988 1357.8325 1384.3913
37815 1400.5983 1401.3435 1422.0612
37816 1446.2781 1473.8433 1481.8290
37817 1488.5992 1497.5403 1852.0731
37818 3009.3540 3055.8226 3082.4059
37819 3097.1174 3145.7036 3163.3400
37820 3182.4882 3681.4640 3734.4101
37821 Zero-point correction (Hartree): 0.156867
37822
37823 diHPCARP_I.mmmmtmpppu
37824 -----
37825 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17935388
37826 Electronic state : 2-A
37827 Cartesian coordinates (Angs):
37828 O -2.378711 -1.061369 -1.248646
37829 O -1.498605 -1.317205 -0.332870
37830 C -0.974555 -0.103382 0.289427
37831 C -0.235482 0.672107 -0.827410
37832 C 1.041690 -0.017018 -1.278297
37833 O 2.001796 0.102195 -0.235970
37834 O 2.820458 -1.048213 -0.216472
37835 H 2.335955 -1.614475 0.409735
37836 C -2.101445 0.699777 0.904776
37837 H -2.679021 0.068425 1.579190
37838 H -2.755357 1.081508 0.124834
37839 H -1.686207 1.538353 1.458797
37840 C -0.024687 -0.631104 1.363025
37841 O 0.470576 -1.723871 1.321623
37842 H 0.157920 0.065404 2.194967
37843 H -0.926042 0.703242 -1.673670
37844 O -0.054029 2.033931 -0.508579
37845 O 0.581503 2.148851 0.758241
37846 H 1.514888 1.987964 0.551236

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37847      H      0.836305      -1.072276      -1.463355
37848      H      1.424532      0.445022      -2.189472
37849 Rotational constants (GHz): 1.1777800      0.8643500      0.7082600
37850 Vibrational harmonic frequencies (cm-1):
37851      60.6440      72.6633      125.6217
37852      159.8101      183.5899      189.5927
37853      213.9993      215.4252      227.6126
37854      247.3742      285.3271      311.1485
37855      323.9534      339.3321      405.3349
37856      419.2525      451.1573      460.4197
37857      477.9826      593.3712      648.3601
37858      717.1836      806.4781      889.1620
37859      924.6786      938.6234      997.8355
37860      1000.7300      1039.0141      1081.3868
37861      1119.4693      1140.6771      1173.5526
37862      1195.3684      1232.4898      1287.3022
37863      1293.2170      1351.7899      1386.7998
37864      1398.6794      1404.9904      1420.0001
37865      1445.0204      1473.1107      1491.8379
37866      1497.0681      1503.9383      1845.0274
37867      3030.2144      3073.7231      3081.8587
37868      3095.9692      3129.6100      3162.1021
37869      3178.7724      3696.2918      3759.3809
37870 Zero-point correction (Hartree): 0.156454
37871
37872 diHPCARP_I.mmpmtpmu
37873 -----
37874 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17870119
37875 Electronic state : 2-A
37876 Cartesian coordinates (Angs):
37877      O      -1.679907      1.788615      -0.838730
37878      O      -1.156326      1.373535      0.272954
37879      C      0.198624      0.852813      0.110389
37880      C      0.123840      -0.428203      -0.772171
37881      C      -0.376610      -1.659600      -0.020979
37882      O      -1.484722      -1.357333      0.795405
37883      O      -2.593856      -1.123861      -0.066211
37884      H      -2.793109      -0.194651      0.111696
37885      C      1.081448      1.916304      -0.518314
37886      H      0.990150      2.850047      0.034997
37887      H      0.785981      2.074631      -1.552354
37888      H      2.117399      1.586870      -0.494520
37889      C      0.635848      0.579853      1.535773
37890      O      1.728022      0.144118      1.782623
37891      H      -0.091131      0.815825      2.328779
37892      H      -0.566987      -0.169934      -1.577711
37893      O      1.332234      -0.672279      -1.449630
37894      O      2.269947      -1.327291      -0.604667
37895      H      2.495546      -0.660539      0.066630
37896      H      -0.621327      -2.451118      -0.729518
37897      H      0.381428      -2.022181      0.669866
37898 Rotational constants (GHz): 1.1275900      0.8802400      0.7265700
37899 Vibrational harmonic frequencies (cm-1):
37900      39.0008      96.4451      109.5567
37901      126.6205      161.2468      173.5720
37902      203.1738      222.1082      228.8229
37903      232.6625      300.0943      308.2254
37904      317.5001      357.1968      369.7504
37905      431.1855      453.7926      477.9758
37906      480.3574      560.7602      636.4022
37907      665.2736      770.4647      889.1458
37908      936.3270      962.0330      975.9465
37909      986.7431      1048.5335      1114.3192
37910      1130.4799      1142.3666      1151.3384
37911      1201.9540      1230.7900      1288.7135
37912      1300.3272      1337.0735      1367.9938
37913      1400.5608      1405.4318      1419.7853
37914      1425.0259      1475.6900      1480.9320
37915      1491.8835      1500.6772      1851.7661
37916      3020.1769      3082.6527      3094.6193
37917      3097.9162      3161.8562      3164.4522
37918      3178.9725      3694.5045      3807.0321

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37919 Zero-point correction (Hartree): 0.156146
37920
37921 diHPCARP_I.mmtppmpppu
37922 -----
37923 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17999023
37924 Electronic state : 2-A
37925 Cartesian coordinates (Angs):
37926 O 2.036957 1.927333 -0.485089
37927 O 1.917332 0.969887 0.380774
37928 C 1.201248 -0.178010 -0.165861
37929 C -0.216675 0.310371 -0.533498
37930 C -1.001488 0.862980 0.651383
37931 O -2.272421 1.334183 0.249704
37932 O -3.133820 0.205688 0.108416
37933 H -3.246887 0.172683 -0.851012
37934 C 1.935225 -0.739775 -1.362806
37935 H 2.955091 -1.004690 -1.084893
37936 H 1.961656 -0.009244 -2.167577
37937 H 1.417469 -1.631643 -1.711486
37938 C 1.185766 -1.184513 0.987683
37939 O 1.089600 -0.852428 2.132329
37940 H 1.282732 -2.239864 0.686570
37941 H -0.096505 1.099431 -1.279373
37942 O -0.924033 -0.690831 -1.234952
37943 O -1.129674 -1.787723 -0.355262
37944 H -1.967662 -1.537938 0.070672
37945 H -1.113973 0.139094 1.457396
37946 H -0.487904 1.736986 1.050928
37947 Rotational constants (GHz): 1.3056400 0.7156700 0.6601100
37948 Vibrational harmonic frequencies (cm-1):
37949 54.5482 81.5533 116.8092
37950 120.2243 153.9232 195.1722
37951 205.1924 210.9552 222.9203
37952 257.5504 300.8559 312.8419
37953 317.4113 332.8061 385.2450
37954 417.6072 462.6698 526.2652
37955 575.3119 585.6394 644.1630
37956 682.0990 802.0305 887.2689
37957 913.4196 952.1480 987.7278
37958 1007.9577 1012.6409 1106.2542
37959 1116.7314 1138.8407 1171.6034
37960 1197.7612 1240.6231 1288.6848
37961 1312.6054 1330.7856 1378.9737
37962 1407.3872 1408.1139 1425.9419
37963 1430.0842 1439.1167 1478.9768
37964 1487.4013 1498.5568 1868.6102
37965 3011.7791 3076.7401 3096.9939
37966 3103.2102 3152.9751 3154.4385
37967 3171.7999 3718.0191 3807.0057
37968 Zero-point correction (Hartree): 0.156613
37969
37970 diHPCARP_I.pmmmtppmu
37971 -----
37972 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17930633
37973 Electronic state : 2-A
37974 Cartesian coordinates (Angs):
37975 O 1.537111 2.071602 0.063794
37976 O 2.042499 0.922161 -0.274566
37977 C 1.138988 -0.191846 -0.040591
37978 C 0.033051 -0.138130 -1.130008
37979 C -0.919461 1.046997 -1.004180
37980 O -1.322207 1.287154 0.331386
37981 O -2.649211 0.834812 0.531708
37982 H -2.544865 -0.130595 0.479925
37983 C 2.003233 -1.429712 -0.205778
37984 H 2.843061 -1.392272 0.485724
37985 H 2.380425 -1.485646 -1.225419
37986 H 1.413457 -2.318038 0.001579
37987 C 0.627105 -0.112332 1.398231
37988 O 0.078747 -1.046749 1.919655
37989 H 0.852186 0.814194 1.942525
37990 H 0.561722 -0.049067 -2.083721

```

37991	O	-0.604799	-1.393033	-1.266964	
37992	O	-1.535358	-1.606119	-0.214049	
37993	H	-0.973799	-1.873600	0.536471	
37994	H	-0.408616	1.947921	-1.340903	
37995	H	-1.795327	0.878621	-1.629932	
37996	Rotational constants (GHz):			1.1892300	0.9109800 0.7641000
37997	Vibrational harmonic frequencies (cm-1):				
37998		60.7957	75.3834		136.2611
37999		141.9075	197.8278		200.2473
38000		217.2412	224.2702		242.1669
38001		254.3114	288.8937		317.7403
38002		323.1785	356.6285		437.5665
38003		464.7862	483.0650		507.1955
38004		533.1311	617.6825		649.2660
38005		696.3295	811.1921		883.2217
38006		903.7833	955.1364		979.7498
38007		1004.4900	1028.1312		1058.1826
38008		1136.4563	1138.4490		1164.7775
38009		1202.9893	1224.0762		1274.8266
38010		1304.9248	1349.3420		1371.5387
38011		1397.1511	1404.0551		1420.9569
38012		1472.5391	1476.4734		1482.5379
38013		1483.5993	1501.9449		1835.5828
38014		3058.0828	3076.1708		3083.9625
38015		3094.8859	3146.7445		3160.2604
38016		3182.1632	3642.8713		3691.5146
38017	Zero-point correction (Hartree): 0.156803				
38018					
38019	diHPCARP_I.pmmpttmu				
38020	-----				
38021	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18238124				
38022	Electronic state : 2-A				
38023	Cartesian coordinates (Angs):				
38024	O	-2.086665	-1.386772	-0.950760	
38025	O	-2.172488	-0.101177	-0.775952	
38026	C	-1.091631	0.442045	0.027381	
38027	C	0.185249	0.477310	-0.842447	
38028	C	0.789249	-0.889044	-1.131357	
38029	O	1.011835	-1.663769	0.028221	
38030	O	2.090899	-1.086825	0.752893	
38031	H	1.621649	-0.620145	1.467571	
38032	C	-1.550576	1.840093	0.405494	
38033	H	-2.521245	1.787724	0.895915	
38034	H	-1.632744	2.457584	-0.487391	
38035	H	-0.825533	2.281290	1.082585	
38036	C	-0.933475	-0.408878	1.288925	
38037	O	-0.200272	-0.084844	2.182247	
38038	H	-1.571574	-1.303583	1.345767	
38039	H	-0.076983	0.947454	-1.798235	
38040	O	1.055631	1.332166	-0.115845	
38041	O	2.302557	1.395717	-0.778553	
38042	H	2.792229	0.696714	-0.315098	
38043	H	0.093490	-1.478775	-1.724431	
38044	H	1.715831	-0.773385	-1.692660	
38045	Rotational constants (GHz):			1.2276100	0.8384300 0.7728400
38046	Vibrational harmonic frequencies (cm-1):				
38047		69.7669	122.8601		144.2413
38048		150.4464	175.2326		190.0426
38049		205.9834	234.8633		247.1041
38050		274.7352	291.0401		309.2778
38051		330.7353	357.3975		394.7758
38052		467.5162	472.8539		511.4765
38053		525.0526	563.1813		651.2758
38054		713.1301	831.1938		872.2762
38055		909.1758	955.5164		967.6986
38056		993.0319	1046.4312		1063.4294
38057		1122.8721	1140.4918		1183.1021
38058		1205.2660	1243.1479		1277.4467
38059		1303.8629	1355.0690		1381.0503
38060		1401.8673	1405.4201		1419.8321
38061		1446.4516	1471.2503		1480.6782
38062		1492.5030	1496.5567		1845.4131

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38063          3029.5600          3034.9584          3081.9250
38064          3104.4629          3157.7653          3158.3936
38065          3188.2413          3679.2126          3736.0717
38066 Zero-point correction (Hartree): 0.156931
38067
38068 diHPCARP_I.ppmptmpu
38069 -----
38070 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18094361
38071 Electronic state : 2-A
38072 Cartesian coordinates (Angs):
38073 O      0.277757      -1.019120          1.816783
38074 O      0.056302          0.221889          1.491122
38075 C      0.646448          0.606383          0.223154
38076 C     -0.122476      -0.038946         -0.954332
38077 C     -1.488451          0.586785         -1.218590
38078 O     -2.247734          0.835947         -0.058803
38079 O     -2.791079         -0.391157          0.396972
38080 H     -2.121909         -0.702318          1.024101
38081 C      0.580392          2.125755          0.191205
38082 H      1.230579          2.545098          0.956828
38083 H     -0.438632          2.460475          0.367220
38084 H      0.929160          2.472070         -0.779957
38085 C      2.116652          0.187006          0.198917
38086 O      2.835063          0.519363         -0.695808
38087 H      2.474844         -0.379763          1.075045
38088 H      0.511591          0.102935         -1.837224
38089 O     -0.352496         -1.413795         -0.756443
38090 O      0.905162         -2.068694         -0.706925
38091 H      0.952749         -2.290566          0.235578
38092 H     -1.352271          1.567224         -1.674389
38093 H     -2.045304         -0.052510         -1.904490
38094 Rotational constants (GHz): 1.3101200      0.8148400      0.7359200
38095 Vibrational harmonic frequencies (cm-1):
38096      71.7615          80.5844          123.2619
38097     157.6697          162.5070          181.7353
38098     211.0667          229.7310          244.3247
38099     265.4358          292.5509          302.1890
38100     319.4620          337.9116          381.8447
38101     382.8781          454.9076          471.8148
38102     516.9193          549.1333          651.3373
38103     697.8180          828.5320          880.2598
38104     908.9944          950.8451          989.2002
38105     998.1042          1029.9456         1067.8741
38106    1142.0151          1148.1693         1173.4525
38107    1216.6619          1225.8261         1284.3638
38108    1310.3378          1360.2117         1368.8894
38109    1395.6842          1399.3682         1412.9508
38110    1429.8657          1433.3405         1466.9416
38111    1490.7966          1512.8486         1869.3051
38112    2994.1845          3048.3452         3083.1486
38113    3088.0483          3141.4192         3159.1337
38114    3179.7132          3762.1175         3776.3936
38115 Zero-point correction (Hartree): 0.156314
38116
38117 diHPCARP_I.ptmpmpmpu
38118 -----
38119 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17626708
38120 Electronic state : 2-A
38121 Cartesian coordinates (Angs):
38122 O     -2.109576          1.821030         -0.313396
38123 O     -1.765234          1.105674          0.711860
38124 C     -1.045792         -0.105144          0.330315
38125 C      0.175941          0.304401         -0.508862
38126 C      1.087758         -0.849691         -0.917426
38127 O      1.786068         -1.391037          0.183639
38128 O      2.985783         -0.655422          0.368375
38129 H      2.676681          0.133182          0.836961
38130 C     -0.732801         -0.815978          1.631898
38131 H     -1.646320         -0.915283          2.216487
38132 H      0.003583         -0.256215          2.202901
38133 H     -0.336246         -1.803568          1.413811
38134 C     -2.013034         -0.926124         -0.525083

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38135	O	-1.801834	-2.063382	-0.827168	
38136	H	-2.926445	-0.391618	-0.837389	
38137	H	-0.185692	0.819228	-1.401948	
38138	O	0.876954	1.241314	0.302834	
38139	O	1.768346	1.955232	-0.543594	
38140	H	1.353918	2.827983	-0.560527	
38141	H	0.499741	-1.666117	-1.335981	
38142	H	1.804289	-0.499639	-1.659765	
38143	Rotational constants (GHz):		1.2389400	0.7955700	0.5984300
38144	Vibrational harmonic frequencies (cm-1):				
38145		36.7039	58.4405		79.1007
38146		100.5591	150.6958		154.6641
38147		201.1908	217.0692		244.8744
38148		256.5703	269.8698		273.5679
38149		296.8106	305.8819		322.9057
38150		405.5031	431.1494		489.8627
38151		501.3837	535.0783		677.0337
38152		710.9580	806.4346		898.3114
38153		902.0179	943.9278		980.4437
38154		993.9194	1040.4590		1048.1271
38155		1118.2101	1141.5715		1160.1832
38156		1208.5155	1260.2586		1292.9436
38157		1320.7139	1352.3618		1383.6496
38158		1403.6217	1407.1143		1412.4941
38159		1424.9560	1429.2485		1468.8773
38160		1483.2658	1497.4604		1870.3710
38161		3000.3316	3078.7869		3085.0760
38162		3094.2586	3147.3319		3164.4773
38163		3185.4042	3782.6294		3810.1737
38164	Zero-point correction (Hartree):		0.155639		
38165	diHPCARP_I.ptmmpptmu				
38166	-----				
38167	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17819786				
38168	Electronic state : 2-A				
38169	Cartesian coordinates (Angs):				
38170	O	-2.361390	1.580765	-0.377618	
38171	O	-1.753872	1.137210	0.680851	
38172	C	-1.020106	-0.087065	0.391197	
38173	C	0.158517	0.272428	-0.519083	
38174	C	1.088236	-0.885666	-0.880274	
38175	O	1.851053	-1.367138	0.210209	
38176	O	2.929337	-0.467826	0.450845	
38177	H	2.610568	0.013606	1.226964	
38178	C	-0.653911	-0.652444	1.752987	
38179	H	-1.558637	-0.804834	2.340811	
38180	H	-0.010206	0.050310	2.278857	
38181	H	-0.131773	-1.598406	1.637331	
38182	C	-2.033846	-1.010346	-0.283711	
38183	O	-1.764522	-1.841456	-1.099189	
38184	H	-3.063808	-0.867982	0.089666	
38185	H	-0.252341	0.691827	-1.441943	
38186	O	0.860442	1.290630	0.179981	
38187	O	1.781140	1.878916	-0.720743	
38188	H	2.566101	1.322454	-0.590934	
38189	H	0.508812	-1.740488	-1.220714	
38190	H	1.760440	-0.576730	-1.681428	
38191	Rotational constants (GHz):		1.3150800	0.7551500	0.6145900
38192	Vibrational harmonic frequencies (cm-1):				
38193		30.7487	60.5899		84.7618
38194		132.0125	172.5239		186.4718
38195		200.0968	226.2564		244.1910
38196		248.2248	284.1549		294.2133
38197		315.2804	327.2605		377.3781
38198		411.9012	484.9079		517.0752
38199		561.4872	566.5965		654.7115
38200		718.3578	808.6503		892.5180
38201		908.7237	951.3319		969.3300
38202		980.5181	1049.8498		1056.3298
38203		1113.1956	1144.6330		1164.8445
38204		1233.3592	1263.7019		1283.9791
38205		1310.5176	1360.8742		1381.1360

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38207      1397.1495          1408.1124          1411.5656
38208      1425.0144          1455.8707          1483.5841
38209      1487.3296          1502.6208          1876.9276
38210      2984.2294          3073.3458          3078.6318
38211      3093.5500          3153.1398          3167.9367
38212      3179.0660          3733.5211          3793.3931
38213      Zero-point correction (Hartree): 0.156459
38214
38215      diHPCARP_I.ptppmtpmu
38216      -----
38217      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18147225
38218      Electronic state : 2-A
38219      Cartesian coordinates (Angs):
38220      O      2.187632      1.188145      -1.010276
38221      O      1.957024      0.682288      0.167546
38222      C      0.532914      0.537169      0.403537
38223      C      -0.019029      -0.586639      -0.520968
38224      C      -1.158309      -1.393269      0.098062
38225      O      -2.235996      -0.589053      0.512569
38226      O      -2.912614      -0.139885      -0.653322
38227      H      -2.564524      0.763529      -0.729256
38228      C      0.397930      0.304318      1.900950
38229      H      0.858258      1.129526      2.443839
38230      H      0.893870      -0.623665      2.176257
38231      H      -0.654524      0.244922      2.168864
38232      C      -0.075278      1.894801      0.077807
38233      O      -1.170166      2.052697      -0.381732
38234      H      0.567458      2.751903      0.342722
38235      H      -0.364599      -0.128593      -1.449239
38236      O      0.997288      -1.455377      -0.964915
38237      O      1.560376      -2.106091      0.170691
38238      H      2.436429      -1.698113      0.199054
38239      H      -1.492288      -2.133354      -0.629763
38240      H      -0.817790      -1.906223      0.996701
38241      Rotational constants (GHz):      1.2089000      0.8661400      0.6528800
38242      Vibrational harmonic frequencies (cm-1):
38243      83.4316      93.9807      122.9173
38244      135.7692      161.3721      172.5464
38245      192.0854      238.2136      261.0366
38246      261.9568      285.6437      296.0539
38247      321.0562      333.5424      374.5593
38248      439.5360      462.0896      529.2144
38249      548.4483      583.0203      619.6014
38250      677.3480      771.1181      915.8823
38251      947.9258      960.9535      972.7269
38252      983.3613      1046.1344      1107.8442
38253      1121.3098      1137.2333      1175.1053
38254      1226.3670      1239.5058      1268.7998
38255      1293.0970      1338.6990      1380.8682
38256      1402.7535      1407.5406      1418.5676
38257      1426.6324      1462.6821      1486.6280
38258      1495.9775      1509.9865      1867.9844
38259      2996.8586      3077.9493      3088.5033
38260      3106.4232      3147.9208      3156.3456
38261      3175.8641      3711.0154      3800.7657
38262      Zero-point correction (Hartree): 0.156785
38263
38264      diHPCARP_I.pttpmtppu
38265      -----
38266      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17868484
38267      Electronic state : 2-A
38268      Cartesian coordinates (Angs):
38269      O      2.104693      -1.109432      -1.448961
38270      O      1.824440      -1.232054      -0.186060
38271      C      1.149282      -0.052143      0.313199
38272      C      -0.231512      0.048946      -0.371528
38273      C      -1.164838      1.049914      0.297108
38274      O      -2.352966      1.232479      -0.445967
38275      O      -3.212255      0.119581      -0.211450
38276      H      -3.118176      -0.373550      -1.038039
38277      C      1.154586      -0.198195      1.827214
38278      H      2.182745      -0.264514      2.183176

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38279	H	0.614418	-1.094919	2.116290	
38280	H	0.687356	0.671530	2.285504	
38281	C	2.032858	1.135444	-0.057683	
38282	O	1.621164	2.250681	-0.191651	
38283	H	3.105703	0.888708	-0.148116	
38284	H	-0.065580	0.364444	-1.403973	
38285	O	-0.837958	-1.218154	-0.541473	
38286	O	-1.245954	-1.729766	0.719310	
38287	H	-2.152462	-1.386732	0.776575	
38288	H	-1.414498	0.754522	1.316762	
38289	H	-0.691073	2.030030	0.311980	
38290	Rotational constants (GHz):		1.3471400	0.7198900	0.5971000
38291	Vibrational harmonic frequencies (cm-1):				
38292		30.1656	59.4339		95.0854
38293		129.8677	157.3719		170.3901
38294		200.2028	225.4169		232.2058
38295		261.0671	286.9533		309.4123
38296		313.3800	343.0722		381.5711
38297		393.9560	475.1105		531.1521
38298		561.0168	571.4194		636.7014
38299		692.9872	823.3130		900.5918
38300		929.4529	953.6369		965.4086
38301		1001.5690	1007.7020		1096.3993
38302		1117.9715	1145.0540		1171.1490
38303		1221.5365	1249.3878		1282.1349
38304		1307.7750	1328.2060		1395.0209
38305		1404.5847	1408.1802		1416.8472
38306		1418.7063	1448.9938		1482.8023
38307		1495.1302	1501.4852		1870.5224
38308		2986.6243	3076.8983		3089.0447
38309		3099.8135	3149.9214		3161.4921
38310		3182.3874	3718.2293		3795.3878
38311	Zero-point correction (Hartree): 0.156422				
38312	diHPCARP_I.tmmptmpu				
38313	-----				
38315	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18157746				
38316	Electronic state : 2-A				
38317	Cartesian coordinates (Angs):				
38318	O	-2.534081	-1.450507	0.240384	
38319	O	-1.530497	-1.147803	-0.524117	
38320	C	-0.927026	0.125267	-0.149823	
38321	C	0.326344	0.231413	-1.066489	
38322	C	1.061548	-1.103194	-1.135583	
38323	O	1.270466	-1.616167	0.167383	
38324	O	2.483871	-1.099098	0.690292	
38325	H	2.253614	-0.184413	0.918578	
38326	C	-1.964761	1.215906	-0.369669	
38327	H	-2.878814	0.949288	0.156577	
38328	H	-2.175477	1.309599	-1.433927	
38329	H	-1.601495	2.168181	0.000060	
38330	C	-0.521195	0.038239	1.315768	
38331	O	0.009433	0.962028	1.874731	
38332	H	-0.751917	-0.905068	1.829270	
38333	H	0.004671	0.555193	-2.061120	
38334	O	1.305820	1.115220	-0.563271	
38335	O	0.776857	2.420014	-0.412148	
38336	H	0.568750	2.412272	0.538301	
38337	H	0.458699	-1.842806	-1.656839	
38338	H	2.017556	-0.977521	-1.642157	
38339	Rotational constants (GHz):		1.1468300	0.9209000	0.7235800
38340	Vibrational harmonic frequencies (cm-1):				
38341		51.6706	84.2574		132.9731
38342		152.3859	172.1220		179.9613
38343		201.9060	217.6043		251.9162
38344		255.9639	291.0305		340.1249
38345		353.8315	368.8082		380.5266
38346		424.0079	480.5469		501.9718
38347		513.8830	591.4240		660.4778
38348		706.1312	836.7405		883.0312
38349		903.9405	964.1900		973.6698
38350		993.8744	1034.7345		1077.1710

```

38351      1118.0773      1135.5379      1169.0533
38352      1186.7429      1245.3656      1282.5534
38353      1304.1045      1341.1824      1370.6636
38354      1390.0123      1404.2111      1422.2506
38355      1462.5458      1468.1724      1475.0367
38356      1485.0496      1499.7079      1834.3164
38357      3052.3051      3062.2871      3087.3991
38358      3105.2566      3162.5082      3166.5228
38359      3199.5038      3696.3858      3740.9193
38360 Zero-point correction (Hartree): 0.156849
38361
38362 diHPCARP_I.tmmmpmtu
38363 -----
38364 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17966454
38365 Electronic state : 2-A
38366 Cartesian coordinates (Angs):
38367 O      -2.826324      -0.982386      -0.457228
38368 O      -1.747587      -0.486472      -0.983155
38369 C      -0.899258      0.153588      0.010318
38370 C      0.345147      0.557335      -0.811295
38371 C      1.086825      -0.651016      -1.372358
38372 O      1.320831      -1.664360      -0.421164
38373 O      2.382929      -1.250724      0.419950
38374 H      1.914465      -0.886589      1.191940
38375 C      -1.619917      1.336302      0.628733
38376 H      -2.546881      0.995762      1.085189
38377 H      -1.835768      2.084969      -0.130917
38378 H      -0.979732      1.773102      1.390927
38379 C      -0.578195      -0.878328      1.089774
38380 O      0.087499      -0.599680      2.049679
38381 H      -1.024369      -1.874275      0.947200
38382 H      0.001466      1.168138      -1.651143
38383 O      1.254311      1.310277      -0.039030
38384 O      0.821400      2.670668      -0.046235
38385 H      1.628844      3.109463      -0.341011
38386 H      0.461332      -1.126546      -2.127977
38387 H      2.028560      -0.329898      -1.817779
38388 Rotational constants (GHz):      1.1035200      0.8827400      0.7057900
38389 Vibrational harmonic frequencies (cm-1):
38390      56.4967      104.6087      126.8517
38391      144.8390      173.8177      177.8029
38392      191.3555      201.5044      233.9314
38393      256.2003      279.4995      291.9023
38394      318.1802      356.7365      376.3802
38395      406.0163      419.3028      463.7010
38396      478.9797      501.0527      644.2626
38397      713.5964      847.7510      874.0272
38398      896.0865      966.8997      978.5907
38399      1004.3060      1040.9943      1066.7928
38400      1131.5290      1139.4026      1170.5358
38401      1184.7343      1259.8524      1286.9552
38402      1316.1354      1349.4169      1372.5589
38403      1398.6958      1402.1233      1415.0512
38404      1422.3156      1463.3691      1480.3998
38405      1485.4991      1500.4317      1842.0336
38406      3026.4922      3066.6375      3084.2331
38407      3087.2085      3143.6646      3166.3723
38408      3180.6582      3684.4902      3828.6265
38409 Zero-point correction (Hartree): 0.156013
38410
38411 diHPCARP_I.tmmmptpmu
38412 -----
38413 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18173772
38414 Electronic state : 2-A
38415 Cartesian coordinates (Angs):
38416 O      -2.758926      -1.236627      0.227107
38417 O      -1.754412      -0.999048      -0.561107
38418 C      -1.010418      0.178784      -0.147310
38419 C      0.165266      0.214379      -1.152108
38420 C      1.029975      -1.040753      -1.089847
38421 O      1.306589      -1.450202      0.235871
38422 O      2.620781      -1.074194      0.604352

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38423	H	2.552954	-0.104406	0.645380		
38424	C	-1.886792	1.412187	-0.269477		
38425	H	-2.773954	1.297788	0.349106		
38426	H	-2.181256	1.557030	-1.307698		
38427	H	-1.328339	2.282330	0.066872		
38428	C	-0.601869	-0.023657	1.314027		
38429	O	-0.103174	0.860307	1.957878		
38430	H	-0.845054	-1.001267	1.750430		
38431	H	-0.290694	0.254482	-2.145795		
38432	O	0.864459	1.440000	-1.103589		
38433	O	1.717382	1.492849	0.031956		
38434	H	1.115284	1.753386	0.752225		
38435	H	0.472338	-1.859587	-1.545647		
38436	H	1.960154	-0.890072	-1.636323		
38437	Rotational constants (GHz):			1.2976000	0.8043500	0.7263700
38438	Vibrational harmonic frequencies (cm-1):					
38439		51.8568	65.3315			121.3336
38440		153.1945	181.1400			191.1403
38441		207.9165	235.2169			238.6151
38442		267.5725	281.5450			309.0873
38443		347.3063	377.7261			417.9816
38444		479.2005	489.5242			511.4118
38445		526.1067	629.2914			642.1734
38446		724.4458	807.8400			882.7782
38447		900.2965	957.8230			977.5908
38448		1014.8991	1027.8622			1060.3656
38449		1132.0857	1139.2685			1166.0833
38450		1180.7527	1257.0078			1283.0857
38451		1305.8614	1346.8440			1378.8272
38452		1396.9623	1401.5625			1421.7621
38453		1466.8606	1478.8006			1482.0784
38454		1486.8381	1501.4109			1838.7592
38455		3057.2316	3074.4713			3083.5759
38456		3087.2574	3143.1937			3165.4985
38457		3176.8467	3654.0840			3682.5143
38458	Zero-point correction (Hartree):			0.156893		
38459	diHPCARP_I.tmmmpptmu					
38460	-----					
38461	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20929472					
38462	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09350630					
38463	T1 diagnostic: 0.020016					
38464	E(MP2/Aug-CC-pVTZ) (Hartree): -721.04858603					
38465	E(MP3/Aug-CC-pVTZ) (Hartree): -721.07077477					
38466	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05165614					
38467	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07259790					
38468	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.53911471					
38469	E(UHF/Aug-CC-pVTZ) (Hartree): -718.53407867					
38470	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18433188					
38471	Electronic state : 2-A					
38472	Cartesian coordinates (Angs):					
38473	O	-3.022273	-0.492127	-0.663552		
38474	O	-1.887274	-0.011214	-1.071934		
38475	C	-1.016495	0.328023	0.040389		
38476	C	0.297770	0.731132	-0.650985		
38477	C	0.955778	-0.425950	-1.388477		
38478	O	1.168791	-1.563532	-0.577113		
38479	O	2.193743	-1.264649	0.360949		
38480	H	1.680011	-1.107599	1.173504		
38481	C	-1.616392	1.462622	0.849085		
38482	H	-2.615599	1.185636	1.177815		
38483	H	-1.666384	2.365031	0.241730		
38484	H	-0.986428	1.645152	1.715562		
38485	C	-0.852485	-0.923269	0.907629		
38486	O	-0.245103	-0.902199	1.942132		
38487	H	-1.346879	-1.831833	0.530597		
38488	H	0.066475	1.514364	-1.383285		
38489	O	1.090277	1.269738	0.390621		
38490	O	2.354339	1.620843	-0.136963		
38491	H	2.865543	0.820014	0.062444		
38492	H	0.283004	-0.775872	-2.172074		
38493	H	1.891202	-0.105130	-1.845260		

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38495 Rotational constants (GHz): 1.3596600 0.7642900 0.7061000
38496 Vibrational harmonic frequencies (cm-1):
38497 77.0530 127.1591 135.5139
38498 137.2782 167.7518 184.2384
38499 229.4617 235.3764 241.4205
38500 266.0336 280.2077 326.3400
38501 336.5985 394.2793 396.0731
38502 427.7244 459.0960 480.9444
38503 531.4750 568.7005 654.9405
38504 733.7519 830.4418 868.9078
38505 904.9814 967.7358 975.1417
38506 992.1681 1046.0534 1063.4220
38507 1125.0703 1137.9928 1180.0046
38508 1196.0333 1263.5817 1288.3045
38509 1300.0585 1361.1232 1380.3521
38510 1400.3612 1401.0742 1419.7433
38511 1445.2602 1472.3266 1481.6003
38512 1488.8517 1497.9556 1847.5391
38513 3020.3581 3033.8640 3083.1205
38514 3095.1796 3144.1195 3165.0590
38515 3181.8512 3682.9498 3734.5300
38516 Zero-point correction (Hartree): 0.156894
38517
38518 diHPCARP_I.tmmmpptpu
38519 -----
38520 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17939884
38521 Electronic state : 2-A
38522 Cartesian coordinates (Angs):
38523 O -2.983767 -0.398640 -0.719549
38524 O -1.812981 0.019862 -1.093368
38525 C -0.970895 0.349998 0.043538
38526 C 0.371699 0.708271 -0.617770
38527 C 0.997220 -0.466283 -1.356621
38528 O 0.990915 -1.655468 -0.594070
38529 O 2.056053 -1.603702 0.339024
38530 H 1.630759 -1.232877 1.131109
38531 C -1.565129 1.512767 0.815829
38532 H -2.581662 1.269563 1.116769
38533 H -1.573839 2.407488 0.194603
38534 H -0.960072 1.688472 1.701413
38535 C -0.878775 -0.887260 0.941898
38536 O -0.279172 -0.863418 1.980623
38537 H -1.428776 -1.773026 0.591318
38538 H 0.182664 1.517830 -1.332343
38539 O 1.187411 1.192116 0.432552
38540 O 2.370497 1.699834 -0.172377
38541 H 2.364374 2.609372 0.149924
38542 H 0.396458 -0.696693 -2.236909
38543 H 2.013718 -0.219766 -1.659805
38544 Rotational constants (GHz): 1.2581600 0.7869800 0.7013300
38545 Vibrational harmonic frequencies (cm-1):
38546 68.9997 84.1268 127.2049
38547 136.7753 163.7588 176.1855
38548 186.2640 206.4840 229.0869
38549 235.5346 262.1819 282.5857
38550 319.4132 347.6896 389.4986
38551 395.2216 413.0941 426.2377
38552 480.3524 565.6389 647.7302
38553 722.4636 843.8655 870.8093
38554 905.8193 971.4912 980.9330
38555 995.3804 1046.1082 1061.8764
38556 1126.8006 1136.2027 1178.0591
38557 1190.6487 1265.7567 1291.0038
38558 1304.6433 1363.0633 1377.9574
38559 1398.4452 1400.7413 1415.7190
38560 1420.6209 1469.4016 1477.2840
38561 1488.8292 1499.5500 1846.5520
38562 3030.8973 3040.1218 3080.8320
38563 3095.1546 3150.3186 3162.0982
38564 3180.3571 3706.8720 3831.0361
38565 Zero-point correction (Hartree): 0.155990
38566

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38567 diHPCARP_I.tmmtmpppu
38568 -----
38569 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17950435
38570 Electronic state : 2-A
38571 Cartesian coordinates (Angs):
38572 O 2.622012 -1.322578 0.384123
38573 O 1.642862 -0.671041 0.932096
38574 C 0.983689 0.226080 -0.002024
38575 C -0.121620 0.843384 0.886954
38576 C -1.246611 -0.131355 1.197021
38577 O -2.003913 -0.322949 0.009414
38578 O -2.499540 -1.644719 -0.023449
38579 H -1.783257 -2.103418 -0.497111
38580 C 1.960767 1.262258 -0.515436
38581 H 2.800371 0.764925 -0.996712
38582 H 2.327426 1.868521 0.311205
38583 H 1.461497 1.912330 -1.229809
38584 C 0.410008 -0.615813 -1.146222
38585 O 0.191099 -1.791183 -1.051228
38586 H 0.219583 -0.056144 -2.074724
38587 H 0.362467 1.106469 1.831581
38588 O -0.578237 2.085810 0.400322
38589 O -0.967698 1.950100 -0.960089
38590 H -1.850085 1.553116 -0.896536
38591 H -0.819714 -1.083540 1.514359
38592 H -1.888379 0.262895 1.986474
38593 Rotational constants (GHz): 1.1877800 0.9043900 0.6689300
38594 Vibrational harmonic frequencies (cm-1):
38595 62.6346 75.0197 132.5872
38596 158.5819 174.9316 190.2276
38597 210.7066 216.8092 236.7516
38598 256.4013 291.1641 316.8328
38599 322.1027 369.2664 385.3348
38600 406.9791 425.9377 474.8621
38601 505.1635 556.5905 641.9485
38602 785.0575 822.9706 863.4582
38603 930.9269 940.0141 991.5961
38604 1000.0947 1040.7909 1082.1852
38605 1120.3843 1136.4847 1173.5601
38606 1194.8701 1247.5962 1278.5176
38607 1289.8485 1355.1503 1376.7065
38608 1400.2254 1405.5532 1417.8984
38609 1448.3168 1474.6571 1491.5336
38610 1499.2205 1505.3862 1846.8977
38611 3023.2856 3072.8135 3082.7055
38612 3085.0355 3130.5812 3162.0855
38613 3175.2886 3692.9813 3754.6645
38614 Zero-point correction (Hartree): 0.156533
38615
38616 diHPCARP_I.tmpmtpmu
38617 -----
38618 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17982062
38619 Electronic state : 2-A
38620 Cartesian coordinates (Angs):
38621 O -1.692512 2.213420 -0.062535
38622 O -1.314334 1.059651 -0.523773
38623 C 0.085519 0.783835 -0.225879
38624 C 0.299333 -0.675064 -0.718763
38625 C -0.192151 -1.737707 0.262176
38626 O -1.457290 -1.411972 0.790477
38627 O -2.413080 -1.571738 -0.251211
38628 H -2.640913 -0.652791 -0.449579
38629 C 0.954856 1.766385 -0.989526
38630 H 0.648132 2.783008 -0.753550
38631 H 0.861298 1.588987 -2.059247
38632 H 1.995712 1.633311 -0.704543
38633 C 0.280998 0.940962 1.274741
38634 O 1.369865 0.829755 1.768462
38635 H -0.617654 1.152683 1.872713
38636 H -0.262175 -0.747538 -1.653837
38637 O 1.628121 -0.903035 -1.123971
38638 O 2.463223 -1.146626 0.000351

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38639      H      2.522568      -0.284579      0.446240
38640      H      -0.213595      -2.711890      -0.226382
38641      H      0.463341      -1.787302      1.129304
38642      Rotational constants (GHz):      1.0677900      0.9336700      0.6839100
38643      Vibrational harmonic frequencies (cm-1):
38644          47.6237      97.2211      114.0231
38645          143.2546      166.3645      179.1052
38646          197.8691      230.1826      242.4283
38647          249.7579      296.2858      310.9580
38648          332.0878      372.8222      383.7502
38649          403.2055      460.0998      474.9254
38650          512.0816      555.8950      636.3857
38651          687.7216      770.4762      886.8786
38652          944.4774      970.0261      976.1352
38653          983.2547      1052.4343      1113.4412
38654          1130.1131      1141.7509      1149.8221
38655          1207.6438      1241.5583      1278.3290
38656          1294.4265      1334.3422      1371.6401
38657          1400.8977      1406.9942      1421.9983
38658          1428.4520      1473.7335      1479.3166
38659          1493.7545      1503.7018      1848.6619
38660          3035.9492      3084.7695      3086.2807
38661          3096.1589      3160.8338      3168.4359
38662          3173.8593      3705.4338      3794.7980
38663      Zero-point correction (Hartree): 0.156521
38664
38665      diHPCARP_I.tmtppppu
38666      -----
38667      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17979834
38668      Electronic state : 2-A
38669      Cartesian coordinates (Angs):
38670      O      -2.999186      -0.967374      -0.445891
38671      O      -1.741919      -0.915142      -0.763207
38672      C      -1.092090      0.271226      -0.236701
38673      C      0.368402      0.078323      -0.694268
38674      C      1.063647      -1.116861      -0.051521
38675      O      2.378158      -1.272509      -0.547697
38676      O      3.214483      -0.335241      0.128679
38677      H      3.404514      0.294959      -0.579179
38678      C      -1.710418      1.519510      -0.824711
38679      H      -2.768227      1.558981      -0.570896
38680      H      -1.598937      1.525370      -1.907690
38681      H      -1.208880      2.395457      -0.417083
38682      C      -1.231329      0.261787      1.293088
38683      O      -1.240014      -0.745341      1.935613
38684      H      -1.324238      1.257300      1.756695
38685      H      0.349298      -0.068199      -1.777825
38686      O      1.104966      1.274763      -0.548279
38687      O      1.177027      1.578146      0.837729
38688      H      1.983165      1.100824      1.097495
38689      H      1.085422      -1.055214      1.035477
38690      H      0.540490      -2.031808      -0.327895
38691      Rotational constants (GHz):      1.5084800      0.6566500      0.6148200
38692      Vibrational harmonic frequencies (cm-1):
38693          56.2928      79.2466      109.0843
38694          123.5287      135.9723      190.2912
38695          199.5174      215.0100      235.9525
38696          252.7948      297.0564      304.8882
38697          321.8317      364.9450      373.5876
38698          392.9027      435.2145      510.1770
38699          580.0880      594.6517      646.8666
38700          705.7218      825.5514      881.1248
38701          917.5176      951.2228      985.3550
38702          1001.5041      1011.4805      1102.8541
38703          1116.2413      1133.2712      1175.8504
38704          1192.1856      1262.4356      1281.6844
38705          1309.5315      1324.0628      1379.2273
38706          1406.7560      1407.7194      1420.4786
38707          1426.0057      1437.6943      1479.9514
38708          1488.6195      1497.7235      1871.1398
38709          3003.3229      3078.2912      3081.8433
38710          3103.9189      3155.0476      3160.8270

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38711          3163.5323          3722.1034          3806.6797
38712 Zero-point correction (Hartree): 0.156484
38713
38714 diHPCARP_I.tpmptmmu
38715 -----
38716 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18007750
38717 Electronic state : 2-A
38718 Cartesian coordinates (Angs):
38719 O      0.760746      -1.781571      -1.637324
38720 O      0.064675      -0.840641      -1.074741
38721 C      0.625378      -0.448003      0.203523
38722 C     -0.218449      0.739067      0.690613
38723 C     -1.591740      0.360631      1.239407
38724 O     -2.269934      -0.618636      0.492438
38725 O     -2.760216      -0.020069     -0.695122
38726 H     -2.023529      -0.153856     -1.310973
38727 C      0.611285      -1.619460      1.174109
38728 H      1.285380      -2.396343      0.821271
38729 H     -0.393117      -2.026477      1.258458
38730 H      0.963402      -1.272024      2.144367
38731 C      2.076109      -0.011506     -0.017948
38732 O      2.755001      0.351247      0.898454
38733 H      2.448796     -0.090676     -1.050576
38734 H      0.355807      1.219908      1.491655
38735 O     -0.458591      1.667642     -0.354641
38736 O      0.789645      2.057408     -0.903108
38737 H      0.965862      2.895137     -0.453914
38738 H     -1.466331     -0.083825      2.226777
38739 H     -2.202383      1.260741      1.327049
38740 Rotational constants (GHz):      1.2377400      0.8126200      0.7127200
38741 Vibrational harmonic frequencies (cm-1):
38742      73.7925          90.5325          106.8049
38743      137.1989         141.4109         174.2502
38744      202.1637         223.0137         242.7029
38745      250.4279         263.7588         282.0113
38746      310.2605         363.3486         368.5086
38747      421.1548         436.0143         454.6670
38748      492.8313         591.4723         640.7377
38749      721.6988         799.3145         879.2372
38750      918.3326         972.6610         989.3214
38751     1002.7170        1030.3184        1060.1266
38752     1146.0159        1155.1805        1160.2522
38753     1205.5400        1248.2247        1286.9541
38754     1312.0096        1364.5470        1376.3875
38755     1394.0823        1400.1242        1405.8765
38756     1413.3372        1450.8165        1465.2368
38757     1487.6500        1515.6362        1860.2958
38758     3025.6879        3038.4785        3081.8020
38759     3085.4393        3136.8160        3163.7080
38760     3179.9229        3768.2037        3800.5816
38761 Zero-point correction (Hartree): 0.156213
38762
38763 diHPCARP_I.tpmptmtu
38764 -----
38765 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17966889
38766 Electronic state : 2-A
38767 Cartesian coordinates (Angs):
38768 O      -0.803683      -1.680759      1.715329
38769 O     -0.091426     -0.775000      1.114637
38770 C     -0.630051     -0.440807     -0.191638
38771 C      0.231334      0.720258     -0.715380
38772 C      1.597191      0.306875     -1.256331
38773 O      2.266213     -0.661223     -0.484677
38774 O      2.752371     -0.041315      0.694036
38775 H      2.025682     -0.196191      1.315718
38776 C     -0.609948     -1.656373     -1.105420
38777 H     -1.291399     -2.413246     -0.724184
38778 H      0.393162     -2.070343     -1.163897
38779 H     -0.953331     -1.351102     -2.092810
38780 C     -2.081779      0.011134     -0.011844
38781 O     -2.756677      0.300820     -0.954679
38782 H     -2.462078      0.009287      1.022107

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38783      H      -0.336590      1.190481      -1.526126
38784      O       0.485006      1.674876       0.295214
38785      O      -0.785351      2.167943       0.718703
38786      H      -0.629566      2.271207       1.665762
38787      H       1.463696      -0.165496      -2.229410
38788      H       2.218312      1.196156      -1.371985
38789      Rotational constants (GHz):      1.2333100      0.8081900      0.7129500
38790      Vibrational harmonic frequencies (cm-1):
38791          60.5173          95.3223          110.2730
38792          128.8768          141.8503          169.9371
38793          200.0173          213.3034          224.6978
38794          245.3893          255.0552          278.8511
38795          308.5427          356.3867          369.1572
38796          389.9695          420.4408          443.6103
38797          490.8398          589.6764          638.4410
38798          722.7007          795.8091          875.4595
38799          917.4057          972.1881          990.3838
38800          1001.5272          1030.1003          1067.5991
38801          1141.4913          1148.7782          1160.6101
38802          1204.0700          1246.7849          1284.4485
38803          1310.9551          1355.0635          1377.6514
38804          1393.7484          1401.9948          1412.4512
38805          1427.7196          1447.2138          1466.2772
38806          1487.9166          1515.0934          1867.4097
38807          3011.7989          3049.2114          3084.5265
38808          3087.0685          3140.1591          3164.2100
38809          3181.5582          3775.5867          3832.4150
38810      Zero-point correction (Hartree): 0.156010
38811
38812      diHPCARP_I.tpmmpttmu
38813      -----
38814      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18109076
38815      Electronic state : 2-A
38816      Cartesian coordinates (Angs):
38817      O       1.554179      -1.686121      -1.361112
38818      O       0.532895      -1.068819      -0.849507
38819      C       0.944744      -0.152793       0.202958
38820      C      -0.287371       0.683194       0.560269
38821      C      -1.401075      -0.070351       1.272161
38822      O      -1.804384      -1.265764       0.645119
38823      O      -2.414386      -0.923566      -0.593454
38824      H      -1.682273      -1.069048      -1.212676
38825      C       1.506671      -0.932513       1.375471
38826      H       2.413006      -1.448770       1.068394
38827      H       0.780408      -1.664326       1.722757
38828      H       1.755141      -0.238875       2.176684
38829      C       2.000271       0.788755      -0.387328
38830      O       2.613869       1.537763       0.312662
38831      H       2.140917       0.734731      -1.478363
38832      H       0.051217       1.482910       1.229266
38833      O      -0.667031       1.241597      -0.691196
38834      O      -1.842159       2.007727      -0.531640
38835      H      -2.521027       1.354122      -0.764164
38836      H      -1.045902      -0.383543       2.254200
38837      H      -2.254795       0.592517       1.415748
38838      Rotational constants (GHz):      1.2575900      0.7941100      0.6610100
38839      Vibrational harmonic frequencies (cm-1):
38840          63.6659          74.9089          101.6227
38841          125.0801          131.1892          188.9598
38842          213.1107          227.4209          234.5976
38843          252.1042          260.6152          327.6049
38844          332.0399          376.1876          404.5445
38845          470.3637          471.8222          480.1194
38846          530.6728          582.4183          642.4426
38847          747.8846          797.2778          862.5910
38848          918.6465          956.8811          990.5146
38849          992.6159          1042.2079          1051.5975
38850          1128.9148          1154.5034          1174.4385
38851          1226.3126          1238.9650          1287.7833
38852          1300.6758          1368.9688          1385.8221
38853          1396.7570          1407.9818          1414.0912
38854          1431.8432          1447.5805          1479.1494

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38855      1488.9595      1511.1132      1872.6221
38856      3018.5870      3045.8846      3083.2106
38857      3091.3525      3136.4120      3168.5510
38858      3169.9903      3744.1227      3759.3958
38859 Zero-point correction (Hartree): 0.156705
38860
38861 diHPCARP_I.tptmpttmu
38862 -----
38863 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18009833
38864 Electronic state : 2-A
38865 Cartesian coordinates (Angs):
38866 O      2.724424      -1.040155      -1.138368
38867 O      1.437724      -0.940738      -0.989681
38868 C      1.107517      -0.196330      0.211917
38869 C     -0.393956      0.072727      0.147026
38870 C     -1.232803      -1.193822      0.020100
38871 O     -2.593817      -0.898401      -0.216486
38872 O     -3.112056      -0.276644      0.949658
38873 H     -2.983565      0.663261      0.747542
38874 C      1.525328      -0.980706      1.441850
38875 H      2.601123      -1.138422      1.416859
38876 H      1.026902      -1.946759      1.476498
38877 H      1.276259      -0.404231      2.330161
38878 C      1.836810      1.151003      0.151612
38879 O      1.891902      1.863418      1.108922
38880 H      2.284879      1.412511      -0.819556
38881 H     -0.652984      0.627941      1.051543
38882 O     -0.573161      0.925026      -0.977412
38883 O     -1.795561      1.631651      -0.822800
38884 H     -2.379742      1.128043      -1.407835
38885 H     -0.923929      -1.762807      -0.856938
38886 H     -1.141963      -1.810014      0.916033
38887 Rotational constants (GHz): 1.4154600 0.6302100 0.5725600
38888 Vibrational harmonic frequencies (cm-1):
38889      53.5934      70.9686      93.9045
38890      118.3767      152.9960      176.1083
38891      200.7884      207.2976      224.0907
38892      252.9917      268.1231      302.3293
38893      327.6047      367.1185      397.1768
38894      416.3540      459.9065      477.1774
38895      518.8659      565.9588      626.2002
38896      670.8392      832.4853      893.0682
38897      943.7943      969.1154      982.2938
38898      996.2895      1037.6532      1091.5404
38899      1128.2662      1149.7859      1166.0051
38900      1226.5911      1249.7039      1282.7418
38901      1311.5553      1341.8530      1381.5536
38902      1398.3347      1410.6420      1422.5315
38903      1430.5904      1441.8843      1473.7539
38904      1485.9969      1506.2823      1873.1229
38905      3020.3852      3077.7847      3087.9391
38906      3090.0017      3142.9749      3171.3766
38907      3174.0638      3747.9252      3786.3583
38908 Zero-point correction (Hartree): 0.156453
38909
38910 diHPCARP_I.tptmptppu
38911 -----
38912 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18007136
38913 Electronic state : 2-A
38914 Cartesian coordinates (Angs):
38915 O     -2.216004      -0.896158      1.634179
38916 O     -1.022298      -0.856626      1.124942
38917 C     -1.049345      -0.293889      -0.215007
38918 C      0.403932      -0.000731      -0.617044
38919 C      1.383332      -1.079248      -0.165123
38920 O      2.688620      -0.823481      -0.640711
38921 O      3.282308      0.157764      0.204588
38922 H      3.239255      0.945193      -0.355453
38923 C     -1.717654      -1.274371      -1.158930
38924 H     -2.689440      -1.554064      -0.758481
38925 H     -1.112165      -2.170104      -1.287446
38926 H     -1.863803      -0.789571      -2.121613

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38927      C      -1.819882      1.029818      -0.148187
38928      O      -2.350764      1.493960      -1.112296
38929      H      -1.820833      1.522007      0.836778
38930      H      0.430347      0.073245      -1.706527
38931      O      0.828717      1.294675      -0.220629
38932      O      0.835926      1.361020      1.197441
38933      H      1.735895      1.060786      1.403967
38934      H      1.397363      -1.187630      0.918249
38935      H      1.109035      -2.038553      -0.603831
38936      Rotational constants (GHz):      1.4780600      0.6419700      0.6060400
38937      Vibrational harmonic frequencies (cm-1):
38938          65.1808          81.4710          88.2643
38939          126.3029          164.2837          191.4945
38940          193.0434          215.0980          234.6426
38941          259.7055          284.7282          305.8610
38942          326.0005          353.4389          381.4172
38943          401.4841          463.2800          506.1380
38944          531.5991          611.3283          633.4204
38945          699.7695          807.4212          879.5093
38946          940.0857          960.4658          978.1903
38947          993.7558          1008.8605          1098.2110
38948          1118.7871          1135.6185          1161.7194
38949          1224.6466          1245.4825          1279.4905
38950          1309.1779          1317.2551          1391.1273
38951          1398.9631          1409.1280          1412.7795
38952          1419.1065          1438.3789          1479.7053
38953          1485.4605          1503.3831          1874.0155
38954          3025.4890          3082.9363          3095.3612
38955          3100.8231          3151.3170          3164.4702
38956          3173.2471          3740.5186          3797.3591
38957      Zero-point correction (Hartree): 0.156556
38958
38959
38960
38961      (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-Ib)
38962      =====
38963
38964      diHPCARP_Ib.mmmmpmtmmu
38965      -----
38966      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17981133
38967      Electronic state : 2-A
38968      Cartesian coordinates (Angs):
38969      O      -2.473915      -0.962563      -1.012460
38970      O      -1.542280      -1.318217      -0.002444
38971      C      -0.832744      -0.151050      0.408422
38972      C      -0.061541      0.390759      -0.814153
38973      C      0.885527      -0.634728      -1.410584
38974      O      1.669908      -1.304816      -0.447694
38975      O      2.737868      -0.452104      -0.072704
38976      H      2.414767      -0.052491      0.753670
38977      C      -1.742853      0.892922      1.035042
38978      H      -2.346946      0.427048      1.813975
38979      H      -2.391134      1.336616      0.282568
38980      H      -1.139317      1.677876      1.484800
38981      C      0.110702      -0.697855      1.479032
38982      O      0.876923      0.008282      2.077027
38983      H      0.004443      -1.772048      1.698080
38984      H      -0.786418      0.703510      -1.564924
38985      O      0.686897      1.566559      -0.444511
38986      O      -0.007023      2.653720      -0.606232
38987      H      -3.315039      -1.063536      -0.549875
38988      H      0.288795      -1.418028      -1.877713
38989      H      1.529278      -0.166114      -2.154995
38990      Rotational constants (GHz):      1.1241200      0.8453400      0.7583100
38991      Vibrational harmonic frequencies (cm-1):
38992          54.2692          102.0056          105.4048
38993          130.5217          170.8742          173.2533
38994          201.5991          214.8976          238.3137
38995          242.7834          253.0165          299.9800
38996          319.5591          328.2183          400.2947
38997          407.9127          433.6877          456.0380
38998          465.5830          500.3675          656.4913

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38999	690.8831	848.1253	870.3976	
39000	913.0820	955.2080	981.3766	
39001	1006.9074	1044.4773	1052.0564	
39002	1125.8004	1145.2721	1173.5777	
39003	1193.8757	1259.0687	1283.2456	
39004	1318.1574	1351.9092	1365.7449	
39005	1398.9497	1401.8732	1407.7158	
39006	1419.7838	1460.8896	1474.6375	
39007	1493.4152	1498.1882	1845.2483	
39008	3015.5787	3074.0745	3089.3143	
39009	3124.1367	3146.3285	3153.1192	
39010	3173.0252	3687.6190	3821.0766	
39011	Zero-point correction (Hartree): 0.155870			
39012				
39013	diHPCARP_Ib.mmmmppttmu			
39014	-----			
39015	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18002533			
39016	Electronic state : 2-A			
39017	Cartesian coordinates (Angs):			
39018	O	-2.574633	0.570595	-1.184048
39019	O	-1.839658	-0.577850	-0.787421
39020	C	-0.970837	-0.225280	0.286181
39021	C	0.012691	0.840556	-0.225192
39022	C	0.832002	0.379872	-1.416902
39023	O	1.376113	-0.911520	-1.249736
39024	O	2.521407	-0.806779	-0.420837
39025	H	2.180394	-1.072536	0.450713
39026	C	-1.723897	0.240766	1.521839
39027	H	-2.490128	-0.488354	1.784591
39028	H	-2.190683	1.206689	1.338780
39029	H	-1.027373	0.332631	2.351873
39030	C	-0.273010	-1.552390	0.590566
39031	O	0.525605	-1.666813	1.480162
39032	H	-0.591169	-2.404360	-0.030647
39033	H	-0.551536	1.732488	-0.498981
39034	O	0.857343	1.207427	0.889157
39035	O	1.519705	2.293732	0.634884
39036	H	-3.472686	0.323699	-0.931341
39037	H	0.171504	0.296825	-2.279939
39038	H	1.622923	1.101449	-1.621294
39039	Rotational constants (GHz): 1.1718500 0.8081700 0.7499600			
39040	Vibrational harmonic frequencies (cm-1):			
39041	58.7636	81.7023	119.4749	
39042	133.4017	163.1681	192.6891	
39043	196.9358	210.1940	229.0638	
39044	235.7680	253.8733	288.5954	
39045	319.0382	331.2051	368.7143	
39046	415.6536	424.9853	459.4123	
39047	470.8811	548.3831	650.8100	
39048	702.6972	843.5760	864.4377	
39049	913.9839	957.5015	976.2044	
39050	1003.0449	1052.0988	1055.6531	
39051	1106.2628	1139.9672	1178.6700	
39052	1196.8861	1274.9719	1288.2594	
39053	1311.2403	1358.1011	1360.7633	
39054	1396.8759	1399.7280	1408.7545	
39055	1420.7069	1462.0561	1472.0885	
39056	1494.3478	1501.8806	1846.5748	
39057	3015.8194	3075.0610	3090.9521	
39058	3113.1266	3148.4071	3152.8558	
39059	3172.1893	3697.9108	3824.9620	
39060	Zero-point correction (Hartree): 0.155898			
39061				
39062	diHPCARP_Ib.pmmmmmmmpu			
39063	-----			
39064	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17968988			
39065	Electronic state : 2-A			
39066	Cartesian coordinates (Angs):			
39067	O	2.011575	0.543383	-1.267933
39068	O	1.656473	-0.781916	-0.899287
39069	C	0.585010	-0.769445	0.022291
39070	C	-0.725003	-0.372822	-0.692324

39071	C	-0.816900	1.076353	-1.139164		
39072	O	-0.378301	2.001036	-0.167275		
39073	O	-1.386834	2.079636	0.839278		
39074	H	-1.588032	3.023173	0.825677		
39075	C	0.516096	-2.208594	0.531040		
39076	H	1.490406	-2.478410	0.933187		
39077	H	0.263712	-2.877283	-0.290121		
39078	H	-0.238089	-2.312397	1.307916		
39079	C	0.895460	0.106041	1.229006		
39080	O	2.005354	0.492377	1.475673		
39081	H	0.044035	0.305162	1.900143		
39082	H	-0.843849	-1.027595	-1.555798		
39083	O	-1.843951	-0.642553	0.187988		
39084	O	-2.368067	-1.811676	-0.031296		
39085	H	2.555584	0.808328	-0.508767		
39086	H	-0.140083	1.223853	-1.977181		
39087	H	-1.841662	1.303681	-1.437340		
39088	Rotational constants (GHz):			1.0762400	0.9322200	0.6987200
39089	Vibrational harmonic frequencies (cm-1):					
39090		55.3129	87.6731			102.0123
39091		127.8500	136.9575			166.7818
39092		185.2709	206.4121			222.1005
39093		234.0368	283.2946			299.7455
39094		309.7469	354.3195			372.8106
39095		405.0863	460.9707			492.0277
39096		511.0983	539.5824			625.3479
39097		766.9722	837.4440			866.7266
39098		929.2014	935.1135			972.4619
39099		1003.2082	1046.6826			1056.0231
39100		1109.3859	1131.3144			1175.5982
39101		1224.2497	1240.6262			1284.6553
39102		1320.2459	1348.2689			1362.9219
39103		1393.7776	1404.2290			1422.5548
39104		1425.0541	1441.3217			1456.6922
39105		1489.5509	1500.5428			1850.1251
39106		3018.7038	3080.4138			3083.9520
39107		3110.7505	3162.4136			3164.5899
39108		3169.2080	3736.0821			3832.6811
39109	Zero-point correction (Hartree):			0.156128		
39110	diHPCARP_Ib.pmmmmmtpu					
39111	-----					
39112	-----					
39113	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.18078123		
39114	Electronic state : 2-A					
39115	Cartesian coordinates (Angs):					
39116	O	-1.850033	-0.881174	-1.344948		
39117	O	-1.829645	0.478261	-0.933205		
39118	C	-0.820403	0.687152	0.033050		
39119	C	0.568885	0.632408	-0.624951		
39120	C	1.024395	-0.732891	-1.108376		
39121	O	0.787818	-1.761896	-0.170755		
39122	O	1.754610	-1.628169	0.869895		
39123	H	2.214401	-2.474286	0.807885		
39124	C	-1.105650	2.089775	0.569336		
39125	H	-2.126707	2.120282	0.943656		
39126	H	-0.998185	2.814346	-0.236877		
39127	H	-0.415156	2.347066	1.368974		
39128	C	-0.965030	-0.272810	1.208065		
39129	O	-1.964941	-0.910603	1.395528		
39130	H	-0.117396	-0.292496	1.912165		
39131	H	0.575004	1.328965	-1.465191		
39132	O	1.498657	1.155886	0.360642		
39133	O	2.663757	1.388099	-0.156188		
39134	H	-2.345991	-1.288912	-0.616671		
39135	H	0.435706	-1.012491	-1.978575		
39136	H	2.083365	-0.687491	-1.365868		
39137	Rotational constants (GHz):			1.2099800	0.8475700	0.6986500
39138	Vibrational harmonic frequencies (cm-1):					
39139		58.1627	82.5441			98.9037
39140		138.1392	156.2179			170.8804
39141		192.8056	198.1871			219.8046
39142		228.6075	264.7369			301.9742

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39143      324.2561      342.2651      359.8400
39144      419.7141      439.0173      475.2383
39145      529.2623      567.5989      667.1070
39146      756.9733      831.9109      865.8047
39147      930.4984      936.6373      967.6113
39148      996.4061      1052.2359     1062.5870
39149      1090.8629     1127.0388     1176.4810
39150      1227.9118     1259.9149     1291.2823
39151      1315.5355     1346.7949     1368.0885
39152      1392.1761     1403.2713     1420.9841
39153      1423.3936     1444.8992     1461.6550
39154      1492.7346     1500.6322     1850.4344
39155      3018.9654     3079.3573     3092.0206
39156      3100.9059     3159.1465     3168.3712
39157      3172.9214     3739.2545     3829.2660
39158 Zero-point correction (Hartree): 0.156260
39159
39160 diHPCARP_Ib.pmpmpmpu
39161 -----
39162 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18088531
39163 Electronic state : 2-A
39164 Cartesian coordinates (Angs):
39165 O      -1.796932      0.908607      -0.985145
39166 O      -0.484041      1.425773      -1.128387
39167 C       0.390226      0.831905      -0.180891
39168 C       0.575640     -0.680700     -0.495006
39169 C      -0.030218     -1.681713      0.492734
39170 O      -1.386323     -1.427976      0.737981
39171 O      -2.106082     -1.800402     -0.428992
39172 H      -2.225085     -0.933892     -0.853997
39173 C       1.674710      1.646057     -0.350244
39174 H       1.422513      2.699778     -0.252696
39175 H       2.098129      1.465191     -1.335910
39176 H       2.411497      1.375000      0.401326
39177 C      -0.106440      1.096835      1.233063
39178 O      -1.037627      1.811158      1.478522
39179 H       0.497519      0.635957      2.034497
39180 H       0.161310     -0.841053     -1.489449
39181 O       1.967263     -1.038441     -0.653509
39182 O       2.613444     -0.977067      0.473228
39183 H      -2.115884      1.409737     -0.215437
39184 H       0.107421     -2.691251      0.102654
39185 H       0.461452     -1.606990      1.461496
39186 Rotational constants (GHz): 1.0879800      0.9383600      0.6805500
39187 Vibrational harmonic frequencies (cm-1):
39188      20.5815      89.4223      114.3104
39189      147.3950      166.5902      203.1700
39190      235.7136      259.1090      268.9150
39191      285.5765      299.9255      333.7712
39192      358.4728      375.3640      391.2038
39193      469.4627      500.8196      541.3828
39194      558.0107      599.1935      627.9642
39195      732.7589      824.9705      903.9850
39196      932.9539      963.6591      987.5307
39197      994.2432      1054.6370     1059.2915
39198      1116.1574     1151.2296     1162.3419
39199      1217.5762     1237.7139     1243.4590
39200      1303.1593     1351.9347     1383.7848
39201      1397.5679     1411.9745     1419.0476
39202      1438.4624     1457.2448     1495.5803
39203      1496.1967     1500.3368     1858.2788
39204      2986.8587     3085.2860     3085.7114
39205      3127.7689     3151.7196     3168.2124
39206      3175.6739     3686.1009     3713.2596
39207 Zero-point correction (Hartree): 0.157474
39208
39209 diHPCARP_Ib.pmpmpmpu
39210 -----
39211 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18081273
39212 Electronic state : 2-A
39213 Cartesian coordinates (Angs):
39214 O       0.597552     -0.451761      1.799923

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39215 O 0.289525 0.763787 1.128067
39216 C 0.553276 0.645899 -0.254802
39217 C -0.384711 -0.304389 -1.014447
39218 C -1.861497 0.075392 -1.031072
39219 O -2.351965 0.666118 0.141229
39220 O -2.374144 -0.330524 1.149072
39221 H -1.562401 -0.135110 1.642611
39222 C 0.376385 2.068022 -0.792797
39223 H 1.115101 2.721132 -0.333069
39224 H -0.618697 2.425344 -0.536846
39225 H 0.505011 2.089061 -1.874751
39226 C 2.015549 0.273816 -0.487497
39227 O 2.829011 0.250684 0.392214
39228 H 2.295206 0.109554 -1.542486
39229 H -0.038225 -0.344107 -2.051480
39230 O -0.283475 -1.664958 -0.528127
39231 O 0.920958 -2.117536 -0.665508
39232 H 1.555406 -0.361274 1.930223
39233 H -2.022071 0.830696 -1.801202
39234 H -2.443040 -0.814218 -1.284263
39235 Rotational constants (GHz): 1.3238300 0.8244000 0.7595300
39236 Vibrational harmonic frequencies (cm-1):
39237 70.6721 94.0692 134.1700
39238 140.2470 172.5514 192.3422
39239 214.9184 238.9464 243.7011
39240 264.0804 291.4215 339.1995
39241 352.9434 375.8351 379.9469
39242 433.1834 467.0450 478.8700
39243 496.3113 591.6876 616.6184
39244 792.2041 846.4418 879.0587
39245 925.5276 929.4227 971.9481
39246 990.6220 1037.0516 1053.9543
39247 1130.0360 1152.8017 1167.8371
39248 1203.2594 1270.4338 1296.2687
39249 1322.8661 1362.0564 1375.5775
39250 1397.8062 1410.9748 1417.5898
39251 1425.9677 1433.3207 1466.5445
39252 1488.1540 1514.4315 1857.2725
39253 2987.1088 3061.4366 3071.3817
39254 3077.8622 3125.4909 3156.9132
39255 3169.9199 3740.2687 3765.8997
39256 Zero-point correction (Hartree): 0.156885
39257
39258 diHPCARP_Ib.ppmpttmu
39259 -----
39260 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18076237
39261 Electronic state : 2-A
39262 Cartesian coordinates (Angs):
39263 O -0.754899 -0.280759 2.121319
39264 O -0.356585 -1.122058 1.043402
39265 C -0.795125 -0.564368 -0.193116
39266 C 0.134934 0.530456 -0.716533
39267 C 1.500502 0.069956 -1.212393
39268 O 2.073021 -1.000451 -0.504143
39269 O 2.381467 -0.548730 0.806714
39270 H 1.691008 -1.002896 1.313467
39271 C -0.869120 -1.735248 -1.169359
39272 H -1.653602 -2.422562 -0.856459
39273 H 0.079924 -2.266061 -1.181233
39274 H -1.099687 -1.367139 -2.168415
39275 C -2.222384 -0.047462 -0.019020
39276 O -2.668814 0.860325 -0.656291
39277 H -2.827472 -0.634244 0.691907
39278 H -0.377022 1.060676 -1.520660
39279 O 0.282375 1.496417 0.359566
39280 O 0.824509 2.599888 -0.050029
39281 H -0.124770 0.455477 2.073781
39282 H 1.399199 -0.311828 -2.229027
39283 H 2.170985 0.931526 -1.225147
39284 Rotational constants (GHz): 1.1662000 0.8461500 0.7433300
39285 Vibrational harmonic frequencies (cm-1):
39286 58.4985 85.6948 92.2201

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39287      135.7349      169.1543      186.0923
39288      197.5582      221.7180      233.7140
39289      260.6241      292.5737      324.7996
39290      351.2806      355.6560      390.1196
39291      423.4850      457.9006      512.8804
39292      545.3766      562.8511      600.4442
39293      729.2900      845.3617      867.6918
39294      930.2740      964.7078      971.9430
39295      994.6371      1036.1571     1048.6006
39296      1098.4177     1147.0552     1172.1778
39297      1224.1627     1252.9536     1293.0703
39298      1310.4501     1352.5316     1377.0424
39299      1396.1022     1400.9983     1421.2211
39300      1441.7308     1457.3260     1471.3783
39301      1489.7986     1511.3505     1873.2720
39302      3005.0494     3075.9307     3080.2360
39303      3110.5256     3133.3644     3153.4447
39304      3170.8743     3742.8357     3760.6752
39305      Zero-point correction (Hartree): 0.156672
39306
39307      diHPCARP_Ib.ppmptmmu
39308      -----
39309      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18021256
39310      Electronic state : 2-A
39311      Cartesian coordinates (Angs):
39312      O      0.180796      0.364874      1.966216
39313      O      0.219458     -0.819497      1.187750
39314      C     -0.531498     -0.657217     -0.012483
39315      C     -0.036676      0.489331     -0.907520
39316      C      1.445489      0.501485     -1.247023
39317      O      2.271458      0.517195     -0.095915
39318      O      2.748463     -0.796339      0.154672
39319      H      2.072155     -1.134256      0.766088
39320      C     -0.362959     -1.985820     -0.743432
39321      H     -0.712099     -2.792257     -0.101530
39322      H      0.679899     -2.164179     -0.996645
39323      H     -0.972378     -1.978605     -1.643805
39324      C     -2.018267     -0.496470      0.341128
39325      O     -2.880310     -0.724804     -0.456851
39326      H     -2.222168     -0.234347      1.390730
39327      H     -0.627317      0.452970     -1.826279
39328      O     -0.255394      1.807569     -0.329969
39329      O     -1.473833      2.000280      0.057763
39330      H      0.943985      0.858010      1.619434
39331      H      1.718402     -0.338770     -1.881452
39332      H      1.657887      1.429353     -1.779885
39333      Rotational constants (GHz):      1.3313300      0.8206900      0.7172600
39334      Vibrational harmonic frequencies (cm-1):
39335      51.9485      87.5660      115.7905
39336      137.0666      173.3135      203.9401
39337      218.7385      226.5432      233.8827
39338      276.6150      287.9920      309.7024
39339      329.7193      345.5261      424.2651
39340      487.0526      503.5280      509.2138
39341      566.2846      590.1416      640.4561
39342      709.0836      801.2844      897.2564
39343      912.8212      951.5967      962.2045
39344      995.5925      1020.8697     1060.1788
39345      1111.2669     1136.6414     1158.7394
39346      1222.7721     1246.2083     1295.3931
39347      1302.8240     1345.3132     1366.6987
39348      1395.3329     1400.5262     1413.5660
39349      1452.4438     1466.7299     1473.8708
39350      1490.6799     1512.1185     1861.3727
39351      3025.1723     3083.4550     3085.8319
39352      3093.0144     3151.3345     3164.3456
39353      3177.6454     3686.7242     3714.1527
39354      Zero-point correction (Hartree): 0.156885
39355
39356      diHPCARP_Ib.ppmptpmu
39357      -----
39358      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17994859

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39359 Electronic state : 2-A
39360 Cartesian coordinates (Angs):
39361 O 0.159777 0.190261 1.948713
39362 O -0.012128 -0.962417 1.141708
39363 C -0.757386 -0.623965 -0.017521
39364 C -0.123503 0.465142 -0.901007
39365 C 1.358870 0.327703 -1.208550
39366 O 2.183150 0.087497 -0.081606
39367 O 2.448369 -1.305453 0.004305
39368 H 1.766158 -1.587786 0.635605
39369 C -0.869222 -1.933263 -0.794256
39370 H -1.290504 -2.702999 -0.149765
39371 H 0.111778 -2.261292 -1.134683
39372 H -1.528901 -1.790530 -1.647240
39373 C -2.163963 -0.191110 0.401928
39374 O -2.987343 0.143147 -0.398629
39375 H -2.367767 -0.257302 1.483897
39376 H -0.679763 0.450787 -1.839687
39377 O -0.442365 1.791283 -0.377719
39378 O 0.541443 2.370278 0.233504
39379 H 0.977050 0.574171 1.580667
39380 H 1.511776 -0.473311 -1.929815
39381 H 1.704176 1.264455 -1.644759
39382 Rotational constants (GHz): 1.2585100 0.8709300 0.7263100
39383 Vibrational harmonic frequencies (cm-1):
39384 76.5897 93.8653 109.4897
39385 143.0487 160.2606 199.3415
39386 214.0934 227.9945 244.5235
39387 270.3670 283.9191 298.2878
39388 327.2700 350.3595 422.7226
39389 490.7389 521.6179 536.5969
39390 548.2186 620.3209 638.2189
39391 711.9877 837.2060 878.6532
39392 919.9015 951.6907 962.4421
39393 976.1058 1018.7927 1065.4343
39394 1092.3002 1142.1895 1163.5191
39395 1232.4638 1249.7472 1263.8369
39396 1312.7093 1355.4858 1390.1505
39397 1397.0967 1403.3594 1413.3488
39398 1455.3282 1464.3335 1472.3158
39399 1493.4872 1511.3246 1870.4503
39400 3005.0430 3078.2569 3096.1133
39401 3105.8617 3148.8308 3156.9802
39402 3168.8033 3685.1482 3714.5710
39403 Zero-point correction (Hartree): 0.157064
39404
39405 diHPCARP_Ib.ppmpttmu
39406 -----
39407 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18226780
39408 Electronic state : 2-A
39409 Cartesian coordinates (Angs):
39410 O 0.229245 -0.597932 1.967259
39411 O 0.222751 -1.367651 0.776456
39412 C -0.607056 -0.744092 -0.194148
39413 C -0.160312 0.659610 -0.613321
39414 C 1.312116 0.851106 -0.940542
39415 O 2.176116 0.441780 0.105853
39416 O 2.707552 -0.838539 -0.201438
39417 H 2.057714 -1.424980 0.221077
39418 C -0.566659 -1.692535 -1.389418
39419 H -0.889818 -2.684560 -1.078706
39420 H 0.445989 -1.764215 -1.784109
39421 H -1.239359 -1.328874 -2.162933
39422 C -2.042168 -0.699146 0.332521
39423 O -2.919224 -0.150773 -0.267200
39424 H -2.208383 -1.252704 1.272196
39425 H -0.763288 0.955296 -1.472670
39426 O -0.520504 1.579063 0.456375
39427 O -0.525147 2.804912 0.034190
39428 H 0.952640 0.030891 1.796185
39429 H 1.585684 0.332054 -1.857482
39430 H 1.476974 1.920548 -1.076067

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39431 Rotational constants (GHz): 1.1627000 0.8794000 0.6882500
39432 Vibrational harmonic frequencies (cm-1):
39433 61.8149 78.5555 85.8153
39434 134.6060 156.3867 182.5149
39435 203.7938 210.2707 238.0292
39436 259.8545 290.7461 293.3742
39437 302.2696 361.9471 405.6412
39438 506.0266 510.4248 537.6168
39439 547.0999 603.9230 616.0854
39440 730.6480 818.7649 890.1885
39441 928.0948 950.9689 974.0202
39442 979.3753 1031.5989 1062.5492
39443 1099.4712 1132.0140 1169.5699
39444 1232.8934 1255.2132 1287.0801
39445 1301.9448 1337.9153 1370.8273
39446 1390.2701 1400.7787 1413.4282
39447 1457.6364 1468.2261 1473.9345
39448 1490.9748 1509.2743 1872.4212
39449 3003.3396 3077.9458 3092.9342
39450 3109.9635 3148.2955 3156.3332
39451 3169.1963 3683.3490 3703.2657
39452 Zero-point correction (Hartree): 0.156650
39453
39454 diHPCARP_Ib.pppppmpu
39455 -----
39456 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18023022
39457 Electronic state : 2-A
39458 Cartesian coordinates (Angs):
39459 O -1.224197 -0.246073 1.864643
39460 O -0.622809 -1.202200 1.002828
39461 C -0.446404 -0.626192 -0.271929
39462 C 0.422677 0.644652 -0.225256
39463 C 1.541271 0.595711 0.810666
39464 O 2.497426 -0.396424 0.521285
39465 O 3.102188 -0.051408 -0.723033
39466 H 4.016913 0.096747 -0.454297
39467 C 0.236284 -1.714342 -1.102861
39468 H -0.395930 -2.600549 -1.119069
39469 H 1.199029 -1.965758 -0.668385
39470 H 0.388188 -1.365508 -2.123274
39471 C -1.804554 -0.368957 -0.926807
39472 O -2.842226 -0.537390 -0.348293
39473 H -1.774807 -0.093458 -1.993047
39474 H 0.828197 0.838951 -1.217809
39475 O -0.330088 1.825196 0.144383
39476 O -1.199366 2.148515 -0.759312
39477 H -2.156672 -0.319519 1.603346
39478 H 2.011720 1.579621 0.864600
39479 H 1.140300 0.322512 1.785040
39480 Rotational constants (GHz): 1.3519600 0.7320600 0.6577100
39481 Vibrational harmonic frequencies (cm-1):
39482 46.8760 56.3414 92.0075
39483 118.4291 172.0069 179.7091
39484 185.5725 198.3019 238.2232
39485 243.6456 260.4173 272.4454
39486 345.4621 367.3441 398.6445
39487 402.4377 414.2425 517.2214
39488 531.6862 586.4846 627.3658
39489 663.1636 834.3217 909.0741
39490 937.1925 949.0231 984.3489
39491 1002.7060 1051.2117 1060.8852
39492 1116.6264 1151.7019 1171.2621
39493 1213.9025 1266.0943 1294.7130
39494 1305.1921 1340.6108 1379.9270
39495 1391.3402 1401.8778 1421.8961
39496 1430.2052 1434.8214 1484.9666
39497 1487.2535 1510.4235 1850.2215
39498 3008.6572 3074.5233 3082.9258
39499 3118.1349 3156.1962 3157.6598
39500 3190.3447 3732.3463 3832.3511
39501 Zero-point correction (Hartree): 0.156403
39502

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39503 diHPCARP_Ib.pppppptpu
39504 -----
39505 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18046145
39506 Electronic state : 2-A
39507 Cartesian coordinates (Angs):
39508 O -1.368318 -0.044026 1.814637
39509 O -0.928737 -1.108815 0.983901
39510 C -0.647336 -0.598251 -0.298610
39511 C 0.423941 0.500834 -0.291888
39512 C 1.474109 0.350966 0.802208
39513 O 2.251209 -0.811704 0.626574
39514 O 2.964308 -0.667952 -0.598745
39515 H 3.872634 -0.582128 -0.284453
39516 C -0.181468 -1.806872 -1.109873
39517 H -0.941014 -2.584676 -1.059312
39518 H 0.753576 -2.183229 -0.703261
39519 H -0.025833 -1.524031 -2.150162
39520 C -1.916325 -0.062274 -0.952532
39521 O -2.999475 -0.135381 -0.446181
39522 H -1.777117 0.376035 -1.958157
39523 H 0.907250 0.554430 -1.266614
39524 O -0.239170 1.777157 -0.096069
39525 O 0.508487 2.762767 -0.489235
39526 H -2.312002 -0.008549 1.594099
39527 H 2.102281 1.244084 0.801173
39528 H 0.996276 0.225288 1.771802
39529 Rotational constants (GHz): 1.2165600 0.7611800 0.6330800
39530 Vibrational harmonic frequencies (cm-1):
39531 54.0281 70.7303 94.3931
39532 112.5701 142.3941 181.1013
39533 191.9884 203.0113 210.1840
39534 231.9585 239.5491 298.6699
39535 325.5448 339.7369 356.4318
39536 408.4566 457.1152 477.4144
39537 489.9475 572.9412 590.2469
39538 717.9489 848.8470 912.8329
39539 935.1906 948.9472 982.1082
39540 1025.2321 1046.4431 1059.6822
39541 1104.2392 1136.1169 1183.2766
39542 1218.5473 1273.8360 1288.8835
39543 1296.4848 1337.9294 1382.6131
39544 1389.5973 1400.2905 1417.0608
39545 1421.7212 1427.4775 1483.5251
39546 1487.4703 1507.0653 1865.3331
39547 2969.4619 3079.2200 3079.8838
39548 3122.7227 3156.7972 3164.1255
39549 3178.4211 3755.2838 3827.0489
39550 Zero-point correction (Hartree): 0.156009
39551
39552 diHPCARP_Ib.pptmmpmpu
39553 -----
39554 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18095138
39555 Electronic state : 2-A
39556 Cartesian coordinates (Angs):
39557 O -1.274405 -0.155956 1.879951
39558 O -1.061999 -1.201147 0.942682
39559 C -0.732036 -0.638939 -0.310397
39560 C 0.511092 0.263253 -0.228169
39561 C 1.526040 -0.245927 0.778844
39562 O 2.808773 0.279931 0.526768
39563 O 3.253585 -0.308208 -0.694091
39564 H 4.059528 -0.751424 -0.403574
39565 C -0.436110 -1.836650 -1.210249
39566 H -1.263708 -2.541516 -1.158604
39567 H 0.474456 -2.339301 -0.890833
39568 H -0.308721 -1.508624 -2.240710
39569 C -1.944974 0.084730 -0.897432
39570 O -2.957168 0.247765 -0.274800
39571 H -1.857710 0.389281 -1.952240
39572 H 0.963923 0.348753 -1.215839
39573 O 0.194726 1.614703 0.186883
39574 O -0.493321 2.242895 -0.711799

```

39575	H	-2.182945	0.109114	1.662274	
39576	H	1.255927	0.110052	1.772554	
39577	H	1.553661	-1.335001	0.786636	
39578	Rotational constants (GHz):			1.3987100	0.6752900 0.6203600
39579	Vibrational harmonic frequencies (cm-1):				
39580		44.5864	58.4088		91.4617
39581		110.3608	153.3566		172.7417
39582		194.9231	201.6176		222.2909
39583		246.2182	252.4037		274.3046
39584		319.4192	363.1771		391.5749
39585		404.3647	440.0850		515.2828
39586		522.7582	583.0497		613.7381
39587		724.2802	862.3741		873.7174
39588		925.9262	940.7555		973.5252
39589		986.4802	1056.0599		1084.3577
39590		1104.9181	1155.1787		1170.7176
39591		1210.4470	1262.3435		1298.4034
39592		1302.6338	1328.6801		1372.8045
39593		1393.1267	1405.4679		1421.0975
39594		1429.9204	1437.9691		1468.1220
39595		1491.2818	1503.7752		1852.1411
39596		3014.9635	3079.2405		3097.2202
39597		3116.4240	3154.5148		3159.4744
39598		3164.4072	3727.2641		3833.9237
39599	Zero-point correction (Hartree): 0.156191				
39600					
39601	diHPCARP_Ib.pptmpmtpu				
39602	-----				
39603	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18215850				
39604	Electronic state : 2-A				
39605	Cartesian coordinates (Angs):				
39606	O	-1.367809	-0.074531	1.852128	
39607	O	-1.496210	-1.033339	0.813391	
39608	C	-1.034148	-0.463277	-0.389668	
39609	C	0.428764	-0.008258	-0.320968	
39610	C	1.274898	-0.878280	0.596675	
39611	O	2.593758	-0.407378	0.704815	
39612	O	3.189488	-0.451430	-0.583769	
39613	H	3.150039	0.484643	-0.831288	
39614	C	-1.204059	-1.565926	-1.432695	
39615	H	-2.227776	-1.933240	-1.402558	
39616	H	-0.527701	-2.391612	-1.220900	
39617	H	-0.989416	-1.182669	-2.429135	
39618	C	-1.916250	0.711248	-0.802124	
39619	O	-2.898680	1.034887	-0.199669	
39620	H	-1.603584	1.233549	-1.725169	
39621	H	0.853252	0.008018	-1.324238	
39622	O	0.470760	1.364622	0.143295	
39623	O	1.521504	1.984504	-0.301759	
39624	H	-2.195876	0.421412	1.756851	
39625	H	0.884509	-0.844142	1.611797	
39626	H	1.258841	-1.907670	0.229861	
39627	Rotational constants (GHz):			1.4915000	0.6521900 0.6076300
39628	Vibrational harmonic frequencies (cm-1):				
39629		72.3268	85.3154		106.1772
39630		132.9158	152.1494		190.1252
39631		200.6179	210.8618		229.2913
39632		238.9858	292.7614		318.9247
39633		330.1409	376.3984		405.2746
39634		439.4161	443.0868		477.2004
39635		486.4311	560.1876		594.6841
39636		758.4558	868.4007		880.0970
39637		933.0959	959.3573		984.4788
39638		993.7735	1051.9941		1071.8304
39639		1101.9315	1146.9107		1182.2344
39640		1217.0538	1280.2557		1294.4674
39641		1301.2835	1333.4904		1389.6757
39642		1402.1941	1413.9505		1418.6911
39643		1427.8607	1431.2312		1468.8176
39644		1489.4600	1505.2778		1868.6554
39645		2972.5832	3070.0888		3079.5224
39646		3119.0759	3158.9070		3161.9722

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39647          3166.2644          3754.1911          3768.2730
39648 Zero-point correction (Hartree): 0.156667
39649
39650 diHPCARP_Ib.pptmppmpu
39651 -----
39652 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18077792
39653 Electronic state : 2-A
39654 Cartesian coordinates (Angs):
39655 O      -1.281497      -0.196555      1.872949
39656 O      -1.103514      -1.215701      0.900546
39657 C      -0.756418      -0.622646     -0.333171
39658 C       0.516790       0.233325     -0.223309
39659 C       1.515501      -0.346663      0.759654
39660 O       2.803308       0.188339      0.576235
39661 O       3.283513      -0.378621     -0.646380
39662 H       3.840319       0.340162     -0.967629
39663 C      -0.505561      -1.798399     -1.275130
39664 H      -1.359720      -2.472253     -1.247428
39665 H       0.384418      -2.347254     -0.974719
39666 H      -0.366271      -1.439552     -2.293739
39667 C      -1.942736       0.164046     -0.892321
39668 O      -2.949536       0.340341     -0.264872
39669 H      -1.842441       0.505561     -1.934801
39670 H       0.968730       0.337910     -1.209272
39671 O       0.247488       1.579157      0.240695
39672 O      -0.397784       2.270610     -0.643712
39673 H      -2.183104       0.100942      1.669793
39674 H       1.229974      -0.070494      1.773686
39675 H       1.546816      -1.433568      0.686075
39676 Rotational constants (GHz): 1.3984500      0.6737500      0.6189200
39677 Vibrational harmonic frequencies (cm-1):
39678 41.3300      58.6118      90.7355
39679 109.6508      156.2458      168.9387
39680 176.6653      196.9228      222.9468
39681 243.0616      252.1779      274.4213
39682 317.8133      360.3124      391.2876
39683 401.4029      436.6364      505.5086
39684 523.6726      583.7451      612.0343
39685 723.5935      857.8948      873.3986
39686 927.2469      941.4873      976.2527
39687 985.5355      1056.0368      1082.2885
39688 1113.4455      1146.6334      1170.5568
39689 1209.5706      1261.7065      1297.4961
39690 1302.6479      1324.9083      1372.5872
39691 1404.6979      1416.7369      1421.4231
39692 1436.7589      1438.7586      1467.4679
39693 1491.0288      1504.6291      1853.2665
39694 3011.6892      3079.2817      3097.9252
39695 3117.7717      3157.7744      3159.6817
39696 3165.0175      3737.1089      3843.5994
39697 Zero-point correction (Hartree): 0.156173
39698
39699 diHPCARP_Ib.pptmpttmu
39700 -----
39701 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18079017
39702 Electronic state : 2-A
39703 Cartesian coordinates (Angs):
39704 O      -1.962518      -0.730326     -1.649961
39705 O      -1.570413       0.572361     -1.235945
39706 C      -1.117833       0.525922      0.110141
39707 C       0.340085       0.082673      0.218521
39708 C       1.307309       1.043169     -0.463961
39709 O       2.601338       0.513449     -0.583696
39710 O       3.121317       0.344508      0.726521
39711 H       2.968571      -0.603152      0.863769
39712 C      -1.304000       1.946800      0.637755
39713 H      -2.366678       2.161920      0.738252
39714 H      -0.878109       2.662870     -0.062794
39715 H      -0.822584       2.055844      1.608304
39716 C      -2.037521      -0.378501      0.926474
39717 O      -1.664571      -0.992073      1.882444
39718 H      -3.090758      -0.360231      0.599721

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39719	H	0.596642	-0.071847	1.265164	
39720	O	0.440392	-1.208281	-0.429184	
39721	O	1.443250	-1.906466	0.008920	
39722	H	-1.130155	-1.127462	-1.943047	
39723	H	0.989215	1.235016	-1.489944	
39724	H	1.335248	1.981285	0.094197	
39725	Rotational constants (GHz):			1.3452800	0.6699700 0.6418100
39726	Vibrational harmonic frequencies (cm-1):				
39727		53.3523	85.0347		96.5133
39728		122.7981	164.7381		190.2829
39729		203.5527	222.0128		227.6144
39730		271.5563	281.2556		297.5584
39731		333.4154	350.5843		384.4269
39732		421.9955	455.4017		478.8982
39733		553.7234	561.2176		585.5561
39734		642.6164	881.2584		895.5183
39735		938.7933	964.1052		981.9818
39736		990.4383	1050.4860		1073.6787
39737		1100.0177	1152.8024		1173.7660
39738		1230.2510	1255.0928		1294.1259
39739		1305.8271	1340.2085		1379.0018
39740		1399.3932	1410.5211		1412.1885
39741		1432.8261	1436.1317		1476.2262
39742		1488.6883	1509.3432		1873.1901
39743		3002.3789	3068.7038		3075.5259
39744		3125.9541	3141.4321		3154.5365
39745		3162.0236	3754.8641		3786.9695
39746	Zero-point correction (Hartree):			0.156515	
39747	diHPCARP_Ib.ptmmmtmmu				
39748	-----				
39749	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18082831				
39750	Electronic state : 2-A				
39751	Cartesian coordinates (Angs):				
39752	O	-2.669415	0.341924	-0.287090	
39753	O	-1.806702	0.255614	0.837961	
39754	C	-0.618623	-0.423890	0.457761	
39755	C	0.116968	0.365253	-0.638060	
39756	C	1.456827	-0.158876	-1.135742	
39757	O	2.347949	-0.649248	-0.163737	
39758	O	2.725779	0.438794	0.671843	
39759	H	3.643642	0.579260	0.407881	
39760	C	0.130951	-0.576574	1.775686	
39761	H	-0.552500	-0.995522	2.512709	
39762	H	0.469308	0.398995	2.118018	
39763	H	0.992354	-1.226073	1.657779	
39764	C	-1.035398	-1.800192	-0.048518	
39765	O	-0.557755	-2.358746	-0.993805	
39766	H	-1.836435	-2.254949	0.562363	
39767	H	-0.535074	0.426766	-1.509921	
39768	O	0.303686	1.729498	-0.182224	
39769	O	-0.743721	2.464387	-0.400207	
39770	H	-2.482662	1.245370	-0.588352	
39771	H	1.265231	-1.020563	-1.771453	
39772	H	1.933217	0.634611	-1.717719	
39773	Rotational constants (GHz):			1.1817300	0.8645600 0.6588500
39774	Vibrational harmonic frequencies (cm-1):				
39775		55.7027	78.1501		100.6329
39776		132.0825	152.0627		178.4663
39777		198.3952	199.9768		211.2392
39778		239.1227	260.0987		296.4465
39779		316.7973	343.5808		351.1072
39780		428.6616	475.7845		501.4708
39781		533.0506	557.6532		644.4432
39782		677.0208	835.0035		872.8191
39783		932.6952	950.0386		964.1200
39784		1007.1125	1044.3210		1052.5668
39785		1120.8879	1157.0609		1171.0033
39786		1237.5680	1261.9597		1294.7579
39787		1324.9353	1365.6329		1374.8873
39788		1391.0502	1402.1741		1411.2673
39789		1432.8277	1435.6861		1462.7683

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39791      1496.2247          1497.6031          1868.5103
39792      2980.8726          3061.8291          3086.8237
39793      3109.3102          3160.3158          3162.5178
39794      3192.9349          3746.3348          3821.9359
39795      Zero-point correction (Hartree): 0.156329
39796
39797      diHPCARP_Ib.ptmmpmmu
39798      -----
39799      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18134078
39800      Electronic state : 2-A
39801      Cartesian coordinates (Angs):
39802      O      -2.432382          1.154446          -0.339777
39803      O      -1.698849          0.755143          0.810610
39804      C      -0.846729          -0.314783          0.443231
39805      C      0.209851          0.141452          -0.577449
39806      C      1.366797          -0.829441          -0.803427
39807      O      2.266671          -0.870985          0.285499
39808      O      3.283394          0.096660          0.076960
39809      H      2.909212          0.887081          0.489876
39810      C      -0.283807          -0.817057          1.765558
39811      H      -1.110396          -1.073181          2.426662
39812      H      0.313030          -0.036427          2.233027
39813      H      0.344304          -1.691160          1.612824
39814      C      -1.728461          -1.401210          -0.168681
39815      O      -1.418569          -2.079249          -1.105396
39816      H      -2.695183          -1.517241          0.353636
39817      H      -0.280779          0.356233          -1.525961
39818      O      0.805855          1.377553          -0.113788
39819      O      0.098605          2.427021          -0.398950
39820      H      -1.903476          1.909584          -0.643434
39821      H      0.965520          -1.834665          -0.918212
39822      H      1.914066          -0.558698          -1.705071
39823      Rotational constants (GHz): 1.2614400      0.7891200      0.6128600
39824      Vibrational harmonic frequencies (cm-1):
39825      70.8017          76.6010          96.2343
39826      142.0061          150.8855          185.5442
39827      195.8580          210.5480          242.8672
39828      248.1970          282.5082          299.4734
39829      321.8515          347.7934          366.7618
39830      443.4438          495.1387          506.4772
39831      523.8834          557.1898          650.8930
39832      679.4068          788.1469          904.3408
39833      929.2687          958.5624          979.9265
39834      1003.9706          1034.3343          1053.0098
39835      1103.7005          1134.0939          1185.5549
39836      1234.9510          1259.0023          1298.5249
39837      1316.8378          1347.8566          1372.5698
39838      1396.2141          1404.8428          1415.8902
39839      1428.6506          1436.6121          1480.8382
39840      1487.4484          1501.2984          1868.6415
39841      2987.8725          3081.3534          3100.8561
39842      3125.5590          3158.1828          3160.7146
39843      3174.4297          3737.4607          3793.2273
39844      Zero-point correction (Hartree): 0.156599
39845
39846      diHPCARP_Ib.ptmpmmmmu
39847      -----
39848      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17936517
39849      Electronic state : 2-A
39850      Cartesian coordinates (Angs):
39851      O      2.419531          0.987515          -0.878933
39852      O      1.873681          0.887955          0.426859
39853      C      0.483190          0.608862          0.343829
39854      C      0.246896          -0.676631          -0.473647
39855      C      -1.186342          -1.065656          -0.785339
39856      O      -2.031996          -0.923415          0.336668
39857      O      -3.250854          -0.333070          -0.081895
39858      H      -2.996810          0.603547          -0.127694
39859      C      0.062625          0.529432          1.810471
39860      H      0.438689          1.412133          2.325685
39861      H      0.500371          -0.355360          2.266625
39862      H      -1.017243          0.482381          1.891658

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39863      C      -0.205204      1.809623      -0.296100
39864      O      -1.383462      1.863170      -0.525371
39865      H       0.463595      2.664858      -0.489313
39866      H       0.769037      -0.585972     -1.425092
39867      O       0.883943      -1.776188      0.219594
39868      O       2.155165      -1.837012     -0.040984
39869      H       2.847174       0.120318     -0.960588
39870      H      -1.545850      -0.426134     -1.588491
39871      H      -1.194006      -2.101171     -1.135571
39872      Rotational constants (GHz):      1.3289800      0.7871300      0.6078200
39873      Vibrational harmonic frequencies (cm-1):
39874          53.2677          72.7208          92.1741
39875          125.5187         131.1501         162.3390
39876          183.1664         202.5717         239.0629
39877          255.3766         279.6261         295.5613
39878          324.8941         346.5974         424.2515
39879          433.2064         497.2533         499.6533
39880          519.4119         566.8071         644.4134
39881          687.9042         807.6263         889.1320
39882          940.6001         956.7063         972.4573
39883         1010.2716         1050.8144        1060.7039
39884         1120.0767         1160.8702        1172.0781
39885         1230.4810         1248.1764        1285.3430
39886         1301.3499         1356.0112        1384.5177
39887         1400.6383         1406.7786        1420.3000
39888         1426.3070         1458.8575        1488.0209
39889         1491.1186         1502.6301        1850.4847
39890         3013.6310         3066.1665        3088.6074
39891         3121.1385         3141.8095        3162.5108
39892         3207.0816         3721.4487        3744.2377
39893      Zero-point correction (Hartree): 0.156501
39894
39895      diHPCARP_Ib.ptmpptmmu
39896      -----
39897      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17869318
39898      Electronic state : 2-A
39899      Cartesian coordinates (Angs):
39900      O       2.501184       0.851591       -0.508463
39901      O       1.793287       0.644939       0.704190
39902      C       0.397076       0.546350       0.434535
39903      C       0.124894      -0.618889      -0.525754
39904      C      -1.306852      -0.932996      -0.931378
39905      O      -2.240375      -1.048681       0.124672
39906      O      -2.833138       0.226991       0.337939
39907      H      -3.710042       0.101583      -0.045897
39908      C      -0.192210       0.400013       1.830520
39909      H       0.199758       1.204213       2.451810
39910      H       0.122281      -0.551165       2.255030
39911      H      -1.274685       0.449362       1.815345
39912      C      -0.016179       1.874201      -0.193524
39913      O      -0.610168       1.989907      -1.225857
39914      H       0.313861       2.748629       0.396629
39915      H       0.680919      -0.441764      -1.446555
39916      O       0.668612      -1.828613       0.059906
39917      O       1.940726      -1.957665      -0.163641
39918      H       2.809287      -0.050161      -0.691411
39919      H      -1.644627      -0.185015      -1.644579
39920      H      -1.298163      -1.915515      -1.406731
39921      Rotational constants (GHz):      1.2379300      0.8395400      0.6510400
39922      Vibrational harmonic frequencies (cm-1):
39923          51.2034          83.8970          99.9558
39924          133.5620         153.8976         173.3826
39925          177.2592         187.7391         217.2793
39926          244.6711         260.2318         282.2625
39927          294.9763         327.8277         372.6794
39928          425.8966         480.3594         513.6485
39929          531.6391         548.3853         643.9717
39930          667.3698         811.8752         899.1375
39931          935.7680         941.1605         949.4700
39932          1011.6397        1043.3135        1053.6953
39933          1114.7907        1150.2585        1161.2187
39934          1236.2350        1267.2707        1296.4932

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39935      1320.7114      1360.9716      1369.0281
39936      1394.9577      1403.9135      1417.2074
39937      1427.2256      1435.3126      1459.3401
39938      1497.4429      1504.6255      1869.9781
39939      2976.4357      3086.0825      3088.6096
39940      3114.7751      3157.5385      3157.8424
39941      3213.6652      3742.4539      3818.3765
39942 Zero-point correction (Hartree): 0.156193
39943
39944 diHPCARP_Ib.ptmtmtmmu
39945 -----
39946 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17887668
39947 Electronic state : 2-A
39948 Cartesian coordinates (Angs):
39949 O      2.704862      0.200174      -0.671232
39950 O      2.049371      0.228096      0.588175
39951 C      0.679893      0.540549      0.387407
39952 C      0.023292      -0.535346      -0.498521
39953 C     -1.453271      -0.428548      -0.815660
39954 O     -2.194555      -0.266866      0.376186
39955 O     -3.562183      -0.309316      0.004798
39956 H     -3.803672      0.625806      0.024147
39957 C      0.130357      0.640094      1.807282
39958 H      0.787484      1.285879      2.387999
39959 H      0.111781      -0.347401      2.263603
39960 H     -0.874787      1.047706      1.797015
39961 C      0.608131      1.920683      -0.258008
39962 O     -0.333007      2.335458      -0.872172
39963 H      1.505687      2.535293      -0.065241
39964 H      0.548908      -0.560887      -1.452615
39965 O      0.239708      -1.827053      0.121156
39966 O      1.399515      -2.325926      -0.179939
39967 H      2.739596      -0.756064      -0.834253
39968 H     -1.612513      0.419806      -1.480622
39969 H     -1.762573      -1.351277      -1.310808
39970 Rotational constants (GHz):      1.2513100      0.7576700      0.5821500
39971 Vibrational harmonic frequencies (cm-1):
39972      21.9881      53.4347      94.3914
39973      122.6887      132.7969      168.8810
39974      187.5745      200.4043      228.9369
39975      244.5926      253.3118      285.5986
39976      294.1914      328.5962      363.4397
39977      378.8191      440.8859      504.4535
39978      524.9940      567.4738      649.0175
39979      706.0563      797.8168      910.7679
39980      937.1408      959.7751      976.6162
39981      1034.3032      1053.2606      1066.9514
39982      1109.8613      1165.1263      1185.7189
39983      1236.1711      1252.5801      1287.0053
39984      1303.9313      1359.1761      1373.7661
39985      1400.0556      1410.0836      1412.6578
39986      1428.2795      1431.0574      1491.1609
39987      1500.4007      1506.4384      1865.7063
39988      2986.6046      3072.9841      3085.9443
39989      3118.7656      3130.7287      3160.3688
39990      3196.9444      3738.9371      3809.9281
39991 Zero-point correction (Hartree): 0.156076
39992
39993 diHPCARP_Ib.ptmtptmmu
39994 -----
39995 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17937154
39996 Electronic state : 2-A
39997 Cartesian coordinates (Angs):
39998 O     -2.743952      0.217855      -0.402669
39999 O     -1.956145      0.119500      0.776322
40000 C     -0.717400      -0.482424      0.439470
40001 C      0.070966      0.418521      -0.529591
40002 C      1.513949      0.054531      -0.819771
40003 O      2.267734      0.175121      0.370962
40004 O      3.600877      -0.177225      0.034387
40005 H      4.055516      0.668683      0.132566
40006 C     -0.055254      -0.738657      1.785885

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40007	H	-0.755501	-1.279492	2.420873	
40008	H	0.195318	0.208737	2.259132	
40009	H	0.854994	-1.318085	1.661720	
40010	C	-1.040963	-1.821172	-0.219778	
40011	O	-0.461138	-2.278379	-1.161717	
40012	H	-1.875452	-2.350148	0.275479	
40013	H	-0.458123	0.443431	-1.481957	
40014	O	0.086895	1.772886	-0.017358	
40015	O	-0.986113	2.435272	-0.321343	
40016	H	-2.573620	1.138361	-0.659649	
40017	H	1.560642	-0.963647	-1.204072	
40018	H	1.903175	0.747123	-1.570056	
40019	Rotational constants (GHz): 1.2491200 0.7408500 0.5838000				
40020	Vibrational harmonic frequencies (cm-1):				
40021		44.7735	62.6298	81.8016	
40022		111.0530	139.1750	169.6206	
40023		190.5483	194.5603	233.2614	
40024		240.8904	249.7010	275.4328	
40025		296.5017	324.7968	357.9553	
40026		377.4921	440.6415	500.4269	
40027		523.1811	560.5597	648.9271	
40028		704.4931	784.1256	922.0883	
40029		930.2566	957.6279	980.5801	
40030		1037.0412	1052.2615	1064.5187	
40031		1107.8645	1153.4434	1187.2364	
40032		1235.2192	1250.2491	1287.1106	
40033		1305.9577	1357.4840	1369.9594	
40034		1402.2150	1408.0514	1415.1479	
40035		1418.0224	1435.5924	1482.5664	
40036		1498.9396	1520.9168	1870.3372	
40037		2979.5206	3062.2980	3082.2960	
40038		3119.8806	3139.9534	3159.3358	
40039		3181.1891	3724.4985	3820.9429	
40040	Zero-point correction (Hartree): 0.155902				
40041	diHPCARP_Ib.ptpmpmmmu				
40042	-----				
40043	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18056862				
40044	Electronic state : 2-A				
40045	Cartesian coordinates (Angs):				
40046	O	2.132392	1.228952	-0.979761	
40047	O	1.601331	1.195537	0.337563	
40048	C	0.295741	0.615704	0.325019	
40049	C	0.350966	-0.791715	-0.300230	
40050	C	-0.920575	-1.626755	-0.179694	
40051	O	-1.999569	-0.997425	-0.836445	
40052	O	-2.939533	-0.555322	0.131131	
40053	H	-2.795154	0.407641	0.116825	
40054	C	-0.131690	0.601099	1.779142	
40055	H	-0.003314	1.595550	2.200820	
40056	H	0.476453	-0.105798	2.339687	
40057	H	-1.180494	0.324896	1.857251	
40058	C	-0.576982	1.557157	-0.510702	
40059	O	-1.694328	1.880780	-0.209800	
40060	H	-0.076887	1.978909	-1.394589	
40061	H	0.662865	-0.724145	-1.341384	
40062	O	1.351304	-1.569823	0.397711	
40063	O	2.554685	-1.388068	-0.050443	
40064	H	2.681805	0.428434	-0.973663	
40065	H	-0.746387	-2.586056	-0.668851	
40066	H	-1.173899	-1.809409	0.863036	
40067	Rotational constants (GHz): 1.3129300 0.8060200 0.6155500				
40068	Vibrational harmonic frequencies (cm-1):				
40069		58.4007	78.3203	113.7105	
40070		143.9400	170.0967	198.1075	
40071		205.3718	220.1432	236.7194	
40072		262.6580	281.4798	294.2074	
40073		334.9667	377.4404	388.9191	
40074		451.1763	515.0813	523.7049	
40075		549.7012	554.7282	593.9356	
40076		671.6110	755.9480	905.3428	
40077		937.0382	958.7718	1006.3248	

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40079      1032.8980      1038.4493      1053.2610
40080      1131.1917      1144.7085      1188.7918
40081      1200.8195      1259.1319      1290.8004
40082      1302.3472      1351.1245      1374.5086
40083      1404.6772      1409.9230      1429.8114
40084      1446.2817      1481.4332      1488.5035
40085      1498.7555      1505.8241      1848.8644
40086      3041.9146      3084.4295      3089.1766
40087      3121.2743      3147.1899      3168.6481
40088      3177.6437      3660.4167      3726.9616
40089      Zero-point correction (Hartree): 0.156938
40090
40091      diHPCARP_Ib.ptpmtmmu
40092      -----
40093      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18060160
40094      Electronic state : 2-A
40095      Cartesian coordinates (Angs):
40096      O      -2.254588      -1.046747      -0.831707
40097      O      -1.803677      -0.821846      0.498820
40098      C      -0.404663      -0.591868      0.446997
40099      C      -0.111591      0.755731      -0.257667
40100      C      1.206881      1.492276      0.026232
40101      O      2.332720      0.980818      -0.627821
40102      O      2.898238      -0.043882      0.176163
40103      H      2.619970      -0.828470      -0.322731
40104      C      0.043695      -0.628212      1.901696
40105      H      -0.282633      -1.560778      2.358726
40106      H      -0.414391      0.200453      2.441127
40107      H      1.126641      -0.550543      1.964468
40108      C      0.171387      -1.796615      -0.290756
40109      O      1.156162      -1.797831      -0.975429
40110      H      -0.413872      -2.714897      -0.114438
40111      H      -0.256816      0.656802      -1.332822
40112      O      -1.087097      1.715957      0.230040
40113      O      -2.206671      1.700899      -0.420032
40114      H      -2.568900      -0.160114      -1.074674
40115      H      1.083705      2.498163      -0.377117
40116      H      1.391341      1.572564      1.098159
40117      Rotational constants (GHz):      1.2688900      0.8158200      0.6304200
40118      Vibrational harmonic frequencies (cm-1):
40119      55.4585      93.8982      102.3744
40120      141.8636      149.8834      208.0954
40121      223.0489      227.7581      252.2700
40122      277.0496      293.3019      306.1187
40123      327.1350      373.2600      400.9760
40124      495.5727      524.8344      526.7956
40125      545.2778      574.1654      581.1875
40126      673.9889      744.4437      928.4724
40127      935.8135      964.1928      992.6687
40128      1003.4336      1048.6906      1058.0713
40129      1113.5676      1155.2684      1192.0426
40130      1232.0985      1248.7141      1293.5536
40131      1312.2067      1329.3164      1384.7486
40132      1401.9559      1413.4820      1420.1506
40133      1439.7143      1456.3199      1478.4991
40134      1500.7587      1506.1144      1863.4345
40135      3005.8554      3075.4351      3081.3071
40136      3120.6549      3135.7099      3152.4795
40137      3171.8571      3714.3504      3725.4438
40138      Zero-point correction (Hartree): 0.157091
40139
40140      diHPCARP_Ib.ptppmmu
40141      -----
40142      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.21209953
40143      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09646428
40144      T1 diagnostic: 0.019983
40145      E(MP2/Aug-CC-pVTZ) (Hartree): -721.05098339
40146      E(MP3/Aug-CC-pVTZ) (Hartree): -721.07382745
40147      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05410426
40148      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07566473
40149      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.54202263
40150      E(UHF/Aug-CC-pVTZ) (Hartree): -718.53690035

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40151 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18634163
40152 Electronic state : 2-A
40153 Cartesian coordinates (Angs):
40154 O -2.164980 -0.967800 -0.994183
40155 O -1.893280 -0.702320 0.376601
40156 C -0.491046 -0.549692 0.523393
40157 C 0.000099 0.737756 -0.174742
40158 C 1.305076 1.324393 0.367655
40159 O 2.360245 0.404730 0.410317
40160 O 2.830429 0.235775 -0.919366
40161 H 2.387858 -0.596371 -1.160907
40162 C -0.261589 -0.554490 2.027687
40163 H -0.708300 -1.448942 2.457964
40164 H -0.738809 0.318334 2.472116
40165 H 0.803697 -0.542318 2.249237
40166 C 0.118159 -1.809538 -0.083849
40167 O 1.054882 -1.853724 -0.830050
40168 H -0.410545 -2.725561 0.231432
40169 H 0.042257 0.589945 -1.252847
40170 O -0.949352 1.799018 0.083968
40171 O -1.959138 1.803578 -0.727856
40172 H -2.365068 -0.075507 -1.322368
40173 H 1.582430 2.192752 -0.230685
40174 H 1.151839 1.643035 1.399758
40175 Rotational constants (GHz): 1.2324500 0.8187200 0.6630100
40176 Vibrational harmonic frequencies (cm-1):
40177 71.5531 90.9862 106.4853
40178 155.9278 164.2514 207.1472
40179 213.6993 235.9962 250.6951
40180 266.0327 286.5417 320.9709
40181 344.2675 375.2949 414.8970
40182 500.9495 521.2958 534.8127
40183 557.6409 573.4304 602.5427
40184 672.3599 742.4343 927.8562
40185 948.5369 962.3617 988.8058
40186 1018.8457 1044.2655 1051.1486
40187 1127.0700 1153.0329 1199.0743
40188 1233.2290 1255.1749 1296.4707
40189 1303.8625 1339.0969 1379.3004
40190 1405.0069 1412.8575 1422.0628
40191 1443.0014 1469.7135 1482.0451
40192 1503.3457 1505.9177 1868.7324
40193 3003.0163 3074.8710 3081.0452
40194 3123.8826 3137.9851 3153.8453
40195 3165.7996 3664.4607 3715.6816
40196 Zero-point correction (Hartree): 0.157357
40197
40198 diHPCARP_Ib.ptppmtpmu
40199 -----
40200 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18454467
40201 Electronic state : 2-A
40202 Cartesian coordinates (Angs):
40203 O 2.180342 1.027503 -1.088172
40204 O 1.966959 0.640838 0.263855
40205 C 0.569279 0.511752 0.457576
40206 C -0.027173 -0.577293 -0.469523
40207 C -1.209402 -1.356267 0.101337
40208 O -2.272185 -0.513998 0.463717
40209 O -2.877873 -0.045307 -0.733064
40210 H -2.485142 0.842094 -0.798574
40211 C 0.419689 0.250123 1.951181
40212 H 0.890717 1.059996 2.506570
40213 H 0.915058 -0.685138 2.203923
40214 H -0.633123 0.196470 2.219780
40215 C -0.037309 1.877288 0.156192
40216 O -1.085241 2.065945 -0.396162
40217 H 0.584437 2.714713 0.517527
40218 H -0.306266 -0.126724 -1.420427
40219 O 0.998480 -1.521884 -0.844643
40220 O 1.431366 -2.211461 0.171313
40221 H 2.462823 0.192666 -1.488575
40222 H -1.539541 -2.093419 -0.632322

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40223      H      -0.914238      -1.867362      1.016746
40224      Rotational constants (GHz):      1.1987900      0.8672100      0.6619600
40225      Vibrational harmonic frequencies (cm-1):
40226      81.7391      102.6062      122.7608
40227      131.9747      166.7453      172.9164
40228      195.9773      246.9469      252.7382
40229      274.4830      292.7132      316.8705
40230      338.9800      351.1698      374.1504
40231      455.6115      462.0710      531.7924
40232      566.1351      586.2019      603.7256
40233      680.3458      782.9926      928.5929
40234      954.2571      968.7566      984.4371
40235      1010.8526      1048.4009      1052.8894
40236      1116.3621      1143.2576      1199.1929
40237      1225.4398      1244.1187      1257.5088
40238      1298.7956      1356.7786      1391.7066
40239      1399.6073      1408.8508      1415.9939
40240      1428.6968      1473.6520      1486.2025
40241      1500.0117      1509.1329      1863.4301
40242      3002.2223      3079.1666      3082.4800
40243      3132.3726      3149.8632      3157.9536
40244      3173.5269      3701.3499      3784.6849
40245      Zero-point correction (Hartree): 0.157244
40246
40247      diHPCARP_Ib.ptppmttmu
40248      -----
40249      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18259133
40250      Electronic state : 2-A
40251      Cartesian coordinates (Angs):
40252      O      -2.347113      -0.487672      -1.073021
40253      O      -2.038578      -0.643515      0.306121
40254      C      -0.624374      -0.655471      0.437882
40255      C      -0.002161      0.650224      -0.090540
40256      C      1.303231      1.076488      0.579542
40257      O      2.295347      0.086482      0.523470
40258      O      2.792746      0.053342      -0.806542
40259      H      2.301794      -0.705502      -1.164640
40260      C      -0.398520      -0.913749      1.921292
40261      H      -0.930026      -1.816921      2.216585
40262      H      -0.789770      -0.077290      2.499183
40263      H      0.662781      -1.037522      2.125879
40264      C      -0.138034      -1.867440      -0.349530
40265      O      0.824697      -1.898513      -1.062927
40266      H      -0.776362      -2.756107      -0.201605
40267      H      0.116842      0.601533      -1.171288
40268      O      -0.963153      1.697231      0.186304
40269      O      -0.760062      2.737907      -0.566368
40270      H      -2.638506      0.434339      -1.105407
40271      H      1.651433      1.998175      0.111813
40272      H      1.129878      1.256878      1.641301
40273      Rotational constants (GHz):      1.0944100      0.8744600      0.6531700
40274      Vibrational harmonic frequencies (cm-1):
40275      63.0241      76.2804      92.6725
40276      110.7371      145.1701      162.5536
40277      199.7971      241.7797      247.3488
40278      274.8248      291.0941      317.4913
40279      341.2995      345.3547      370.4822
40280      433.7686      463.7225      532.1913
40281      554.4686      568.8043      592.5565
40282      649.8348      783.5183      927.0739
40283      951.1625      963.0974      986.6434
40284      1043.3287      1048.6944      1064.2191
40285      1104.1460      1145.9539      1195.6476
40286      1231.4086      1267.3483      1283.5637
40287      1297.6549      1335.6859      1387.1358
40288      1398.6279      1405.6884      1411.9277
40289      1420.6929      1470.2348      1482.2744
40290      1503.8327      1506.4956      1867.5040
40291      2996.8677      3075.2820      3080.9585
40292      3128.7042      3141.9906      3153.3138
40293      3168.5440      3701.9429      3793.2921
40294      Zero-point correction (Hartree): 0.156737

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40295
40296 diHPCARP_Ib.pttmmmtmmu
40297 -----
40298 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18304856
40299 Electronic state : 2-A
40300 Cartesian coordinates (Angs):
40301 O 2.014912 -0.600128 -1.464068
40302 O 2.098714 -0.426451 -0.056428
40303 C 1.019119 0.392604 0.347650
40304 C -0.330251 -0.296737 0.080473
40305 C -1.510041 0.342222 0.786901
40306 O -2.734091 -0.184560 0.324242
40307 O -2.882421 0.218100 -1.030553
40308 H -3.518353 0.940731 -0.956152
40309 C 1.276160 0.658023 1.825962
40310 H 2.271719 1.079861 1.952951
40311 H 1.219658 -0.277355 2.380769
40312 H 0.543836 1.360938 2.219256
40313 C 1.128793 1.706767 -0.422727
40314 O 0.204427 2.421974 -0.682386
40315 H 2.168832 1.958956 -0.696992
40316 H -0.523640 -0.354222 -0.988863
40317 O -0.266116 -1.652596 0.583996
40318 O 0.285884 -2.475687 -0.251345
40319 H 1.535826 -1.444323 -1.516357
40320 H -1.492505 0.088768 1.848208
40321 H -1.478526 1.424160 0.659960
40322 Rotational constants (GHz): 1.1408900 0.7908500 0.6313000
40323 Vibrational harmonic frequencies (cm-1):
40324 51.0243 54.4130 90.8703
40325 118.6555 156.9696 181.8416
40326 194.5799 205.3746 220.2090
40327 240.8247 261.1559 274.8335
40328 294.9980 316.6529 376.2177
40329 402.7891 493.2716 524.9596
40330 542.8598 577.2356 597.6395
40331 673.2218 824.0745 878.1622
40332 931.5067 964.5618 971.5293
40333 1009.6408 1053.2854 1084.0288
40334 1102.0426 1159.0992 1185.6079
40335 1236.4465 1257.7270 1298.5889
40336 1306.6231 1333.7884 1374.5161
40337 1399.3121 1401.3700 1410.8620
40338 1429.7261 1442.7777 1473.0209
40339 1492.7115 1504.2911 1868.5028
40340 2989.8742 3075.4629 3085.7694
40341 3138.7505 3147.7902 3156.3158
40342 3160.0812 3695.8377 3817.8779
40343 Zero-point correction (Hartree): 0.156082
40344
40345 diHPCARP_Ib.pttmtmmu
40346 -----
40347 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18232147
40348 Electronic state : 2-A
40349 Cartesian coordinates (Angs):
40350 O -1.993963 0.762708 -1.424839
40351 O -2.068977 0.555431 -0.020954
40352 C -1.049692 -0.355981 0.342110
40353 C 0.344215 0.239650 0.077162
40354 C 1.485888 -0.495658 0.751906
40355 O 2.737485 0.022066 0.369329
40356 O 2.942433 -0.386651 -0.983215
40357 H 3.298512 0.424291 -1.365100
40358 C -1.309988 -0.650045 1.814203
40359 H -2.335904 -0.991776 1.940290
40360 H -1.169007 0.256628 2.400803
40361 H -0.634773 -1.425356 2.171886
40362 C -1.267036 -1.632637 -0.466905
40363 O -0.397025 -2.390374 -0.784008
40364 H -2.329754 -1.811823 -0.710672
40365 H 0.526611 0.311596 -0.993350
40366 O 0.380453 1.584403 0.614539

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40367      O      -0.099812      2.468452      -0.202349
40368      H      -1.459510      1.573377      -1.462271
40369      H      1.452906      -0.336541      1.830402
40370      H      1.425857      -1.560652      0.529126
40371      Rotational constants (GHz):      1.1489900      0.7812800      0.6264300
40372      Vibrational harmonic frequencies (cm-1):
40373      44.3678      53.6745      89.0500
40374      114.6595      156.8222      181.1163
40375      186.0360      200.4734      214.7585
40376      235.1184      255.9362      275.6605
40377      294.9641      315.7989      372.5134
40378      399.6428      485.7936      520.1417
40379      523.1360      572.1479      594.7825
40380      670.7656      820.6310      878.1053
40381      930.3583      962.7321      971.6352
40382      1010.1401      1052.1497      1080.3882
40383      1108.2828      1149.2584      1185.8047
40384      1237.2058      1256.5586      1297.5437
40385      1308.5543      1331.8257      1371.3894
40386      1398.5849      1408.6512      1412.6599
40387      1433.4321      1441.0324      1471.2928
40388      1492.6010      1504.2292      1871.7648
40389      2983.9364      3075.9844      3091.3021
40390      3138.9556      3151.4145      3156.7943
40391      3160.8687      3716.5071      3840.4546
40392      Zero-point correction (Hartree): 0.155964
40393
40394      diHPCARP_Ib.pttpttmu
40395      -----
40396      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17993700
40397      Electronic state : 2-A
40398      Cartesian coordinates (Angs):
40399      O      -1.765459      1.437033      -1.264475
40400      O      -1.935801      1.072472      0.099513
40401      C      -1.210516      -0.126321      0.325584
40402      C      0.281498      0.073979      0.034240
40403      C      1.205544      -1.000479      0.592393
40404      O      2.559549      -0.653854      0.431931
40405      O      2.838929      -0.591853      -0.958742
40406      H      2.833398      0.365966      -1.104018
40407      C      -1.525928      -0.476109      1.774765
40408      H      -2.605299      -0.486858      1.917269
40409      H      -1.091324      0.270024      2.438261
40410      H      -1.129940      -1.459148      2.021891
40411      C      -1.803223      -1.202898      -0.579021
40412      O      -1.182355      -2.120778      -1.029391
40413      H      -2.885636      -1.070725      -0.760125
40414      H      0.437377      0.176816      -1.037183
40415      O      0.642367      1.340695      0.634466
40416      O      1.579298      1.942962      -0.032928
40417      H      -1.203852      2.220739      -1.190316
40418      H      1.090896      -1.087229      1.673045
40419      H      0.977911      -1.952029      0.110420
40420      Rotational constants (GHz):      1.2451000      0.7438200      0.6189900
40421      Vibrational harmonic frequencies (cm-1):
40422      44.0302      62.5760      84.6047
40423      90.8409      124.5842      161.6111
40424      177.1969      208.4757      238.3893
40425      262.8565      282.0199      296.1544
40426      305.8955      317.2080      364.3779
40427      427.4532      441.2073      458.4410
40428      535.3400      551.4176      582.3161
40429      653.0570      871.2267      892.6789
40430      931.0972      960.6071      968.3045
40431      1026.5599      1049.9323      1080.5004
40432      1092.7936      1141.9787      1186.6210
40433      1236.0035      1271.3094      1295.0904
40434      1309.2967      1332.0492      1382.3120
40435      1395.8392      1406.8215      1411.2108
40436      1411.9629      1432.5018      1477.2948
40437      1494.5751      1504.2658      1874.0646
40438      2982.1950      3076.2959      3087.1560

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40439          3140.3850          3151.6864          3157.0703
40440          3163.4339          3768.5129          3799.8717
40441 Zero-point correction (Hartree): 0.155903
40442
40443 diHPCARP_Ib.pttpmtmmu
40444 -----
40445 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18156114
40446 Electronic state : 2-A
40447 Cartesian coordinates (Angs):
40448 O      -2.140741      1.256488      -0.968500
40449 O      -1.871612      0.940851      0.390593
40450 C      -1.072731     -0.226390      0.418527
40451 C       0.307006      0.031824     -0.214207
40452 C       1.348593     -1.039549      0.061694
40453 O      -2.542708     -0.786710     -0.647640
40454 O       3.404827     -0.013705      0.174221
40455 H       3.196628      0.892100     -0.089623
40456 C      -1.004298     -0.604945      1.892549
40457 H      -2.013945     -0.674049      2.293699
40458 H      -0.459329      0.159046      2.445095
40459 H      -0.508847     -1.565825      2.017579
40460 C      -1.828148     -1.313893     -0.341372
40461 O      -1.306165     -2.192039     -0.964774
40462 H      -2.924766     -1.229538     -0.237846
40463 H       0.206422      0.179200     -1.288845
40464 O       0.842593      1.265862      0.328912
40465 O       0.392624      2.321885     -0.277857
40466 H      -1.454834      1.921236     -1.143209
40467 H       1.574311     -1.113935      1.125328
40468 H       0.967962     -1.991578     -0.304958
40469 Rotational constants (GHz): 1.2627900      0.7363100      0.5818300
40470 Vibrational harmonic frequencies (cm-1):
40471 56.9360      61.0771      96.8186
40472 117.7259     146.9440     177.5037
40473 198.4737     207.5599     236.8875
40474 243.0706     264.0707     290.9525
40475 307.1226     322.7941     367.7723
40476 394.0130     501.8661     520.4474
40477 522.6832     570.5368     588.8832
40478 667.6427     818.4165     872.3818
40479 931.8046     961.3669     970.0152
40480 1014.6243    1052.3379    1085.7389
40481 1115.8840    1138.0215    1188.3461
40482 1237.3718    1254.8358    1293.7643
40483 1313.0617    1332.0796    1370.9782
40484 1400.3324    1408.4079    1411.5667
40485 1423.4706    1437.5886    1470.1658
40486 1493.5212    1503.1567    1871.0171
40487 2987.3636    3076.3303    3094.7464
40488 3125.5458    3157.0596    3157.4967
40489 3163.4396    3728.4513    3808.3371
40490 Zero-point correction (Hartree): 0.156125
40491
40492 diHPCARP_Ib.pttpptmmu
40493 -----
40494 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18077193
40495 Electronic state : 2-A
40496 Cartesian coordinates (Angs):
40497 O      -1.977357      1.157796     -1.226775
40498 O      -1.942734      0.871356      0.164319
40499 C      -1.090213     -0.239138      0.360942
40500 C       0.358553      0.091695     -0.041412
40501 C       1.379198     -0.929243      0.436231
40502 O       2.511846     -0.996496     -0.395920
40503 O       3.155158      0.272347     -0.353002
40504 H       3.986168      0.053521      0.085731
40505 C      -1.239481     -0.569817      1.841309
40506 H      -2.288950     -0.746587      2.070948
40507 H      -0.888009      0.269838      2.438811
40508 H      -0.669439     -1.461701      2.094744
40509 C      -1.647404     -1.392549     -0.471153
40510 O      -0.991414     -2.286889     -0.921196

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40511	H	-2.743812	-1.339361	-0.597234	
40512	H	0.438178	0.218209	-1.120036	
40513	O	0.709879	1.357299	0.571196	
40514	O	0.319342	2.377623	-0.124238	
40515	H	-1.297893	1.850156	-1.287151	
40516	H	1.667080	-0.704762	1.467813	
40517	H	0.955000	-1.929292	0.375806	
40518	Rotational constants (GHz):		1.2026800	0.7787200	0.6024100
40519	Vibrational harmonic frequencies (cm-1):				
40520		37.2495	48.1817		95.2129
40521		110.0555	145.8174		177.4607
40522		195.9273	203.5832		217.9351
40523		227.9820	247.2952		286.3255
40524		314.8960	335.3120		352.9540
40525		398.3861	470.3818		519.8120
40526		542.5582	575.7210		600.1202
40527		675.3147	823.7496		888.2742
40528		932.5637	962.2259		973.7097
40529		1007.8434	1054.7664		1085.9489
40530		1120.5609	1139.4689		1176.5616
40531		1235.3456	1255.7929		1303.1504
40532		1311.0203	1329.0263		1366.6753
40533		1395.2989	1400.2466		1411.0985
40534		1435.7068	1441.2791		1466.1434
40535		1490.4562	1504.4117		1869.7930
40536		2985.2556	3055.2985		3077.3197
40537		3132.3527	3156.5318		3158.8838
40538		3163.1867	3710.8440		3826.8895
40539	Zero-point correction (Hartree):		0.155886		
40540	diHPCARP_Ib.pttmtmmu				
40541	-----				
40542	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18141307				
40543	Electronic state : 2-A				
40544	Cartesian coordinates (Angs):				
40545	O	-2.409036	0.614255	-1.097233	
40546	O	-2.167140	0.391511	0.285296	
40547	C	-1.020803	-0.427415	0.402633	
40548	C	0.231562	0.293807	-0.125745	
40549	C	1.533902	-0.345485	0.295786	
40550	O	2.527191	0.231974	-0.524569	
40551	O	3.764663	-0.331403	-0.115530	
40552	H	4.234154	0.449650	0.201915	
40553	C	-0.944255	-0.763448	1.886056	
40554	H	-1.880912	-1.218429	2.203629	
40555	H	-0.786516	0.148315	2.460282	
40556	H	-0.130568	-1.460376	2.078787	
40557	C	-1.291552	-1.704405	-0.390852	
40558	O	-0.457896	-2.329114	-0.978693	
40559	H	-2.350941	-2.016433	-0.350834	
40560	H	0.187828	0.385900	-1.210166	
40561	O	0.263271	1.636083	0.420335	
40562	O	-0.470267	2.470525	-0.246323	
40563	H	-1.964990	1.469348	-1.225851	
40564	H	1.738246	-0.123322	1.346833	
40565	H	1.494284	-1.423622	0.141866	
40566	Rotational constants (GHz):		1.2349400	0.6962200	0.5545400
40567	Vibrational harmonic frequencies (cm-1):				
40568		58.3214	64.2909		96.7285
40569		114.6202	125.9833		184.0683
40570		199.0628	199.4845		215.2190
40571		233.4792	256.5820		285.3976
40572		293.5688	324.0021		367.6135
40573		373.2363	427.5602		517.0935
40574		534.7525	578.3025		614.8780
40575		683.5484	817.6588		891.3641
40576		930.3278	964.7592		1002.8056
40577		1037.3188	1054.2939		1087.7639
40578		1121.9983	1150.9700		1197.0524
40579		1236.9472	1258.5924		1279.5748
40580		1307.3458	1324.5683		1363.4195
40581		1400.6365	1409.4499		1412.5917
40582					


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40583      1432.1878      1443.8809      1491.1595
40584      1502.3707      1514.1596      1873.0565
40585      2983.9129      3060.6030      3076.5989
40586      3127.4639      3134.3581      3156.5660
40587      3161.2975      3709.0972      3827.3986
40588      Zero-point correction (Hartree): 0.156035
40589
40590      diHPCARP_Ib.ptttptmmu
40591      -----
40592      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18164996
40593      Electronic state : 2-A
40594      Cartesian coordinates (Angs):
40595      O      -2.408512      0.528111      -1.131728
40596      O      -2.184649      0.326850      0.257115
40597      C      -1.008580      -0.443588      0.403892
40598      C      0.223855      0.319469      -0.111295
40599      C      1.539661      -0.275543      0.334443
40600      O      2.524203      0.293642      -0.502212
40601      O      3.778208      -0.166089      -0.022768
40602      H      4.056585      -0.751772      -0.737788
40603      C      -0.945004      -0.758199      1.892675
40604      H      -1.867112      -1.248582      2.199965
40605      H      -0.836573      0.167204      2.456364
40606      H      -0.105710      -1.416250      2.110497
40607      C      -1.215271      -1.737601      -0.381015
40608      O      -0.351906      -2.326033      -0.964557
40609      H      -2.258755      -2.099259      -0.342876
40610      H      0.191941      0.400137      -1.197091
40611      O      0.198121      1.665722      0.421460
40612      O      -0.557044      2.464231      -0.264799
40613      H      -1.995760      1.399023      -1.259282
40614      H      1.740077      -0.009251      1.375141
40615      H      1.519978      -1.359960      0.222781
40616      Rotational constants (GHz):      1.2334400      0.6967200      0.5563100
40617      Vibrational harmonic frequencies (cm-1):
40618      57.8963      65.8205      101.9070
40619      117.3147      125.5513      183.7262
40620      190.8096      199.8383      210.8256
40621      233.0287      257.4822      286.5779
40622      292.0153      325.0693      367.2061
40623      376.2989      426.3864      517.7513
40624      536.2944      578.8662      614.6789
40625      684.1225      818.6640      894.0697
40626      930.3926      964.9628      1003.5272
40627      1037.9454      1054.3942      1091.3969
40628      1123.2908      1151.1672      1197.3487
40629      1236.4329      1259.4688      1280.8689
40630      1306.2490      1329.2607      1364.8653
40631      1399.6892      1408.7510      1411.6387
40632      1433.5767      1443.6142      1491.0866
40633      1502.5548      1513.8890      1870.4625
40634      2984.3421      3066.8646      3076.1288
40635      3124.9376      3132.1867      3156.3120
40636      3160.5382      3699.2418      3822.0186
40637      Zero-point correction (Hartree): 0.156035
40638
40639      diHPCARP_Ib.tmmmmmtmu
40640      -----
40641      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17926774
40642      Electronic state : 2-A
40643      Cartesian coordinates (Angs):
40644      O      2.940610      -0.014239      0.739921
40645      O      1.569114      0.099251      1.079632
40646      C      0.810467      0.468240      -0.059475
40647      C      -0.573011      0.744386      0.544786
40648      C      -1.193955      -0.442943      1.258771
40649      O      -1.139559      -1.633825      0.506821
40650      O      -2.106264      -1.525124      -0.537404
40651      H      -2.634065      -2.317755      -0.381657
40652      C      1.353197      1.714742      -0.753849
40653      H      2.367184      1.532735      -1.098302
40654      H      1.363055      2.543702      -0.047060

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40655	H	0.725868	1.980106	-1.602682	
40656	C	0.779763	-0.671194	-1.075612	
40657	O	1.614788	-1.535048	-1.097849	
40658	H	-0.020031	-0.620513	-1.832938	
40659	H	-0.484633	1.574138	1.248146	
40660	O	-1.409294	1.197624	-0.544971	
40661	O	-2.531285	1.680906	-0.112366	
40662	H	2.943956	-0.865699	0.271725	
40663	H	-0.602794	-0.655174	2.148944	
40664	H	-2.222190	-0.207296	1.535826	
40665	Rotational constants (GHz):			1.3314500	0.7738300 0.6367700
40666	Vibrational harmonic frequencies (cm-1):				
40667		48.4147	74.8354	92.7777	
40668		127.1967	147.7489	160.0942	
40669		169.4786	179.1921	205.7500	
40670		228.5991	257.7676	297.0827	
40671		320.0322	337.3558	362.9755	
40672		389.9278	452.1089	463.5560	
40673		529.5070	553.5431	667.4447	
40674		771.7629	829.2398	859.7728	
40675		917.2219	932.8192	969.2154	
40676		1002.7111	1047.7095	1061.6515	
40677		1104.8874	1135.9853	1175.6686	
40678		1215.5534	1279.3132	1292.9178	
40679		1312.4056	1351.1012	1366.7085	
40680		1394.3565	1402.7353	1421.9666	
40681		1425.1143	1458.1031	1466.4738	
40682		1490.1415	1502.2850	1848.6784	
40683		3009.7089	3080.8624	3087.1125	
40684		3099.0177	3150.9664	3157.4140	
40685		3179.2687	3713.7833	3832.7350	
40686	Zero-point correction (Hartree): 0.155856				
40687	diHPCARP_Ib.tnmpmnmumu				
40688	-----				
40689	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18104313				
40690	Electronic state : 2-A				
40691	Cartesian coordinates (Angs):				
40692	O	1.632449	-2.106896	-0.792799	
40693	O	0.816462	-0.984395	-1.079755	
40694	C	-0.124749	-0.792881	-0.038993	
40695	C	-1.009552	0.337294	-0.600982	
40696	C	-0.243166	1.605973	-0.915429	
40697	O	0.477553	2.030260	0.230955	
40698	O	1.854435	2.121876	-0.085991	
40699	H	2.211262	1.325288	0.342564	
40700	C	-0.941590	-2.044477	0.262791	
40701	H	-0.280942	-2.848216	0.576338	
40702	H	-1.475807	-2.351970	-0.634468	
40703	H	-1.666880	-1.848370	1.050312	
40704	C	0.583157	-0.348789	1.234136	
40705	O	1.784905	-0.360994	1.344757	
40706	H	-0.067548	-0.070896	2.077801	
40707	H	-1.529654	-0.029385	-1.485594	
40708	O	-2.012602	0.671781	0.382990	
40709	O	-3.124967	0.025593	0.194727	
40710	H	2.294959	-1.710959	-0.205682	
40711	H	0.449000	1.421082	-1.733142	
40712	H	-0.944877	2.392906	-1.196337	
40713	Rotational constants (GHz):			1.0922600	0.9380700 0.6433200
40714	Vibrational harmonic frequencies (cm-1):				
40715		39.9700	89.0236	98.7830	
40716		158.3246	165.6529	192.5341	
40717		206.3880	219.0291	239.4654	
40718		254.6220	304.3156	316.4482	
40719		351.4477	369.3722	388.6058	
40720		424.3545	459.6131	481.3310	
40721		498.5229	547.7231	617.1281	
40722		754.2073	836.1462	897.7100	
40723		912.0743	925.1130	973.8841	
40724		1014.9351	1047.5712	1061.6207	
40725		1123.3853	1131.9541	1171.2125	

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40727      1210.9333      1259.4904      1284.3153
40728      1296.4558      1344.5345      1353.5284
40729      1397.4402      1404.6351      1420.2039
40730      1444.1982      1475.5257      1479.5220
40731      1486.8386      1503.2484      1820.9897
40732      3021.8753      3084.4490      3085.0548
40733      3117.3867      3160.7125      3161.9042
40734      3175.6104      3704.7364      3759.8779
40735 Zero-point correction (Hartree): 0.156569
40736
40737 diHPCARP_Ib.tmmppmtmu
40738 -----
40739 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18151216
40740 Electronic state : 2-A
40741 Cartesian coordinates (Angs):
40742 O      2.600379      -0.763869      -0.826736
40743 O      1.268430      -0.349770      -1.076448
40744 C      0.427714      -0.784886      -0.024328
40745 C     -0.973063      -0.433367      -0.546537
40746 C     -1.163547      1.033141      -0.878765
40747 O     -0.779437      1.836031      0.225826
40748 O      0.289212      2.682648      -0.157226
40749 H      1.050975      2.248680      0.262457
40750 C      0.546692      -2.280511      0.253579
40751 H      1.550496      -2.523557      0.590723
40752 H      0.343626      -2.828362      -0.665492
40753 H     -0.172128      -2.581603      1.013205
40754 C      0.747456      -0.018143      1.253453
40755 O      1.713529      0.697878      1.350476
40756 H      0.080107      -0.200804      2.109764
40757 H     -1.197578      -1.050673      -1.417162
40758 O     -1.889204      -0.820817      0.507027
40759 O     -3.113947      -0.858711      0.081580
40760 H      2.909671      -0.056686      -0.239895
40761 H     -0.568181      1.298609      -1.748775
40762 H     -2.220187      1.209870      -1.085226
40763 Rotational constants (GHz): 1.1614500 0.8827900 0.6402400
40764 Vibrational harmonic frequencies (cm-1):
40765      47.7357      77.7919      118.6405
40766      151.9148      165.1065      182.1221
40767      196.1365      202.7457      230.0357
40768      252.4258      299.6015      306.9105
40769      345.9585      361.1393      388.8193
40770      422.3758      452.7496      489.8062
40771      494.2873      558.8251      654.3467
40772      743.8285      837.3591      892.4769
40773      907.4335      924.8671      975.7308
40774      1011.1256      1049.8990      1069.6949
40775      1102.7891      1131.0690      1172.5192
40776      1216.5783      1272.3628      1284.0650
40777      1301.6154      1345.3029      1359.6145
40778      1396.0713      1403.3569      1419.7938
40779      1441.8015      1475.8627      1477.6620
40780      1489.9542      1503.1957      1823.7500
40781      3030.3758      3082.2442      3089.4121
40782      3109.0087      3159.9850      3160.8793
40783      3176.2955      3707.1160      3762.5580
40784 Zero-point correction (Hartree): 0.156526
40785
40786 diHPCARP_Ib.tmpppmpmu
40787 -----
40788 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18056308
40789 Electronic state : 2-A
40790 Cartesian coordinates (Angs):
40791 O      2.529072      -0.731902      -0.656725
40792 O      1.316760      -0.022062      -0.832969
40793 C      0.237832      -0.710851      -0.205847
40794 C     -0.963345      0.193641      -0.569942
40795 C     -1.175979      1.408775      0.334588
40796 O      0.013253      2.109288      0.575835
40797 O      0.445973      2.657918      -0.661768
40798 H      1.143287      2.028585      -0.905216

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40799	C	0.073872	-2.119491	-0.766225		
40800	H	1.020012	-2.647320	-0.682585		
40801	H	-0.212205	-2.063961	-1.815546		
40802	H	-0.693276	-2.667126	-0.222633		
40803	C	0.467595	-0.792244	1.300345		
40804	O	1.491025	-0.455242	1.828520		
40805	H	-0.366177	-1.223561	1.878426		
40806	H	-0.814068	0.505797	-1.603103		
40807	O	-2.200629	-0.544172	-0.618211		
40808	O	-2.498887	-1.072213	0.531295		
40809	H	2.757624	-0.485382	0.255113		
40810	H	-1.931973	2.060135	-0.108272		
40811	H	-1.515610	1.080924	1.318478		
40812	Rotational constants (GHz):			1.0514000	0.9442700	0.6869300
40813	Vibrational harmonic frequencies (cm-1):					
40814		54.1526	96.5950			113.1012
40815		140.2075	156.4670			184.0573
40816		208.2600	226.6963			244.4893
40817		262.4628	303.7788			319.0700
40818		346.8986	359.9981			377.4555
40819		438.8346	490.2925			515.2738
40820		550.3984	590.0557			594.7855
40821		726.1612	832.7674			893.6256
40822		928.0868	961.0917			997.1509
40823		1003.8461	1056.3313			1073.6345
40824		1111.6980	1144.2735			1179.4390
40825		1205.4662	1249.7467			1257.8919
40826		1304.5448	1353.0158			1386.2460
40827		1402.9180	1415.5532			1422.8749
40828		1444.6901	1458.6081			1490.1485
40829		1492.7878	1505.0902			1855.1878
40830		3011.5192	3070.9965			3082.0357
40831		3119.6840	3134.2435			3159.4623
40832		3176.8285	3714.9885			3740.2735
40833	Zero-point correction (Hartree):			0.157048		
40834	diHPCARP_Ib.tmtmpmtmu					
40835	-----					
40836	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18035487					
40837	Electronic state : 2-A					
40838	Cartesian coordinates (Angs):					
40839	O	-2.853707	-0.865030	-0.947464		
40840	O	-1.438772	-0.858569	-0.870297		
40841	C	-1.014233	0.325960	-0.227609		
40842	C	0.519312	0.202926	-0.264224		
40843	C	1.039787	-1.103436	0.327654		
40844	O	2.432775	-1.082238	0.506043		
40845	O	3.032359	-0.996187	-0.778787		
40846	H	3.266618	-0.056450	-0.808553		
40847	C	-1.482756	1.586998	-0.941823		
40848	H	-2.568203	1.645077	-0.930662		
40849	H	-1.143328	1.556637	-1.975991		
40850	H	-1.070731	2.471591	-0.458520		
40851	C	-1.498303	0.349590	1.220493		
40852	O	-2.144494	-0.537263	1.706005		
40853	H	-1.231665	1.250791	1.798724		
40854	H	0.867570	0.328536	-1.288495		
40855	O	1.025451	1.314710	0.504527		
40856	O	2.221736	1.660617	0.137467		
40857	H	-3.082281	-1.264542	-0.093948		
40858	H	0.638739	-1.264696	1.329857		
40859	H	0.737642	-1.927495	-0.319321		
40860	Rotational constants (GHz):			1.4972700	0.6135700	0.5665500
40861	Vibrational harmonic frequencies (cm-1):					
40862		46.6861	75.2179			97.8118
40863		126.0324	152.1303			166.9480
40864		182.9415	211.8064			221.4110
40865		253.9232	276.3163			309.0942
40866		351.9594	373.0537			383.8023
40867		441.4063	444.1849			467.1691
40868		478.0870	565.8303			575.9665
40869		749.9572	836.5992			882.0542
40870						

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40871      926.1766      959.7473      986.2227
40872      1014.7786     1048.6671     1086.4056
40873      1095.4933     1146.4154     1184.1335
40874      1222.1671     1276.8790     1295.1899
40875      1305.1052     1332.0671     1364.4851
40876      1402.3919     1412.2026     1420.0116
40877      1435.3081     1441.8519     1472.7406
40878      1488.7070     1503.0135     1856.4921
40879      2997.1559     3080.0748     3080.8770
40880      3124.0260     3139.6575     3157.5593
40881      3171.3523     3755.8925     3766.4230
40882      Zero-point correction (Hartree): 0.156328
40883
40884      diHPCARP_Ib.tpmmpmmmu
40885      -----
40886      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.1808814
40887      Electronic state : 2-A
40888      Cartesian coordinates (Angs):
40889      O      1.199604      -1.911073      -1.005208
40890      O      0.340077      -0.802978      -0.806916
40891      C      0.564579      -0.239804      0.473238
40892      C      -0.515559      0.831146      0.665535
40893      C      -1.940947      0.332453      0.884239
40894      O      -2.306626      -0.813787      0.167231
40895      O      -2.389036      -0.464280      -1.204344
40896      H      -1.508213      -0.728658      -1.517383
40897      C      0.487466      -1.268235      1.602669
40898      H      1.321862      -1.960909      1.536085
40899      H      -0.441274      -1.827139      1.514404
40900      H      0.522113      -0.767534      2.570940
40901      C      1.951918      0.399443      0.515743
40902      O      2.793400      0.192399      -0.312302
40903      H      2.160449      1.013129      1.410596
40904      H      -0.235096      1.439316      1.529295
40905      O      -0.524292      1.735411      -0.466623
40906      O      0.581403      2.409603      -0.524744
40907      H      2.018004      -1.459543      -1.269654
40908      H      -2.051273      0.043996      1.930206
40909      H      -2.627541      1.154966      0.670226
40910      Rotational constants (GHz):      1.2470200      0.8480200      0.6903100
40911      Vibrational harmonic frequencies (cm-1):
40912      70.0771      96.9024      115.0457
40913      136.0364      179.2872      190.8996
40914      197.5695      226.6673      247.6285
40915      271.8902      292.4545      306.4594
40916      365.4054      372.9844      398.1789
40917      446.3202      490.7330      520.6099
40918      542.5794      583.1671      606.0084
40919      798.1780      842.8141      858.3714
40920      920.3124      930.9009      971.0761
40921      1008.9261      1036.3604      1070.0496
40922      1126.4389      1149.1744      1187.8569
40923      1209.6501      1255.5738      1287.7566
40924      1322.7493      1354.7848      1381.0966
40925      1397.9511      1411.8080      1422.0652
40926      1453.3145      1464.2137      1466.4101
40927      1487.7568      1512.7692      1858.7567
40928      2976.5208      3068.6177      3075.9925
40929      3080.2055      3127.4366      3156.5388
40930      3178.7797      3725.6110      3732.3651
40931      Zero-point correction (Hartree): 0.157116
40932
40933
40934
40935      (2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-Ic)
40936      =====
40937
40938      diHPCARP_Ic.mmpptpmu
40939      -----
40940      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17969857
40941      Electronic state : 2-A
40942      Cartesian coordinates (Angs):

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40943 O -1.749592 1.745598 -0.460777
40944 O -0.797670 1.488969 0.556094
40945 C 0.363342 0.889827 -0.016569
40946 C 0.008090 -0.508324 -0.569177
40947 C -0.588999 -1.474058 0.449376
40948 O -1.910121 -1.049297 0.851500
40949 O -2.735503 -1.004734 -0.148070
40950 H -2.441998 1.098326 -0.253724
40951 C 0.972052 1.767800 -1.106934
40952 H 1.179398 2.762287 -0.712977
40953 H 0.267884 1.857780 -1.930967
40954 H 1.893626 1.316588 -1.466954
40955 C 1.330681 0.916580 1.154332
40956 O 2.330609 0.252411 1.222271
40957 H 1.080109 1.652881 1.935957
40958 H -0.744807 -0.334001 -1.340639
40959 O 1.068626 -1.117475 -1.272829
40960 O 1.862840 -1.901377 -0.391598
40961 H 2.396611 -1.228579 0.066852
40962 H -0.666443 -2.463992 0.004672
40963 H -0.028894 -1.525017 1.378882
40964 Rotational constants (GHz): 1.1661500 0.8733700 0.6603100
40965 Vibrational harmonic frequencies (cm-1):
40966 34.0834 77.4302 101.6901
40967 143.3741 167.0245 183.7703
40968 204.6958 214.5164 223.8221
40969 252.9851 265.1857 306.6428
40970 313.3694 338.9306 405.6698
40971 439.2012 463.0515 490.1830
40972 556.6404 570.3428 628.7808
40973 667.7732 789.1347 909.2923
40974 948.1165 965.6837 983.9204
40975 996.1229 1042.5830 1063.9313
40976 1110.1416 1156.7912 1174.9694
40977 1190.5154 1236.4766 1284.4757
40978 1315.4722 1340.8198 1378.2406
40979 1396.7792 1411.2393 1429.1659
40980 1449.5783 1484.6474 1486.1603
40981 1488.0964 1502.2057 1853.0389
40982 3008.7811 3078.2412 3098.1629
40983 3115.6401 3157.8864 3175.6052
40984 3182.1203 3661.6031 3744.4348
40985 Zero-point correction (Hartree): 0.156417
40986
40987 diHPCARP_Ic.mmtmptpmu
40988 -----
40989 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18020395
40990 Electronic state : 2-A
40991 Cartesian coordinates (Angs):
40992 O 1.275481 2.142324 0.373675
40993 O 0.333630 1.703377 -0.588368
40994 C -0.604547 0.817658 0.017742
40995 C 0.150388 -0.459244 0.464977
40996 C 0.935568 -1.120544 -0.663829
40997 O 2.316509 -1.327539 -0.287842
40998 O 2.943064 -0.210202 -0.100813
40999 H 2.032596 1.566363 0.172145
41000 C -1.331446 1.459989 1.192975
41001 H -1.814390 2.383204 0.875406
41002 H -0.616406 1.689469 1.979515
41003 H -2.081081 0.771037 1.575682
41004 C -1.619167 0.633810 -1.101171
41005 O -2.521077 -0.159543 -1.066160
41006 H -1.507170 1.335058 -1.944957
41007 H 0.864006 -0.101815 1.210607
41008 O -0.637622 -1.365210 1.205598
41009 O -1.389744 -2.205664 0.344007
41010 H -2.123277 -1.631469 0.063572
41011 H 0.550256 -2.113122 -0.872535
41012 H 0.948766 -0.509086 -1.564372
41013 Rotational constants (GHz): 1.1450900 0.8597100 0.6209000
41014 Vibrational harmonic frequencies (cm-1):

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41015      50.2699      61.0823      84.1545
41016      129.6498     161.6022     183.0576
41017      212.3870     221.4359     244.5226
41018      261.1974     273.1595     294.4976
41019      307.6954     343.3732     459.1735
41020      460.3233     482.5545     546.0291
41021      560.2349     579.2443     605.6338
41022      682.1544     851.5591     906.3113
41023      917.9017     958.4376     981.7103
41024     1002.3499     1016.8098    1062.9422
41025     1110.2599     1158.7921    1171.0430
41026     1193.6244     1261.0544    1264.2641
41027     1330.2311     1338.8304    1378.7687
41028     1398.5224     1419.4360    1425.9306
41029     1473.0904     1481.9688    1484.8633
41030     1488.6962     1502.9749    1854.2319
41031     3003.5615     3079.9124    3094.1368
41032     3112.8468     3159.8805    3174.5662
41033     3193.9812     3677.5525    3698.2181
41034 Zero-point correction (Hartree): 0.156812
41035
41036 diHPCARP_Ic.mmtpppppu
41037 -----
41038 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18066307
41039 Electronic state : 2-A
41040 Cartesian coordinates (Angs):
41041 O      1.904008      1.980532      -0.226475
41042 O      1.829758      0.808158      0.580549
41043 C      1.159842     -0.202050     -0.166927
41044 C     -0.238930      0.326808     -0.564758
41045 C     -0.994487      0.861941      0.646192
41046 O     -2.295520      1.322195      0.239035
41047 O     -3.141441      0.344303      0.122273
41048 H      2.858404      2.101674     -0.294627
41049 C      1.945178     -0.645949     -1.385351
41050 H      2.931704     -0.999251     -1.084540
41051 H      2.056558      0.177012     -2.088148
41052 H      1.417125     -1.456245     -1.885856
41053 C      1.049690     -1.366991      0.830811
41054 O      0.938891     -1.209090      2.010736
41055 H      1.102630     -2.368601      0.375103
41056 H     -0.096521      1.134694     -1.284337
41057 O     -0.973392     -0.621610     -1.300234
41058 O     -1.268190     -1.726024     -0.457452
41059 H     -2.141485     -1.467862     -0.116670
41060 H     -1.125071      0.114910      1.425100
41061 H     -0.484018      1.733405      1.046713
41062 Rotational constants (GHz): 1.2801100      0.7396600      0.6606700
41063 Vibrational harmonic frequencies (cm-1):
41064      48.3721      81.1380      112.9804
41065     127.5692     159.5705     176.8515
41066     194.1621     199.0821     219.0915
41067     224.0471     271.3967     300.9249
41068     319.3521     326.1563     331.8239
41069     412.6278     490.0094     520.1332
41070     545.0678     584.3425     641.3207
41071     677.0127     802.0789     890.3980
41072     925.2281     977.3386     986.4961
41073     1005.0063     1022.1785     1046.7059
41074     1107.9400     1151.9679     1190.5838
41075     1207.8976     1241.2199     1257.6800
41076     1320.0930     1336.8401     1381.5190
41077     1396.0538     1405.5943     1411.9129
41078     1431.8280     1437.3151     1484.5126
41079     1489.4258     1503.0424     1865.6494
41080     3007.8157     3072.6151     3107.6958
41081     3126.1142     3149.5213     3162.4021
41082     3189.4997     3719.4363     3836.0685
41083 Zero-point correction (Hartree): 0.156307
41084
41085 diHPCARP_Ic.mptpptppu
41086 -----

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41087 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18186226
41088 Electronic state : 2-A
41089 Cartesian coordinates (Angs):
41090 O -0.531160 2.233877 0.450242
41091 O -1.374549 1.357508 -0.276009
41092 C -1.226317 0.038756 0.211405
41093 C 0.180802 -0.549752 -0.012332
41094 C 1.205434 -0.220176 1.062674
41095 O 2.406835 -0.983996 0.832420
41096 O 3.170041 -0.442061 -0.065999
41097 H 0.200339 2.310857 -0.183761
41098 C -1.702563 -0.080598 1.656020
41099 H -2.758126 0.181897 1.715338
41100 H -1.145644 0.605015 2.291181
41101 H -1.577824 -1.103316 2.011240
41102 C -2.210942 -0.742857 -0.663356
41103 O -2.207964 -1.937307 -0.724947
41104 H -2.952312 -0.122919 -1.195140
41105 H 0.050020 -1.635822 -0.026704
41106 O 0.655939 -0.280602 -1.318154
41107 O 1.164528 1.044558 -1.401107
41108 H 2.109428 0.877521 -1.247363
41109 H 1.473775 0.830515 1.101827
41110 H 0.852505 -0.551819 2.035354
41111 Rotational constants (GHz): 1.3128300 0.7141400 0.6471900
41112 Vibrational harmonic frequencies (cm-1):
41113 78.6240 84.7659 95.1592
41114 151.1193 170.3196 187.6157
41115 206.2110 220.2048 241.6540
41116 272.7188 287.1116 301.3043
41117 324.9592 354.5776 414.6100
41118 459.8973 504.6138 524.8308
41119 557.0878 572.4621 638.4307
41120 702.6114 837.0711 911.6649
41121 930.3032 952.6141 972.4652
41122 998.6921 1009.9753 1061.1602
41123 1127.1451 1137.0028 1180.0627
41124 1207.3566 1253.8051 1274.9084
41125 1313.0296 1343.9665 1391.4182
41126 1394.4329 1406.5936 1409.2580
41127 1445.0084 1471.4765 1483.7258
41128 1489.5441 1513.2441 1872.6288
41129 2999.8942 3071.8608 3082.0741
41130 3134.4381 3147.8868 3162.3211
41131 3198.4033 3709.1595 3725.6007
41132 Zero-point correction (Hartree): 0.157128
41133
41134 diHPCARP_Ic.mtmmpttmu
41135 -----
41136 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18134188
41137 Electronic state : 2-A
41138 Cartesian coordinates (Angs):
41139 O -1.499503 2.223784 0.519623
41140 O -1.867370 1.087122 -0.240836
41141 C -1.108106 -0.056180 0.137472
41142 C 0.197044 -0.083584 -0.671804
41143 C 1.143265 -1.244377 -0.370105
41144 O 1.775796 -1.101188 0.915870
41145 O 2.776568 -0.274996 0.881789
41146 H -0.682492 2.501080 0.077098
41147 C -0.935870 -0.162904 1.648824
41148 H -1.896929 0.014848 2.128870
41149 H -0.223723 0.574918 2.006797
41150 H -0.576353 -1.155360 1.917477
41151 C -2.034623 -1.190371 -0.297985
41152 O -1.694949 -2.133591 -0.952620
41153 H -3.068953 -1.068216 0.067713
41154 H -0.064665 -0.149420 -1.731494
41155 O 0.820793 1.163184 -0.423387
41156 O 1.909636 1.308635 -1.317466
41157 H 2.642567 1.000192 -0.759104
41158 H 0.600629 -2.184176 -0.332500

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41159      H      1.931889      -1.292979      -1.117051
41160 Rotational constants (GHz):      1.1826100      0.8005900      0.6396000
41161 Vibrational harmonic frequencies (cm-1):
41162      62.2127      83.7418      91.7883
41163      160.8271      171.8135      181.5354
41164      195.0610      224.1765      252.8572
41165      266.7744      285.2386      308.3626
41166      336.9383      353.1251      395.0687
41167      452.2628      463.6232      524.6503
41168      528.5483      541.4483      688.3975
41169      713.1197      795.3806      893.1264
41170      917.7560      954.9109      979.7091
41171      1008.5650      1051.9034      1057.2841
41172      1072.3774      1149.6166      1187.0419
41173      1231.0448      1250.9306      1270.1942
41174      1325.5850      1353.9665      1382.5481
41175      1390.3459      1403.0333      1417.3288
41176      1448.9480      1460.2623      1485.8242
41177      1488.0827      1497.3249      1866.7432
41178      2995.8655      3076.4904      3080.7430
41179      3123.4649      3155.4097      3177.8161
41180      3192.4097      3717.3482      3751.8849
41181 Zero-point correction (Hartree): 0.156949
41182
41183 diHPCARP_Ic.mttptppu
41184 -----
41185 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18204411
41186 Electronic state : 2-A
41187 Cartesian coordinates (Angs):
41188      O      1.838147      -2.022330      -0.247149
41189      O      1.951323      -0.688771      -0.708726
41190      C      1.167352      0.190807      0.084018
41191      C      -0.278181      0.198737      -0.458174
41192      C      -1.253813      0.957433      0.425345
41193      O      -2.545810      1.014612      -0.208482
41194      O      -3.230931      -0.072728      -0.027196
41195      H      1.013334      -2.309748      -0.667175
41196      C      1.314052      -0.087997      1.578010
41197      H      2.372978      -0.147865      1.827330
41198      H      0.837872      -1.027377      1.838980
41199      H      0.864435      0.721066      2.153954
41200      C      1.838557      1.537328      -0.172971
41201      O      1.243654      2.565430      -0.328373
41202      H      2.941421      1.487590      -0.171439
41203      H      -0.258661      0.666761      -1.444943
41204      O      -0.740139      -1.108087      -0.759048
41205      O      -1.039979      -1.812338      0.441067
41206      H      -1.996393      -1.652428      0.504401
41207      H      -1.380633      0.487497      1.397434
41208      H      -0.932285      1.990358      0.527347
41209 Rotational constants (GHz):      1.2663000      0.7988100      0.5732800
41210 Vibrational harmonic frequencies (cm-1):
41211      69.0300      82.4431      105.7789
41212      133.5914      174.9877      197.7758
41213      206.4126      220.5885      249.9411
41214      281.7387      289.0421      308.8562
41215      330.1146      347.1951      407.8086
41216      455.4598      469.4695      519.7698
41217      541.8349      583.9560      621.9219
41218      710.4093      811.2172      900.8624
41219      928.8976      968.1907      976.8761
41220      998.8104      1017.2976      1059.4144
41221      1124.1508      1134.7299      1189.3260
41222      1219.4528      1252.4152      1261.2998
41223      1312.4297      1342.0834      1388.7727
41224      1395.9627      1400.6138      1410.7045
41225      1435.1199      1444.6434      1485.0538
41226      1494.7238      1501.3406      1864.5604
41227      2994.4833      3076.0493      3097.1565
41228      3121.5118      3145.1444      3188.2749
41229      3193.2519      3725.5683      3767.1554
41230 Zero-point correction (Hartree): 0.157047

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41231
41232 diHPCARP_Ic.pmmmpmpu
41233 -----
41234 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18143046
41235 Electronic state : 2-A
41236 Cartesian coordinates (Angs):
41237 O -1.822248 -1.366334 -0.977411
41238 O -1.999538 0.025958 -0.750535
41239 C -0.890604 0.545112 -0.038640
41240 C 0.363741 0.523188 -0.954462
41241 C 1.039374 -0.825976 -1.165232
41242 O 1.272210 -1.551995 0.063048
41243 O 2.414062 -1.265622 0.607416
41244 H -2.135544 -1.728281 -0.132809
41245 C -1.281632 1.989194 0.264933
41246 H -2.238533 1.993918 0.783181
41247 H -1.375507 2.544241 -0.666929
41248 H -0.523638 2.465422 0.881638
41249 C -0.757293 -0.166541 1.308380
41250 O -1.559198 -0.976274 1.687500
41251 H 0.079988 0.162028 1.940473
41252 H -0.005668 0.829395 -1.937355
41253 O 1.292234 1.546497 -0.653090
41254 O 1.713393 1.423056 0.698626
41255 H 2.472445 0.823474 0.632287
41256 H 0.393381 -1.476447 -1.745355
41257 H 2.004238 -0.685895 -1.649432
41258 Rotational constants (GHz): 1.2008600 0.8770600 0.7343300
41259 Vibrational harmonic frequencies (cm-1):
41260 46.1513 65.5754 114.2333
41261 130.9340 181.8084 199.9496
41262 216.4522 229.2287 233.5318
41263 249.4888 293.1939 328.8934
41264 346.4405 375.9026 395.2790
41265 430.2040 481.1554 518.3229
41266 539.4322 548.0960 629.4397
41267 777.6721 813.5214 863.4438
41268 931.8110 954.3610 965.8697
41269 1019.7548 1032.7872 1052.6225
41270 1080.8123 1132.5566 1186.7256
41271 1217.1626 1235.2104 1270.4256
41272 1324.5807 1358.8753 1373.6112
41273 1397.8390 1401.6201 1415.7575
41274 1435.4782 1436.6269 1466.9236
41275 1489.8433 1498.7141 1845.3898
41276 3043.5991 3079.1082 3081.6026
41277 3113.4460 3160.5205 3176.9024
41278 3193.7176 3728.7534 3751.1685
41279 Zero-point correction (Hartree): 0.156880
41280
41281 diHPCARP_Ic.pmmmpmtmu
41282 -----
41283 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18485661
41284 Electronic state : 2-A
41285 Cartesian coordinates (Angs):
41286 O -1.815122 -1.252416 -1.110142
41287 O -1.870983 0.163628 -1.001846
41288 C -0.921668 0.634316 -0.066852
41289 C 0.504310 0.601396 -0.659045
41290 C 1.006875 -0.770902 -1.073719
41291 O 1.048714 -1.651075 0.065635
41292 O 2.112229 -1.451371 0.787326
41293 H -2.338345 -1.519840 -0.337624
41294 C -1.339211 2.081371 0.195899
41295 H -2.355972 2.096043 0.582667
41296 H -1.305117 2.635620 -0.741192
41297 H -0.663782 2.550033 0.907344
41298 C -1.033407 -0.097006 1.265672
41299 O -1.977822 -0.782857 1.547950
41300 H -0.218101 0.093756 1.981205
41301 H 0.507534 1.234066 -1.553249
41302 O 1.315926 1.177943 0.348346

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41303	O	2.650295	1.258467	-0.115204	
41304	H	3.026378	0.452652	0.274812	
41305	H	0.327550	-1.231606	-1.781976	
41306	H	2.012565	-0.704328	-1.480231	
41307	Rotational constants (GHz):		1.2927200	0.8076500	0.6832900
41308	Vibrational harmonic frequencies (cm-1):				
41309		52.3272	73.5288		129.1704
41310		132.9205	173.7164		195.2893
41311		196.3715	221.5321		237.6160
41312		258.9401	301.4490		323.7966
41313		331.1893	344.9466		405.0374
41314		442.2111	492.8694		507.7870
41315		531.5253	570.9986		659.6028
41316		746.2956	831.9762		882.1866
41317		931.4240	938.1927		983.1351
41318		1006.6245	1042.5554		1055.8589
41319		1081.6934	1142.8500		1179.7914
41320		1227.0260	1241.8935		1272.1916
41321		1315.1522	1354.0980		1373.9347
41322		1398.6752	1404.2001		1418.3969
41323		1439.1891	1446.0655		1484.3280
41324		1492.5392	1500.1931		1850.2323
41325		3021.9459	3053.7806		3078.7844
41326		3133.3812	3158.3337		3174.7007
41327		3206.9053	3720.8512		3735.0655
41328	Zero-point correction (Hartree):		0.156982		
41329					
41330	diHPCARP_Ic.pmpmtpmu				
41331	-----				
41332	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18072794				
41333	Electronic state : 2-A				
41334	Cartesian coordinates (Angs):				
41335	O	-1.092785	-1.939365	-0.677019	
41336	O	-0.320554	-1.831423	0.514421	
41337	C	0.621191	-0.782500	0.357029	
41338	C	-0.065018	0.597865	0.556204	
41339	C	-1.016186	1.075180	-0.548433	
41340	O	-2.373189	1.172386	-0.055240	
41341	O	-2.909162	0.017794	0.179339	
41342	H	-1.902877	-1.462353	-0.422186	
41343	C	1.640206	-1.021133	1.469519	
41344	H	2.089166	-2.006142	1.352635	
41345	H	1.132435	-0.980422	2.432434	
41346	H	2.410362	-0.255285	1.442453	
41347	C	1.349210	-0.994832	-0.955525	
41348	O	1.960674	-0.132543	-1.531550	
41349	H	1.337230	-2.033636	-1.320060	
41350	H	-0.652648	0.467383	1.469065	
41351	O	0.858602	1.611544	0.906385	
41352	O	1.413218	2.226101	-0.247396	
41353	H	1.906168	1.504387	-0.682154	
41354	H	-0.762290	2.090819	-0.831982	
41355	H	-1.028390	0.431815	-1.424489	
41356	Rotational constants (GHz):		1.1192600	0.8834600	0.6556300
41357	Vibrational harmonic frequencies (cm-1):				
41358		28.3856	72.2677		105.3530
41359		143.1139	168.3772		205.3578
41360		209.0751	233.3974		247.0017
41361		258.6374	303.0765		314.2956
41362		326.9414	358.4745		395.8868
41363		462.3382	546.0361		559.6801
41364		576.2748	597.5635		649.4360
41365		661.6671	863.9652		928.5080
41366		934.0402	959.3865		964.2896
41367		997.9832	1023.0698		1056.6126
41368		1093.1847	1146.3840		1182.9321
41369		1205.9698	1253.7950		1275.7122
41370		1321.5114	1340.2718		1356.1934
41371		1400.7032	1416.9720		1420.0184
41372		1467.9052	1486.0208		1493.3042
41373		1498.7010	1520.6350		1844.5498
41374		3028.8512	3077.9545		3081.9825

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41375          3129.9243          3153.7584          3179.0426
41376          3199.8360          3604.4538          3643.5449
41377 Zero-point correction (Hartree): 0.157136
41378
41379 diHPCARP_Ic.pmpmpmpmu
41380 -----
41381 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18128181
41382 Electronic state : 2-A
41383 Cartesian coordinates (Angs):
41384 O      -0.626509      -2.003865      -0.970984
41385 O      -0.181170      -1.842487      0.373260
41386 C       0.664042      -0.700754      0.431514
41387 C      -0.166297      0.599370      0.543536
41388 C      -1.143662      0.901953      -0.587560
41389 O      -2.321986      0.070182      -0.467208
41390 O      -3.049996      0.401780      0.555925
41391 H      -1.558384      -1.748936      -0.903061
41392 C       1.476753      -0.895905      1.709975
41393 H       2.115477      -1.773699      1.624884
41394 H       0.790219      -1.046862      2.542416
41395 H       2.082223      -0.012622      1.897235
41396 C       1.644444      -0.804380      -0.723345
41397 O       2.190139      0.122098      -1.261434
41398 H       1.880003      -1.844820      -1.000282
41399 H      -0.762486      0.484829      1.453624
41400 O       0.649917      1.725250      0.804075
41401 O       0.982041      2.390478      -0.406915
41402 H       1.670315      1.807628      -0.777715
41403 H      -1.459327      1.939092      -0.519168
41404 H      -0.749208      0.686183      -1.576400
41405 Rotational constants (GHz): 1.1194700      0.8744600      0.6658800
41406 Vibrational harmonic frequencies (cm-1):
41407      54.2184          81.3831          102.4408
41408      144.2041         165.2688         200.9320
41409      216.5649         226.7120         243.5283
41410      262.5339         292.2966         307.1278
41411      347.5786         367.1134         416.8714
41412      425.7265         502.5040         540.7106
41413      582.4412         594.4916         614.3384
41414      663.1436         803.2556         927.1600
41415      952.1964         956.6027         982.2957
41416      995.2321        1045.5015        1056.1768
41417      1110.3057        1143.6947        1188.5778
41418      1206.1385        1239.4554        1284.7103
41419      1322.0310        1337.9631        1374.3234
41420      1399.3490        1411.6601        1425.6538
41421      1430.8736        1482.5522        1490.5839
41422      1496.5230        1502.9440        1852.0736
41423      3018.1296        3074.6282        3076.5572
41424      3127.2758        3150.3103        3175.5459
41425      3193.5243        3621.6276        3769.2641
41426 Zero-point correction (Hartree): 0.157141
41427
41428 diHPCARP_Ic.pmtmppppu
41429 -----
41430 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18129774
41431 Electronic state : 2-A
41432 Cartesian coordinates (Angs):
41433 O      -1.293614          1.983630      -0.494537
41434 O      -1.533809          1.229739      0.686889
41435 C      -1.039734         -0.086267      0.540802
41436 C       0.506258         -0.117947      0.534775
41437 C       1.176471          0.833082     -0.448766
41438 O       2.583280          0.515031     -0.514375
41439 O       3.188012          0.786882      0.602828
41440 H      -2.026642          1.683290     -1.055580
41441 C      -1.548051         -0.819126      1.781046
41442 H      -2.635243         -0.869819      1.769578
41443 H      -1.230110         -0.272960      2.667893
41444 H      -1.133694         -1.824759      1.812846
41445 C      -1.665976         -0.788527     -0.657262
41446 O      -2.478650         -0.264490     -1.371990

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41447	H	-1.376772	-1.841110	-0.792823	
41448	H	0.839693	0.141554	1.541798	
41449	O	0.979423	-1.448041	0.382371	
41450	O	0.956873	-1.802997	-0.994118	
41451	H	1.892487	-1.718957	-1.227618	
41452	H	0.817355	0.713118	-1.465831	
41453	H	1.067001	1.864329	-0.130375	
41454	Rotational constants (GHz):		1.3546700	0.6998100	0.6250400
41455	Vibrational harmonic frequencies (cm-1):				
41456		37.4475	72.5809		90.4620
41457		128.7432	164.0860		191.5969
41458		213.2387	230.2828		258.8780
41459		268.6729	295.7046		320.4474
41460		334.1713	368.5545		377.6195
41461		391.9807	453.7263		510.3575
41462		533.4226	569.8752		676.9646
41463		713.4767	831.3126		882.6072
41464		931.5994	963.5953		981.9499
41465		994.0461	1034.7563		1054.2005
41466		1112.8464	1125.7054		1189.1736
41467		1235.2119	1239.9561		1254.9178
41468		1308.5774	1343.5179		1371.5561
41469		1398.3295	1407.1427		1414.5671
41470		1427.9267	1446.0183		1476.5809
41471		1492.8232	1502.2232		1843.4961
41472		3035.7281	3076.8333		3094.9298
41473		3140.7966	3157.2590		3167.4585
41474		3206.2809	3730.3747		3783.5527
41475	Zero-point correction (Hartree):		0.156875		
41476	diHPCARP_Ic.pmtpppppu				
41477	-----				
41479	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.18482211		
41480	Electronic state :		2-A		
41481	Cartesian coordinates (Angs):				
41482	O	-1.774804	-1.793073	-0.596849	
41483	O	-1.978586	-0.435988	-0.966795	
41484	C	-1.072657	0.397215	-0.269447	
41485	C	0.395161	0.053142	-0.661110	
41486	C	1.004643	-1.080096	0.159764	
41487	O	2.362803	-1.312107	-0.253717	
41488	O	3.195556	-0.484761	0.299976	
41489	H	-2.313309	-1.844649	0.208469	
41490	C	-1.425415	1.806513	-0.731745	
41491	H	-2.487533	1.978254	-0.566789	
41492	H	-1.205116	1.906857	-1.792615	
41493	H	-0.841551	2.541952	-0.183794	
41494	C	-1.330590	0.324070	1.230455	
41495	O	-2.145898	-0.408090	1.723840	
41496	H	-0.733045	1.019472	1.842315	
41497	H	0.364526	-0.234391	-1.714335	
41498	O	1.230453	1.188196	-0.663688	
41499	O	1.370243	1.652340	0.673017	
41500	H	2.216548	1.241385	0.916690	
41501	H	1.018902	-0.858482	1.225987	
41502	H	0.475587	-2.007616	-0.029711	
41503	Rotational constants (GHz):		1.3877000	0.7059100	0.6135600
41504	Vibrational harmonic frequencies (cm-1):				
41505		47.8811	80.0052		105.5637
41506		150.3838	186.0355		198.2652
41507		200.5568	237.5044		241.0581
41508		273.5403	301.9741		310.4714
41509		340.1169	370.9208		383.8317
41510		440.9618	500.5872		521.2464
41511		527.8181	571.9659		643.9434
41512		720.9222	833.7638		897.1444
41513		935.7766	965.6943		981.1376
41514		1002.6130	1025.0930		1052.2702
41515		1110.1111	1129.8184		1189.5844
41516		1222.1659	1224.1146		1253.5735
41517		1326.9300	1336.2457		1372.1828
41518		1398.9159	1400.5797		1416.9083

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41519      1437.0035      1438.2220      1486.0509
41520      1489.9439      1497.7678      1847.0382
41521      3012.1697      3082.1020      3097.7741
41522      3111.1324      3163.0288      3174.2282
41523      3195.7142      3720.5771      3746.4162
41524 Zero-point correction (Hartree): 0.157033
41525
41526 diHPCARP_Ic.ppmmttmu
41527 -----
41528 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18126868
41529 Electronic state : 2-A
41530 Cartesian coordinates (Angs):
41531 O      -0.265493      -1.151835      1.785381
41532 O      -0.756711      -1.534275      0.510275
41533 C      -1.117177      -0.374372      -0.217216
41534 C      0.087814      0.476671      -0.649093
41535 C      1.225751      -0.333248      -1.267230
41536 O      1.924280      -1.082405      -0.252851
41537 O      2.822987      -0.362116      0.351477
41538 H      0.688486      -1.083506      1.632087
41539 C      -1.873113      -0.908336      -1.430834
41540 H      -2.740819      -1.472833      -1.094344
41541 H      -1.246435      -1.575512      -2.019476
41542 H      -2.209578      -0.075862      -2.044559
41543 C      -2.097707      0.479944      0.587310
41544 O      -2.512593      1.522175      0.171602
41545 H      -2.434738      0.035476      1.537849
41546 H      -0.264931      1.197136      -1.392421
41547 O      0.545086      1.181788      0.486251
41548 O      1.459531      2.169183      0.037222
41549 H      2.306232      1.745092      0.244965
41550 H      0.860269      -1.074636      -1.972716
41551 H      1.951425      0.320576      -1.743855
41552 Rotational constants (GHz):      1.3179700      0.7961200      0.6830900
41553 Vibrational harmonic frequencies (cm-1):
41554      48.0416      79.3820      86.0811
41555      131.9185      167.2559      191.3657
41556      201.8928      208.9091      225.4877
41557      243.0020      285.8803      301.4405
41558      311.1243      343.6568      367.9737
41559      384.8816      474.1591      511.9023
41560      532.7091      547.7610      614.9688
41561      728.4704      822.3319      888.0905
41562      934.8648      954.9301      974.0514
41563      1015.4615      1041.5291      1050.1351
41564      1063.0231      1141.5379      1181.1390
41565      1233.5477      1247.5343      1263.2359
41566      1320.2590      1347.8041      1374.4320
41567      1382.2044      1398.9704      1409.5500
41568      1427.7416      1441.2597      1477.7420
41569      1486.8342      1511.7043      1868.9752
41570      3011.5821      3071.9658      3082.1160
41571      3122.2954      3157.1022      3171.0350
41572      3184.7777      3762.9620      3780.0493
41573 Zero-point correction (Hartree): 0.156262
41574
41575 diHPCARP_Ic.pppmpmpu
41576 -----
41577 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18103660
41578 Electronic state : 2-A
41579 Cartesian coordinates (Angs):
41580 O      2.094142      -0.699678      -1.434988
41581 O      0.898482      -1.363185      -1.035429
41582 C      0.431022      -0.805532      0.188907
41583 C      -0.362509      0.482010      -0.048097
41584 C      -1.582196      0.319021      -0.946548
41585 O      -2.646462      -0.391202      -0.284305
41586 O      -3.094635      0.268288      0.740390
41587 H      1.779364      0.174834      -1.713194
41588 C      -0.397202      -1.906348      0.839817
41589 H      0.256970      -2.716246      1.159379
41590 H      -1.109740      -2.305196      0.120677

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41591      H      -0.947525      -1.519544      1.696103
41592      C      1.650354      -0.536085      1.063626
41593      O      1.833684      0.483653      1.670150
41594      H      2.351475      -1.384676      1.126208
41595      H      -0.680766      0.900779      0.906041
41596      O      0.487516      1.418206      -0.706365
41597      O      0.670863      2.567883      0.099100
41598      H      1.271039      2.227130      0.785003
41599      H      -1.949821      1.304847      -1.222436
41600      H      -1.356518      -0.272029      -1.832434
41601      Rotational constants (GHz):      1.1836700      0.7647700      0.6592100
41602      Vibrational harmonic frequencies (cm-1):
41603      40.4650      64.4761      92.0727
41604      124.2231      131.8990      191.0444
41605      199.0472      210.3066      233.9815
41606      269.5279      274.0128      313.6392
41607      346.3796      362.4740      389.3773
41608      426.2026      460.1930      516.7134
41609      537.7273      575.8181      600.9198
41610      660.2455      784.7053      922.4194
41611      951.0777      972.1504      987.9975
41612      1025.8907      1038.4008      1052.2021
41613      1117.2529      1137.2118      1174.1878
41614      1229.0409      1249.5894      1265.6391
41615      1299.8132      1335.5231      1377.5227
41616      1401.2709      1408.4730      1417.2815
41617      1460.4076      1478.6948      1484.8389
41618      1489.3724      1503.3474      1855.0202
41619      3009.5248      3075.4954      3105.3650
41620      3121.8266      3154.7016      3162.7299
41621      3171.4400      3700.6871      3745.6899
41622      Zero-point correction (Hartree): 0.156482
41623
41624      diHPCARP_Ic.pppmttptu
41625      -----
41626      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18114148
41627      Electronic state : 2-A
41628      Cartesian coordinates (Angs):
41629      O      2.300552      0.315812      -1.371464
41630      O      1.352078      -0.740043      -1.275288
41631      C      0.738785      -0.711900      0.005181
41632      C      -0.373052      0.334922      0.092078
41633      C      -1.519841      0.110152      -0.883812
41634      O      -2.440165      -0.881003      -0.388170
41635      O      -3.074425      -0.456481      0.662826
41636      H      1.745059      1.093988      -1.529719
41637      C      0.197701      -2.122870      0.213210
41638      H      1.029879      -2.820207      0.296893
41639      H      -0.413913      -2.417896      -0.637550
41640      H      -0.408036      -2.167421      1.116419
41641      C      1.801601      -0.465913      1.070967
41642      O      1.580709      0.109319      2.096961
41643      H      2.779958      -0.921480      0.842049
41644      H      -0.756922      0.354219      1.114158
41645      O      0.238791      1.583681      -0.205046
41646      O      -0.645989      2.619250      0.181455
41647      H      -0.307376      2.845010      1.059049
41648      H      -2.065799      1.040704      -1.019281
41649      H      -1.166419      -0.277541      -1.837955
41650      Rotational constants (GHz):      1.1410800      0.7493500      0.6543100
41651      Vibrational harmonic frequencies (cm-1):
41652      52.2047      65.3234      83.5222
41653      111.1447      126.8933      183.1090
41654      200.6703      206.4547      235.0128
41655      259.3841      283.3380      299.1436
41656      319.6740      343.3569      350.1316
41657      393.3733      434.0828      468.7903
41658      546.2896      562.9373      616.9105
41659      653.0187      794.1737      928.1298
41660      957.1887      972.9069      982.5442
41661      1035.9497      1043.6479      1056.8597
41662      1108.7784      1131.4028      1182.1339

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41663      1230.9130      1252.9774      1258.7449
41664      1309.4417      1339.7979      1388.5156
41665      1401.1962      1408.3532      1413.3190
41666      1426.4230      1453.2923      1482.7611
41667      1490.4174      1503.1450      1869.2999
41668      3000.4182      3076.3640      3099.3744
41669      3108.3946      3154.8879      3165.1089
41670      3173.1982      3760.5717      3792.7528
41671      Zero-point correction (Hartree): 0.156164
41672
41673      diHPCARP_Ic.pppppmpmu
41674      -----
41675      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18276858
41676      Electronic state : 2-A
41677      Cartesian coordinates (Angs):
41678      O      -2.010734      0.430428      1.356136
41679      O      -1.014727      -0.583808      1.286672
41680      C      -0.418531      -0.625887      0.002531
41681      C      0.583704      0.518980      -0.220882
41682      C      1.756344      0.495093      0.751113
41683      O      2.774197      -0.431627      0.327639
41684      O      3.345573      -0.045809      -0.772382
41685      H      -2.787517      -0.067326      1.056406
41686      C      0.291536      -1.982231      -0.036996
41687      H      -0.450911      -2.776524      0.001746
41688      H      0.953371      -2.078437      0.821185
41689      H      0.887226      -2.080604      -0.943720
41690      C      -1.464378      -0.687171      -1.100005
41691      O      -2.620006      -0.941602      -0.898041
41692      H      -1.069660      -0.557467      -2.122212
41693      H      0.971779      0.456054      -1.243963
41694      O      0.025615      1.796635      0.001225
41695      O      -1.104225      1.942442      -0.838319
41696      H      -1.814513      1.811854      -0.189555
41697      H      2.200963      1.486512      0.801798
41698      H      1.451664      0.159968      1.740315
41699      Rotational constants (GHz):      1.4460400      0.6919200      0.6099600
41700      Vibrational harmonic frequencies (cm-1):
41701      63.1702      69.0680      118.6322
41702      151.4372      185.8705      207.8603
41703      222.0893      232.6219      243.1156
41704      270.0668      301.1543      315.0494
41705      345.7863      371.7640      391.4524
41706      433.4996      468.2805      528.7262
41707      564.5099      590.2311      615.5368
41708      700.2313      845.3262      918.4596
41709      925.0010      966.7015      992.6775
41710      1003.1353      1047.2097      1066.4710
41711      1118.9758      1150.3747      1169.1365
41712      1209.4696      1239.6535      1280.2840
41713      1314.1957      1332.5563      1391.8592
41714      1403.2717      1411.5291      1423.0865
41715      1434.4157      1451.6108      1484.0712
41716      1494.2519      1513.8407      1849.4842
41717      2993.7890      3050.2903      3078.6877
41718      3111.2299      3160.1199      3165.0606
41719      3175.2495      3739.6825      3754.5149
41720      Zero-point correction (Hartree): 0.157321
41721
41722      diHPCARP_Ic.pppppmpmu
41723      -----
41724      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18313675
41725      Electronic state : 2-A
41726      Cartesian coordinates (Angs):
41727      O      -2.039449      0.842354      1.008330
41728      O      -1.140904      -0.227701      1.264615
41729      C      -0.510592      -0.675974      0.074714
41730      C      0.540195      0.287895      -0.508940
41731      C      1.659318      0.661367      0.455129
41732      O      2.633504      -0.401672      0.545426
41733      O      3.232034      -0.607918      -0.586975
41734      H      -2.794571      0.373772      0.614489

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41735	C	0.127758	-2.003043	0.491086	
41736	H	-0.651813	-2.708058	0.772180	
41737	H	0.780245	-1.841160	1.346488	
41738	H	0.723408	-2.417135	-0.321386	
41739	C	-1.533166	-0.998705	-1.001512	
41740	O	-2.718858	-1.004920	-0.816090	
41741	H	-1.105834	-1.276914	-1.981549	
41742	H	1.000950	-0.216311	-1.363313	
41743	O	-0.039041	1.443300	-1.082115	
41744	O	-0.188478	2.445356	-0.086535	
41745	H	-1.031465	2.187508	0.327715	
41746	H	2.160933	1.556208	0.096066	
41747	H	1.306605	0.802475	1.473198	
41748	Rotational constants (GHz):			1.3396600	0.7381200 0.6049100
41749	Vibrational harmonic frequencies (cm-1):				
41750		43.7872	66.9273		108.8236
41751		149.9945	155.8229		200.2668
41752		216.0354	244.1306		267.5632
41753		273.7872	295.5633		318.5516
41754		323.3441	349.6392		385.5740
41755		464.6633	506.3596		535.7135
41756		576.1716	616.3374		662.0456
41757		730.3167	841.0071		901.6570
41758		927.6828	951.3007		979.0980
41759		994.7796	1036.2250		1053.6175
41760		1113.2244	1151.3610		1166.6757
41761		1210.3916	1238.3259		1279.8816
41762		1310.9817	1336.6085		1386.1304
41763		1404.7337	1411.0516		1425.8070
41764		1439.7974	1474.0971		1480.4767
41765		1486.9830	1508.4736		1857.0360
41766		2980.6072	3076.6804		3080.2562
41767		3122.0016	3159.6875		3165.5209
41768		3188.4321	3639.1895		3707.1935
41769	Zero-point correction (Hartree):			0.157144	
41770	diHPCARP_Ic.ppptmpmu				
41771	-----				
41772	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18143252				
41773	Electronic state : 2-A				
41774	Cartesian coordinates (Angs):				
41775	O	-1.889899	0.649371	1.295164	
41776	O	-0.903026	-0.372022	1.276972	
41777	C	-0.488501	-0.674371	-0.045350	
41778	C	0.382813	0.407552	-0.715115	
41779	C	1.667642	0.718299	0.041385	
41780	O	2.675320	-0.210858	-0.421098	
41781	O	3.377341	-0.714470	0.545867	
41782	H	-2.680649	0.164389	1.005306	
41783	C	0.295396	-1.978158	0.121015	
41784	H	-0.372977	-2.760313	0.474826	
41785	H	1.086489	-1.835410	0.855258	
41786	H	0.749729	-2.280970	-0.821246	
41787	C	-1.677633	-0.981073	-0.938635	
41788	O	-2.805229	-1.082557	-0.540972	
41789	H	-1.429374	-1.152414	-2.001786	
41790	H	0.664159	0.018360	-1.699084	
41791	O	-0.338713	1.582856	-1.021386	
41792	O	-0.317630	2.454145	0.099488	
41793	H	-1.061499	2.112326	0.627401	
41794	H	2.003858	1.721157	-0.211262	
41795	H	1.576658	0.607668	1.118502	
41796	Rotational constants (GHz):			1.3268300	0.7232300 0.5881800
41797	Vibrational harmonic frequencies (cm-1):				
41798		36.6774	51.4438		100.3146
41799		124.1564	166.8015		184.6666
41800		217.0919	247.8261		265.4561
41801		283.8378	306.1754		313.9777
41802		326.1596	349.9284		383.9733
41803		435.1228	507.6303		538.0655
41804		563.9146	618.4239		668.1158
41805		747.1490	844.8888		903.5198

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41807          926.9967          965.5352          980.3480
41808          990.2863          1026.0526          1054.1550
41809          1115.9193          1153.5495          1167.6193
41810          1211.5956          1225.9273          1293.9656
41811          1315.3479          1331.1106          1381.1811
41812          1404.0784          1408.8183          1425.0440
41813          1441.6193          1474.3042          1481.1588
41814          1491.9416          1507.8826          1858.0644
41815          2976.4026          3061.6640          3077.7845
41816          3116.4099          3159.7264          3163.1601
41817          3183.7458          3644.7609          3717.5810
41818 Zero-point correction (Hartree): 0.157009
41819
41820 diHPCARP_Ic.pptmpmpmu
41821 -----
41822 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18087131
41823 Electronic state : 2-A
41824 Cartesian coordinates (Angs):
41825 O          1.673600          -1.213934          1.103394
41826 O          1.315393          0.150043          1.277059
41827 C          0.817671          0.698513          0.067504
41828 C          -0.554113          0.150669          -0.371483
41829 C          -1.563766          0.136802          0.756483
41830 O          -2.878787          -0.137226          0.238317
41831 O          -3.307773          0.844614          -0.492594
41832 H          2.543424          -1.128830          0.678456
41833 C          0.762824          2.201530          0.345076
41834 H          1.767423          2.573725          0.535582
41835 H          0.152723          2.398842          1.223555
41836 H          0.336313          2.731294          -0.505351
41837 C          1.804028          0.498223          -1.073770
41838 O          2.910907          0.060998          -0.923338
41839 H          1.444513          0.827064          -2.064646
41840 H          -0.931095          0.821401          -1.148801
41841 O          -0.448543          -1.091526          -1.050431
41842 O          -0.549156          -2.187544          -0.158849
41843 H          0.326144          -2.189916          0.265906
41844 H          -1.363574          -0.654495          1.470338
41845 H          -1.600864          1.103088          1.253639
41846 Rotational constants (GHz): 1.4626700 0.6775800 0.5905800
41847 Vibrational harmonic frequencies (cm-1):
41848 18.6873 43.9704 104.9867
41849 125.8431 134.0586 171.7314
41850 209.2809 234.6758 258.8802
41851 269.5663 275.8000 319.9568
41852 336.9789 351.8811 385.5798
41853 449.8124 483.9050 522.6036
41854 563.1812 629.9724 666.9548
41855 744.6829 854.5776 868.9870
41856 925.7729 945.9579 978.7406
41857 982.9345 1008.1201 1052.0838
41858 1138.2003 1147.1248 1175.5222
41859 1206.4810 1253.2624 1272.1608
41860 1319.6032 1330.8986 1389.8100
41861 1404.2862 1416.1624 1423.5938
41862 1437.6202 1470.3043 1481.1561
41863 1486.9569 1509.9117 1859.0784
41864 2989.8193 3076.9939 3082.4430
41865 3128.8613 3160.9927 3166.7054
41866 3201.9227 3672.9544 3715.8868
41867 Zero-point correction (Hartree): 0.156827
41868
41869 diHPCARP_Ic.pptmpmtmu
41870 -----
41871 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18169000
41872 Electronic state : 2-A
41873 Cartesian coordinates (Angs):
41874 O          -1.369768          -0.176005          1.852874
41875 O          -1.446560          -1.102928          0.780497
41876 C          -1.000736          -0.474377          -0.402189
41877 C          0.438980          0.054840          -0.293930
41878 C          1.276423          -0.817390          0.621064

```

41879	O	2.650937	-0.378879	0.580541	
41880	O	3.215134	-0.685860	-0.548782	
41881	H	-2.197157	0.317529	1.736745	
41882	C	-1.112618	-1.550206	-1.477663	
41883	H	-2.113158	-1.977571	-1.460090	
41884	H	-0.388590	-2.342808	-1.296645	
41885	H	-0.921655	-1.122217	-2.460565	
41886	C	-1.920903	0.681825	-0.779902	
41887	O	-2.913586	0.952786	-0.166453	
41888	H	-1.626549	1.239818	-1.686227	
41889	H	0.886162	0.077470	-1.289795	
41890	O	0.393163	1.393043	0.187221	
41891	O	1.457965	2.118480	-0.408298	
41892	H	2.163124	2.032772	0.247867	
41893	H	0.963971	-0.692878	1.654102	
41894	H	1.248700	-1.865365	0.329529	
41895	Rotational constants (GHz):		1.4332600	0.6588100	0.6010600
41896	Vibrational harmonic frequencies (cm-1):				
41897		58.2555	71.3090		95.0546
41898		115.4490	119.7912		163.7997
41899		203.7039	206.8606		223.8625
41900		242.2484	283.4460		317.0496
41901		330.7835	339.7480		378.1979
41902		406.2847	436.2569		486.9358
41903		495.4527	560.4644		590.9438
41904		753.6297	868.8365		897.6802
41905		931.9520	965.4295		982.1603
41906		993.8431	1033.7435		1060.0455
41907		1121.5097	1132.5317		1184.8429
41908		1217.3453	1248.5125		1281.5551
41909		1310.9560	1323.9612		1383.5699
41910		1403.9980	1412.3635		1418.2167
41911		1421.3127	1431.0017		1474.7397
41912		1490.2643	1503.9230		1865.1631
41913		2986.6439	3076.5412		3092.7513
41914		3116.4490	3155.7004		3162.4151
41915		3191.1184	3745.5800		3795.7831
41916	Zero-point correction (Hartree):		0.156196		
41917	diHPCARP_Ic.pptmtpu				
41918	-----				
41919	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18409519				
41920	Electronic state : 2-A				
41921	Cartesian coordinates (Angs):				
41922	O	1.493956	1.842508	-0.745582	
41923	O	1.236532	0.569539	-1.321396	
41924	C	1.107384	-0.397904	-0.295005	
41925	C	-0.287507	-0.446379	0.354094	
41926	C	-1.361557	-0.891858	-0.625785	
41927	O	-2.628474	-1.038365	0.045038	
41928	O	-3.252282	0.088645	0.194076	
41929	H	0.595079	2.180344	-0.594408	
41930	C	1.456258	-1.723616	-0.973369	
41931	H	2.520605	-1.747735	-1.202526	
41932	H	0.912802	-1.819243	-1.912144	
41933	H	1.216556	-2.561011	-0.319409	
41934	C	2.178681	-0.171043	0.769154	
41935	O	2.076473	-0.578619	1.889148	
41936	H	3.088052	0.326529	0.394235	
41937	H	-0.224245	-1.159394	1.179458	
41938	O	-0.650393	0.747012	1.028148	
41939	O	-1.031966	1.749618	0.098047	
41940	H	-1.990579	1.599630	0.035180	
41941	H	-1.483039	-0.190949	-1.448875	
41942	H	-1.145562	-1.886072	-1.005861	
41943	Rotational constants (GHz):		1.3937600	0.6958600	0.6356700
41944	Vibrational harmonic frequencies (cm-1):				
41945		59.2665	88.5411		102.6416
41946		156.6883	167.6501		196.4291
41947		224.4431	243.9561		269.7572
41948		284.5362	307.4175		311.1467
41949		319.6730	353.8095		397.5028

41951	486.7149	537.5448	547.1944			
41952	578.4725	614.2961	620.5827			
41953	678.4379	833.4080	912.5062			
41954	938.3755	962.1578	975.6766			
41955	990.8692	1008.3962	1060.3230			
41956	1124.9886	1132.2686	1171.2641			
41957	1223.0867	1250.8197	1262.8477			
41958	1307.9265	1340.1974	1392.7170			
41959	1397.5835	1402.8625	1409.5995			
41960	1435.3762	1464.2232	1485.7210			
41961	1489.2388	1513.8277	1869.9366			
41962	3007.9964	3070.8027	3097.6371			
41963	3120.0410	3148.3809	3156.8776			
41964	3185.6901	3683.6479	3703.5272			
41965	Zero-point correction (Hartree): 0.157370					
41966	diHPCARP_Ic.pptppmpu					
41967	-----					
41968	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18512530					
41969	Electronic state : 2-A					
41970	Cartesian coordinates (Angs):					
41971	O	1.331997	1.922732	0.576284		
41972	O	1.670348	1.165693	-0.579562		
41973	C	1.097358	-0.124110	-0.505239		
41974	C	-0.438545	-0.087908	-0.708475		
41975	C	-1.170455	1.035494	0.014036		
41976	O	-2.564923	0.989879	-0.358072		
41977	O	-3.236506	0.123554	0.335890		
41978	H	1.960355	1.560384	1.222407		
41979	C	1.726225	-0.887405	-1.670423		
41980	H	2.794558	-1.018337	-1.508253		
41981	H	1.576076	-0.319114	-2.587152		
41982	H	1.249217	-1.861051	-1.770022		
41983	C	1.543905	-0.859567	0.754889		
41984	O	2.284481	-0.370545	1.566102		
41985	H	1.216060	-1.905234	0.832602		
41986	H	-0.616762	0.039177	-1.779615		
41987	O	-1.011337	-1.356040	-0.449005		
41988	O	-1.078665	-1.561958	0.954734		
41989	H	-1.975314	-1.234345	1.141563		
41990	H	-1.102616	0.971055	1.095485		
41991	H	-0.815649	2.001927	-0.326709		
41992	Rotational constants (GHz):			1.4155900	0.6960400	0.6302600
41993	Vibrational harmonic frequencies (cm-1):					
41994	46.8697	84.2424	122.5990			
41995	172.2234	197.9511	215.3495			
41996	239.4970	247.4899	263.2963			
41997	280.5975	302.1367	312.9493			
41998	348.7309	361.3533	395.5218			
41999	461.8049	530.7897	551.4509			
42000	572.2565	583.7983	657.8086			
42001	708.5390	834.4225	885.8763			
42002	932.7821	968.0744	985.8411			
42003	1003.4173	1029.5379	1053.6525			
42004	1106.4456	1133.1316	1182.4987			
42005	1228.5264	1250.0840	1255.9227			
42006	1315.8927	1347.9905	1376.8724			
42007	1398.6987	1405.1603	1428.4281			
42008	1449.0536	1452.5201	1475.5781			
42009	1491.8530	1503.4863	1841.7716			
42010	3050.4140	3074.3350	3078.7607			
42011	3141.0027	3156.3804	3162.6695			
42012	3209.4169	3715.8697	3719.3704			
42013	Zero-point correction (Hartree): 0.157884					
42014	diHPCARP_Ic.pptppmtmu					
42015	-----					
42016	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18163734					
42017	Electronic state : 2-A					
42018	Cartesian coordinates (Angs):					
42019	O	-1.115420	-0.398269	1.879173		
42020	O	-1.442706	-1.142435	0.715712		
42021						
42022						

42023	C	-1.103324	-0.384860	-0.425356			
42024	C	0.386920	0.008925	-0.464267			
42025	C	1.235397	-1.059789	0.205817			
42026	O	2.613655	-0.984257	-0.216335			
42027	O	3.266940	-0.044373	0.391779			
42028	H	-1.890968	0.179538	1.959672			
42029	C	-1.473065	-1.277802	-1.604378			
42030	H	-2.499216	-1.621819	-1.491264			
42031	H	-0.816260	-2.145564	-1.643442			
42032	H	-1.379985	-0.727155	-2.539262			
42033	C	-1.944848	0.885971	-0.499372			
42034	O	-2.806486	1.142978	0.292079			
42035	H	-1.729143	1.543871	-1.359409			
42036	H	0.691687	0.129688	-1.506406			
42037	O	0.514832	1.273617	0.169130			
42038	O	1.542401	2.008138	-0.475179			
42039	H	2.317164	1.772964	0.057344			
42040	H	1.197026	-0.952173	1.286811			
42041	H	0.917488	-2.057197	-0.089589			
42042	Rotational constants (GHz):				1.4590300	0.6611200	0.5982600
42043	Vibrational harmonic frequencies (cm-1):						
42044		44.7267	70.8234			91.6855	
42045		118.1413	148.9765			176.2787	
42046		200.3812	208.5161			226.1554	
42047		243.1756	301.6826			321.8398	
42048		332.2112	368.0312			409.2838	
42049		431.0476	439.2200			479.4118	
42050		489.5513	546.0694			590.6849	
42051		741.9545	860.0232			917.1267	
42052		932.2537	966.2692			974.1690	
42053		996.0775	1042.9956			1061.8503	
42054		1109.2947	1128.8522			1181.6373	
42055		1216.5748	1258.7565			1278.3824	
42056		1305.5700	1335.6340			1380.2785	
42057		1403.6836	1411.6405			1417.8694	
42058		1433.3504	1434.4642			1467.3733	
42059		1490.4850	1504.1586			1865.4478	
42060		2989.0090	3074.9798			3082.3994	
42061		3119.7088	3152.9590			3161.8092	
42062		3186.8603	3743.4699			3760.1520	
42063	Zero-point correction (Hartree):				0.156340		
42064	diHPCARP_Ic.ptmmmtmpu						
42065	-----						
42067	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.17988999		
42068	Electronic state : 2-A						
42069	Cartesian coordinates (Angs):						
42070	O	2.562132	-0.778215	-0.352159			
42071	O	1.759900	-0.529202	0.794616			
42072	C	0.744748	0.401787	0.431148			
42073	C	-0.226343	-0.236290	-0.581678			
42074	C	-1.482391	0.565132	-0.891962			
42075	O	-2.359324	0.655562	0.247600			
42076	O	-3.320485	-0.218174	0.200696			
42077	H	2.108442	-1.542318	-0.743793			
42078	C	0.108147	0.790808	1.758362			
42079	H	0.891263	1.083956	2.455992			
42080	H	-0.439633	-0.056231	2.167507			
42081	H	-0.583147	1.619049	1.624212			
42082	C	1.456557	1.617392	-0.151232			
42083	O	1.022907	2.301358	-1.034096			
42084	H	2.422846	1.831669	0.340182			
42085	H	0.293617	-0.359473	-1.535679			
42086	O	-0.685822	-1.500116	-0.135934			
42087	O	0.313010	-2.480928	-0.390279			
42088	H	0.619656	-2.672148	0.507061			
42089	H	-1.214473	1.583234	-1.160916			
42090	H	-2.041419	0.077014	-1.685944			
42091	Rotational constants (GHz):				1.2224500	0.8014800	0.6098200
42092	Vibrational harmonic frequencies (cm-1):						
42093		47.8187	57.6060			77.3148	
42094		105.7245	156.0805			184.0430	

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42095      197.4388      211.7950      247.3891
42096      247.9442      280.8858      295.4179
42097      315.5049      342.5907      383.0576
42098      410.1482      511.9853      533.8268
42099      544.5729      592.4397      651.3799
42100      680.9772      786.3495      893.3820
42101      929.5110      958.1661      972.9290
42102     1020.5320     1047.9119     1057.0221
42103     1078.6272     1145.8553     1180.8316
42104     1237.5942     1241.5681     1277.3216
42105     1332.4094     1348.3903     1380.7639
42106     1393.0935     1404.2290     1416.0242
42107     1416.9232     1438.5709     1473.9911
42108     1490.1610     1500.2588     1867.7295
42109     2981.8535     3076.8363     3079.7243
42110     3118.7391     3157.8490     3171.8739
42111     3187.6295     3713.4716     3796.2824
42112 Zero-point correction (Hartree): 0.156397
42113
42114 diHPCARP_Ic.ptmmmtppu
42115 -----
42116 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17991917
42117 Electronic state : 2-A
42118 Cartesian coordinates (Angs):
42119 O      2.238557      -1.451942      -0.545165
42120 O      1.588821      -1.072818      0.660929
42121 C      0.899041      0.137643      0.423063
42122 C     -0.110649     -0.024711     -0.737729
42123 C     -1.218077      1.014906     -0.814038
42124 O     -2.149992      0.993154      0.289947
42125 O     -3.131911      0.171657      0.089412
42126 H      1.585334     -2.060727     -0.922022
42127 C      0.329678      0.523946      1.784180
42128 H      1.148156      0.595475      2.500214
42129 H     -0.374017     -0.232889      2.117943
42130 H     -0.173949      1.486808      1.729161
42131 C      1.930044      1.198718      0.050708
42132 O      1.721795      2.096912     -0.715389
42133 H      2.892315      1.085222      0.582205
42134 H      0.449210      0.120774     -1.665703
42135 O     -0.566853     -1.355227     -0.879819
42136 O     -1.177152     -1.797068      0.325492
42137 H     -2.115488     -1.649268      0.136581
42138 H     -0.776586      2.009629     -0.798659
42139 H     -1.801318      0.864613     -1.720076
42140 Rotational constants (GHz):      1.3290200      0.7989800      0.6402000
42141 Vibrational harmonic frequencies (cm-1):
42142      67.7756      78.8145      97.0753
42143     124.5616     162.8922     181.3222
42144     196.3211     216.5950     237.5716
42145     257.6550     259.6105     307.1002
42146     328.2730     363.6210     410.3922
42147     452.2549     469.9216     502.8990
42148     537.0379     542.0188     673.4328
42149     680.3711     811.1481     903.9469
42150     931.7354     956.2225     970.1638
42151     996.3201    1032.8511    1052.9609
42152    1078.3611    1155.4592    1193.5068
42153    1233.0115    1252.6556    1285.3318
42154    1339.7424    1359.1220    1389.7067
42155    1393.1236    1399.6933    1412.0380
42156    1425.0297    1432.6176    1473.9992
42157    1488.3430    1504.1730    1862.7228
42158    2986.4909    3080.4600    3083.0526
42159    3107.4378    3155.5650    3173.1580
42160    3184.2692    3765.0634    3768.8302
42161 Zero-point correction (Hartree): 0.156706
42162
42163 diHPCARP_Ic.ptmmmttmu
42164 -----
42165 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18419716
42166 Electronic state : 2-A

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42167 Cartesian coordinates (Angs):
42168 O -2.023862 1.796351 -0.114295
42169 O -1.654129 0.928834 0.946231
42170 C -1.014558 -0.208165 0.393058
42171 C 0.165096 0.202039 -0.506952
42172 C 1.156321 -0.913783 -0.824113
42173 O 1.958546 -1.272232 0.317276
42174 O 2.925487 -0.430232 0.521012
42175 H -1.272214 2.408350 -0.123772
42176 C -0.643144 -1.040719 1.614440
42177 H -1.534433 -1.198791 2.220348
42178 H 0.099582 -0.509544 2.206096
42179 H -0.240685 -2.006660 1.317188
42180 C -2.050048 -0.975894 -0.421356
42181 O -1.797357 -1.611928 -1.404951
42182 H -3.071113 -0.913901 -0.002510
42183 H -0.233111 0.535173 -1.469025
42184 O 0.780527 1.294236 0.146834
42185 O 1.754736 1.837488 -0.728963
42186 H 2.554304 1.383729 -0.415158
42187 H 0.628254 -1.817826 -1.115461
42188 H 1.835828 -0.601534 -1.613316
42189 Rotational constants (GHz): 1.2779100 0.7758200 0.6340700
42190 Vibrational harmonic frequencies (cm-1):
42191 65.9431 83.8956 93.3061
42192 134.4628 160.0911 187.2181
42193 190.5594 233.9632 252.3728
42194 261.0523 285.7058 302.8513
42195 310.6086 330.1097 418.3748
42196 458.9381 504.9023 523.1119
42197 531.8283 545.2707 659.5109
42198 715.1100 794.1977 892.4814
42199 928.9804 958.8141 986.1045
42200 1001.6891 1051.4509 1055.6840
42201 1075.1795 1162.3234 1189.5382
42202 1241.2830 1245.9472 1281.7713
42203 1327.6091 1360.7984 1384.6882
42204 1391.9170 1401.3835 1413.6263
42205 1422.7860 1449.3700 1487.2856
42206 1488.1134 1503.0230 1865.2577
42207 2981.0122 3075.9465 3078.5410
42208 3120.6637 3156.9709 3169.5711
42209 3185.4038 3726.1029 3762.7883
42210 Zero-point correction (Hartree): 0.156892
42211
42212 diHPCARP_Ic.ptmtmtmpu
42213 -----
42214 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18026004
42215 Electronic state : 2-A
42216 Cartesian coordinates (Angs):
42217 O 2.712060 -0.062366 -0.397250
42218 O 1.898658 -0.053803 0.768491
42219 C 0.637894 0.514832 0.425836
42220 C -0.113659 -0.413638 -0.548829
42221 C -1.556124 -0.051067 -0.845704
42222 O -2.358303 -0.243795 0.338166
42223 O -3.609357 -0.010993 0.087519
42224 H 2.512462 -0.937137 -0.767867
42225 C -0.050310 0.722411 1.767644
42226 H 0.626614 1.253912 2.434879
42227 H -0.305483 -0.240781 2.205421
42228 H -0.962438 1.301012 1.645040
42229 C 0.927271 1.875658 -0.197394
42230 O 0.288732 2.366028 -1.084114
42231 H 1.786377 2.392615 0.267162
42232 H 0.401856 -0.394002 -1.512566
42233 O -0.150871 -1.749102 -0.071449
42234 O 1.092408 -2.382506 -0.347901
42235 H 1.473481 -2.441824 0.539327
42236 H -1.639565 0.986539 -1.158181
42237 H -1.950365 -0.717209 -1.610232
42238 Rotational constants (GHz): 1.2339100 0.7593900 0.5879000

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42239 Vibrational harmonic frequencies (cm-1):
42240         42.8373          50.6661          90.4461
42241         120.6306         146.0815         187.9251
42242         195.9600         207.3509         241.9537
42243         255.7091         272.6781         302.0868
42244         319.2207         351.2954         380.5053
42245         407.4530         421.7456         519.8677
42246         553.4798         586.5583         659.9627
42247         715.3770         772.7095         915.7620
42248         929.5732         956.5417         967.7028
42249         1031.3353        1047.1652        1051.3905
42250         1108.9980        1143.8983        1177.5736
42251         1238.4939        1247.1303        1294.9785
42252         1296.6226        1358.7973        1381.7654
42253         1399.1693        1406.0799        1417.0604
42254         1418.7906        1436.2329        1488.0708
42255         1490.8095        1498.7627        1869.3193
42256         2983.4520        3078.3387        3080.3175
42257         3111.9808        3158.6615        3172.7390
42258         3179.9425        3727.9453        3795.6516
42259 Zero-point correction (Hartree): 0.156427
42260
42261 diHPCARP_Ic.ptppmtmmu
42262 -----
42263 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18175398
42264 Electronic state : 2-A
42265 Cartesian coordinates (Angs):
42266 O      -1.619557      1.527401      -1.137300
42267 O      -1.800606      1.065803      0.195281
42268 C      -1.142448      -0.179880      0.320439
42269 C       0.367447      -0.003683      0.070138
42270 C       1.205300      -1.182032      0.496920
42271 O       2.513253      -1.188083      -0.139934
42272 O       2.905165      -0.040552      -0.592779
42273 H      -0.857404      2.120127      -1.028589
42274 C      -1.462561      -0.634822      1.738198
42275 H      -2.541081      -0.652812      1.886185
42276 H      -1.022409      0.066122      2.445865
42277 H      -1.067832      -1.634206      1.915720
42278 C      -1.770635      -1.144773      -0.676636
42279 O      -1.208476      -2.100453      -1.132670
42280 H      -2.818371      -0.900807      -0.927755
42281 H       0.530903      0.178055      -0.991004
42282 O       0.831557      1.117272      0.813145
42283 O       0.954536      2.229914      -0.051263
42284 H       1.845206      2.087998      -0.408822
42285 H       1.386942      -1.156752      1.572163
42286 H       0.754453      -2.126994      0.206050
42287 Rotational constants (GHz):  1.1816700    0.8107800    0.6273300
42288 Vibrational harmonic frequencies (cm-1):
42289         46.9936          58.8695          78.3151
42290         104.0707         110.4200         177.7977
42291         191.4892         213.3037         232.8090
42292         269.2518         279.8764         300.2651
42293         319.1483         352.1893         379.8066
42294         445.8946         479.3547         524.9176
42295         538.0567         576.7632         640.4307
42296         681.1772         853.6486         898.7606
42297         933.2639         938.3526         968.2599
42298         1012.6820        1053.0555        1061.9352
42299         1122.2356        1138.6506        1175.8543
42300         1240.2048        1261.0068        1270.4617
42301         1278.0708        1339.9459        1376.4013
42302         1400.0434        1410.0039        1420.5109
42303         1436.3439        1461.3984        1482.5253
42304         1491.7580        1506.0854        1864.0279
42305         2989.7743        3073.0456        3091.0243
42306         3123.3455        3154.6611        3157.3818
42307         3175.1970        3716.8325        3748.6769
42308 Zero-point correction (Hartree): 0.156343
42309
42310 diHPCARP_Ic.pttmtmmu

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42311 -----
42312 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18248302
42313 Electronic state : 2-A
42314 Cartesian coordinates (Angs):
42315 O -1.940700 0.981180 -1.315179
42316 O -2.003853 0.656729 0.066876
42317 C -1.045525 -0.352317 0.323443
42318 C 0.381789 0.181311 0.082360
42319 C 1.463098 -0.714045 0.650533
42320 O 2.761946 -0.235597 0.243806
42321 O 2.929468 -0.343442 -1.038478
42322 H -1.377340 1.770694 -1.287892
42323 C -1.291307 -0.741219 1.776075
42324 H -2.341728 -0.991202 1.914877
42325 H -1.041067 0.098993 2.422053
42326 H -0.687467 -1.606489 2.044536
42327 C -1.370398 -1.542124 -0.571879
42328 O -0.584549 -2.398273 -0.864605
42329 H -2.423353 -1.568328 -0.904208
42330 H 0.559887 0.300506 -0.986915
42331 O 0.554955 1.432974 0.733898
42332 O 0.119620 2.473961 -0.127734
42333 H 0.961318 2.867315 -0.392895
42334 H 1.487863 -0.665209 1.737478
42335 H 1.340860 -1.736165 0.301103
42336 Rotational constants (GHz): 1.1297400 0.7987800 0.6238400
42337 Vibrational harmonic frequencies (cm-1):
42338 45.4410 54.6928 88.2126
42339 108.0780 139.2414 185.1133
42340 214.9167 218.7978 235.7189
42341 258.9801 272.6636 296.4368
42342 302.7221 321.2825 364.9682
42343 383.5184 499.4162 517.6865
42344 518.9689 577.1186 602.3833
42345 676.9713 827.6769 891.1913
42346 933.6986 966.9614 980.5769
42347 1005.2360 1048.9500 1054.9404
42348 1121.8678 1148.3621 1187.8577
42349 1240.4801 1250.9363 1259.9999
42350 1315.3548 1322.9146 1385.1472
42351 1396.9007 1406.6281 1411.5838
42352 1415.0224 1450.7470 1481.8429
42353 1493.2518 1505.0800 1865.7886
42354 2988.1203 3074.7378 3108.1469
42355 3115.8321 3156.3824 3159.2942
42356 3182.7163 3748.0607 3809.7433
42357 Zero-point correction (Hartree): 0.156272
42358
42359 diHPCARP_Ic.pttmtmpu
42360 -----
42361 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18239302
42362 Electronic state : 2-A
42363 Cartesian coordinates (Angs):
42364 O 1.981017 -0.675278 -1.435325
42365 O 2.030211 -0.476687 -0.029073
42366 C 0.976720 0.410688 0.325340
42367 C -0.388394 -0.258430 0.065047
42368 C -1.550345 0.498021 0.676439
42369 O -2.799210 -0.036751 0.198124
42370 O -2.962443 0.206965 -1.065915
42371 H 1.390077 -1.443851 -1.503744
42372 C 1.209623 0.712489 1.799987
42373 H 2.230749 1.059449 1.948727
42374 H 1.051633 -0.189104 2.389865
42375 H 0.524486 1.489872 2.134172
42376 C 1.171195 1.693502 -0.477034
42377 O 0.316250 2.514230 -0.649760
42378 H 2.200534 1.824229 -0.854622
42379 H -0.567730 -0.351506 -1.007554
42380 O -0.438173 -1.543727 0.666145
42381 O 0.213286 -2.484908 -0.177488
42382 H 1.018552 -2.664056 0.327722

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42383      H      -1.586765      0.353983      1.754854
42384      H      -1.501842      1.552611      0.418255
42385      Rotational constants (GHz):      1.1216200      0.8009500      0.6238900
42386      Vibrational harmonic frequencies (cm-1):
42387          44.1785          59.8934          90.0614
42388          116.7802          153.6053          189.7401
42389          206.2294          225.2149          236.7295
42390          260.5977          271.7511          296.8546
42391          305.8395          351.1698          378.2105
42392          403.5155          504.8674          521.6552
42393          566.7325          597.0448          613.6305
42394          680.0283          822.4634          894.9251
42395          933.1131          966.2991          986.4311
42396          1002.9295          1047.4832          1048.9723
42397          1121.3028          1152.6128          1184.2788
42398          1237.9584          1248.4812          1258.3297
42399          1321.4335          1326.5223          1382.2038
42400          1400.2051          1407.6720          1413.7831
42401          1422.6232          1443.8096          1482.6575
42402          1494.1715          1503.3290          1868.2431
42403          2992.6497          3076.0274          3101.1967
42404          3113.8655          3157.2554          3159.5505
42405          3183.1887          3709.8884          3796.2639
42406      Zero-point correction (Hartree): 0.156593
42407
42408      diHPCARP_Ic.pttmmtpmu
42409      -----
42410      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18152857
42411      Electronic state : 2-A
42412      Cartesian coordinates (Angs):
42413      O      2.014563      -0.504862      -1.585886
42414      O      1.992366      -0.629208      -0.170283
42415      C      1.011190      0.266393      0.330493
42416      C      -0.388846      -0.134066      -0.206593
42417      C      -1.517480      0.206041      0.743106
42418      O      -2.787946      -0.055809      0.119900
42419      O      -3.005718      0.756009      -0.869295
42420      H      1.343325      -1.153384      -1.850762
42421      C      1.178060      0.217423      1.847317
42422      H      2.205015      0.473943      2.104916
42423      H      0.952156      -0.775022      2.229639
42424      H      0.513824      0.940070      2.317833
42425      C      1.364524      1.679489      -0.113263
42426      O      0.551202      2.553970      -0.194655
42427      H      2.439750      1.842289      -0.307633
42428      H      -0.577180      0.390030      -1.145477
42429      O      -0.413044      -1.495579      -0.597202
42430      O      -0.171986      -2.314854      0.538458
42431      H      0.786963      -2.439703      0.481664
42432      H      -1.505416      -0.428695      1.625961
42433      H      -1.478614      1.261457      1.009195
42434      Rotational constants (GHz):      1.1677200      0.7869700      0.6308500
42435      Vibrational harmonic frequencies (cm-1):
42436          59.8687          61.3179          90.9469
42437          134.5732          148.4342          172.4596
42438          185.6864          224.9509          237.4116
42439          258.1564          279.7353          306.2739
42440          321.2006          378.8382          398.9904
42441          440.1654          489.7518          516.8538
42442          533.2259          583.5219          618.3864
42443          705.0589          822.4376          915.1240
42444          946.3089          969.4212          973.7519
42445          998.1391          1008.8191          1051.2219
42446          1129.6729          1136.8995          1192.7853
42447          1231.3773          1252.4738          1255.1245
42448          1319.0229          1329.5499          1390.1199
42449          1396.2280          1411.1686          1412.5061
42450          1426.8151          1438.4964          1477.7051
42451          1497.8738          1503.3852          1869.4373
42452          2987.6877          3079.3409          3104.0393
42453          3108.8356          3154.0304          3172.1019
42454          3178.0815          3743.5953          3769.9782

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42455 Zero-point correction (Hartree): 0.156736
42456
42457 diHPCARP_Ic.pttmtppu
42458 -----
42459 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18029380
42460 Electronic state : 2-A
42461 Cartesian coordinates (Angs):
42462 O 1.930324 -0.752576 -1.621738
42463 O 1.961998 -0.854022 -0.205086
42464 C 1.097860 0.132070 0.320934
42465 C -0.343230 -0.057123 -0.219867
42466 C -1.402618 0.520182 0.697113
42467 O -2.714192 0.273303 0.155854
42468 O -2.904210 0.918093 -0.955186
42469 H 1.267498 -1.424533 -1.840627
42470 C 1.257809 0.000047 1.832799
42471 H 2.311027 0.103622 2.091104
42472 H 0.907336 -0.976467 2.157902
42473 H 0.699116 0.782974 2.342878
42474 C 1.623533 1.504425 -0.080204
42475 O 0.930420 2.479072 -0.153593
42476 H 2.713367 1.534426 -0.260786
42477 H -0.424964 0.443169 -1.185886
42478 O -0.602840 -1.405808 -0.559622
42479 O -0.676275 -2.185144 0.628768
42480 H -1.600092 -2.467408 0.606569
42481 H -1.417238 0.029309 1.666418
42482 H -1.257975 1.593949 0.802598
42483 Rotational constants (GHz): 1.1814400 0.7731000 0.6314700
42484 Vibrational harmonic frequencies (cm-1):
42485 45.6413 60.4025 80.9539
42486 103.1600 133.4358 154.8977
42487 177.5473 218.6386 246.9550
42488 258.5510 285.1721 294.2565
42489 309.0750 325.6839 373.7191
42490 379.2785 466.6857 492.7526
42491 530.0817 576.4155 627.9881
42492 711.7696 810.3793 916.3145
42493 942.8769 968.7273 973.7708
42494 998.6549 1009.1207 1053.6576
42495 1126.1375 1142.2055 1197.8390
42496 1234.9452 1250.5112 1262.1683
42497 1312.6042 1325.9398 1391.6575
42498 1394.4002 1408.2409 1409.1453
42499 1415.2872 1426.8071 1485.0643
42500 1498.9619 1506.7091 1865.7267
42501 2983.9706 3078.4975 3113.7021
42502 3117.8855 3152.2746 3175.3274
42503 3183.9286 3768.1676 3809.9946
42504 Zero-point correction (Hartree): 0.156202
42505
42506 diHPCARP_Ic.pttpmtmmu
42507 -----
42508 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18167513
42509 Electronic state : 2-A
42510 Cartesian coordinates (Angs):
42511 O -2.103855 1.251215 -0.956959
42512 O -1.907718 0.852640 0.393138
42513 C -1.068253 -0.286254 0.393941
42514 C 0.336374 0.068148 -0.135901
42515 C 1.376619 -0.994649 0.164637
42516 O 2.554293 -0.716542 -0.613497
42517 O 3.461824 -0.085593 0.069954
42518 H -1.443251 1.957899 -1.033595
42519 C -1.052872 -0.738071 1.848726
42520 H -2.074276 -0.867756 2.202297
42521 H -0.563500 0.022444 2.455468
42522 H -0.523740 -1.684211 1.950515
42523 C -1.741598 -1.354890 -0.457581
42524 O -1.154431 -2.215686 -1.049937
42525 H -2.844066 -1.283380 -0.459786
42526 H 0.294982 0.222007 -1.215476

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42527	O	0.816788	1.248012	0.488376	
42528	O	0.356155	2.380388	-0.235200	
42529	H	1.182188	2.712745	-0.609677	
42530	H	1.665487	-0.989859	1.213621	
42531	H	1.020103	-1.971053	-0.153300	
42532	Rotational constants (GHz):		1.2242200	0.7460100	0.5812000
42533	Vibrational harmonic frequencies (cm-1):				
42534		54.9372	61.0474		72.2669
42535		108.0466	124.3212		177.5519
42536		211.7921	216.4767		238.1072
42537		249.3634	279.8228		296.0529
42538		308.8885	320.6748		362.5102
42539		378.7806	508.0907		522.9314
42540		543.4985	560.1479		586.4366
42541		674.0184	825.5904		892.5582
42542		932.4999	965.7125		984.6378
42543		1014.2424	1049.4107		1054.7788
42544		1118.8978	1147.2099		1189.5048
42545		1242.1078	1254.1720		1263.2369
42546		1313.9155	1337.1733		1382.8871
42547		1397.9953	1403.3884		1407.4359
42548		1414.7152	1451.8071		1471.9168
42549		1493.1188	1504.7603		1865.4605
42550		2987.1824	3074.7401		3098.7172
42551		3113.6228	3157.1385		3158.4261
42552		3185.8399	3740.0861		3813.8661
42553	Zero-point correction (Hartree): 0.156201				
42554					
42555	diHPCARP_Ic.pttpmtmpu				
42556	-----				
42557	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18125087				
42558	Electronic state : 2-A				
42559	Cartesian coordinates (Angs):				
42560	O	-2.203647	1.025672	-1.045194	
42561	O	-1.942281	0.766404	0.327499	
42562	C	-1.022259	-0.314699	0.398886	
42563	C	0.348633	0.108933	-0.166505	
42564	C	1.455865	-0.873522	0.166902	
42565	O	2.606182	-0.566448	-0.638573	
42566	O	3.549329	0.011085	0.042627	
42567	H	-1.513207	1.676546	-1.254658	
42568	C	-0.966361	-0.670237	1.878544	
42569	H	-1.973983	-0.840888	2.253700	
42570	H	-0.514602	0.149573	2.435216	
42571	H	-0.378665	-1.574334	2.028868	
42572	C	-1.636297	-1.478217	-0.371038	
42573	O	-1.003186	-2.341277	-0.908523	
42574	H	-2.740928	-1.473183	-0.363043	
42575	H	0.291113	0.214479	-1.252021	
42576	O	0.772048	1.336803	0.400019	
42577	O	0.133886	2.411490	-0.280041	
42578	H	-0.452533	2.747008	0.411996	
42579	H	1.756561	-0.798773	1.209951	
42580	H	1.150115	-1.883811	-0.093247	
42581	Rotational constants (GHz):		1.2260600	0.7379200	0.5751200
42582	Vibrational harmonic frequencies (cm-1):				
42583		45.1393	58.4285		71.1360
42584		112.8999	139.4655		180.8637
42585		205.4918	219.7769		235.1868
42586		251.7782	276.3949		296.2001
42587		310.9010	347.6238		378.2343
42588		398.1180	507.3635		542.2260
42589		559.5457	579.6203		609.0521
42590		676.5231	816.7439		892.5897
42591		930.5220	963.8340		988.3277
42592		1016.2083	1047.2994		1049.3476
42593		1122.0258	1147.8175		1188.5159
42594		1239.9668	1254.2371		1262.8230
42595		1318.4761	1336.9484		1378.6625
42596		1401.1819	1402.5674		1412.6008
42597		1421.2392	1441.9486		1474.8795
42598		1493.0815	1502.4560		1868.6464

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42599      2987.9975      3075.2347      3089.8946
42600      3111.4366      3156.6111      3158.6048
42601      3183.1683      3711.6963      3799.2485
42602 Zero-point correction (Hartree): 0.156393
42603
42604 diHPCARP_Ic.pttpmtppu
42605 -----
42606 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18495270
42607 Electronic state : 2-A
42608 Cartesian coordinates (Angs):
42609 O      1.920928      -1.352783      -1.274363
42610 O      1.771049      -1.189024      0.128904
42611 C      1.120629      0.043321      0.355961
42612 C      -0.248255      0.083613      -0.373279
42613 C      -1.227822      1.048306      0.271947
42614 O      -2.442395      1.096260      -0.498413
42615 O      -3.232643      0.105091      -0.217201
42616 H      1.144405      -1.895098      -1.479907
42617 C      1.065308      0.161182      1.876336
42618 H      2.074901      0.079708      2.277465
42619 H      0.454731      -0.640697      2.283929
42620 H      0.655175      1.126063      2.170073
42621 C      2.009443      1.166119      -0.162675
42622 O      1.585871      2.226277      -0.528537
42623 H      3.089573      0.934316      -0.138694
42624 H      -0.080649      0.404928      -1.402747
42625 O      -0.795818      -1.206135      -0.542963
42626 O      -1.205884      -1.722147      0.714143
42627 H      -2.150502      -1.497053      0.694839
42628 H      -1.492302      0.755905      1.285011
42629 H      -0.820012      2.056382      0.247725
42630 Rotational constants (GHz):      1.3263100      0.7419600      0.6092300
42631 Vibrational harmonic frequencies (cm-1):
42632      72.1114      86.8247      107.0949
42633      132.0948      163.5445      183.4640
42634      189.6413      222.3256      237.6883
42635      265.6665      299.5553      309.6027
42636      320.1132      374.0061      385.0284
42637      465.0565      504.5420      531.7165
42638      541.7251      584.5976      620.0523
42639      701.2747      820.0030      916.9443
42640      938.7169      968.8373      975.8374
42641      1006.9629      1013.5116      1053.5949
42642      1116.5210      1150.6153      1195.8866
42643      1236.1149      1258.1076      1262.0276
42644      1317.3817      1341.0506      1392.4417
42645      1393.9612      1401.7150      1407.6268
42646      1422.3478      1451.2880      1484.4345
42647      1497.2902      1505.8952      1862.7211
42648      2985.4687      3077.3512      3103.7196
42649      3118.5588      3151.7741      3172.8599
42650      3185.1422      3735.2251      3766.3645
42651 Zero-point correction (Hartree): 0.157162
42652
42653 diHPCARP_Ic.ptttmtmmu
42654 -----
42655 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18194890
42656 Electronic state : 2-A
42657 Cartesian coordinates (Angs):
42658 O      -2.353811      0.723675      -1.036281
42659 O      -2.118218      0.401417      0.327827
42660 C      -0.999812      -0.462893      0.385253
42661 C      0.277515      0.258269      -0.086499
42662 C      1.546165      -0.471495      0.289938
42663 O      2.604395      0.127298      -0.484211
42664 O      3.768022      -0.296622      -0.100870
42665 H      -1.909334      1.584262      -1.096370
42666 C      -0.932400      -0.888356      1.846369
42667 H      -1.891025      -1.304799      2.150832
42668 H      -0.715093      -0.017842      2.463608
42669 H      -0.160220      -1.642138      1.991667
42670 C      -1.312328      -1.677393      -0.480251

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42671	O	-0.487086	-2.322313	-1.062190	
42672	H	-2.387265	-1.931859	-0.505297	
42673	H	0.250324	0.387345	-1.169943	
42674	O	0.387949	1.532295	0.535065	
42675	O	-0.340487	2.487897	-0.220846	
42676	H	0.374405	3.010272	-0.607135	
42677	H	1.788988	-0.336686	1.343091	
42678	H	1.488269	-1.526525	0.032739	
42679	Rotational constants (GHz):		1.2043900	0.7138900	0.5593300
42680	Vibrational harmonic frequencies (cm-1):				
42681		49.0900	61.1709		92.4064
42682		106.6618	120.8520		179.6045
42683		206.0140	224.9411		237.2233
42684		256.9204	276.3407		293.2271
42685		306.1105	322.5219		364.3117
42686		374.3585	435.2061		506.1789
42687		524.5398	573.2409		623.6316
42688		686.3429	824.8614		880.6046
42689		931.9782	966.8707		998.4529
42690		1033.9447	1053.9972		1055.6266
42691		1129.5427	1138.7651		1192.1094
42692		1242.0944	1259.9117		1275.5266
42693		1297.5760	1324.6631		1381.0646
42694		1399.2086	1406.8844		1411.4756
42695		1420.3571	1452.1810		1483.2531
42696		1493.6202	1505.4335		1866.9836
42697		2985.2535	3074.8609		3097.4060
42698		3105.4592	3156.5392		3158.6866
42699		3173.0823	3753.8716		3811.0429
42700	Zero-point correction (Hartree):		0.156200		
42701	diHPCARP_Ic.pttmtmpu				
42702	-----				
42703	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18183335				
42704	Electronic state : 2-A				
42705	Cartesian coordinates (Angs):				
42706	O	2.362175	-0.507489	-1.141820	
42707	O	2.119713	-0.336061	0.248195	
42708	C	0.954570	0.465461	0.391788	
42709	C	-0.286722	-0.295353	-0.111786	
42710	C	-1.585824	0.357437	0.304431	
42711	O	-2.620762	-0.208224	-0.521246	
42712	O	-3.794433	0.171959	-0.123494	
42713	H	1.852931	-1.313424	-1.331061	
42714	C	0.890490	0.780198	1.880149	
42715	H	1.831240	1.222094	2.203965	
42716	H	0.719029	-0.137705	2.440643	
42717	H	0.084122	1.482574	2.084992	
42718	C	1.199724	1.755037	-0.384069	
42719	O	0.338050	2.408355	-0.898054	
42720	H	2.262953	2.054711	-0.406489	
42721	H	-0.264669	-0.373624	-1.200938	
42722	O	-0.344029	-1.598475	0.448954	
42723	O	0.520368	-2.462653	-0.277498	
42724	H	1.221962	-2.614074	0.370963	
42725	H	-1.828336	0.132780	1.342444	
42726	H	-1.561319	1.430700	0.132112	
42727	Rotational constants (GHz):		1.2103000	0.7124000	0.5589000
42728	Vibrational harmonic frequencies (cm-1):				
42729		50.1260	57.1822		95.7955
42730		115.5407	124.1904		189.5887
42731		193.9887	211.1340		230.7275
42732		260.1758	277.5304		292.2732
42733		306.9559	348.5287		368.4951
42734		399.4799	432.2181		516.4702
42735		564.4809	603.0261		623.8974
42736		689.1372	819.5952		883.8719
42737		929.9881	964.2047		998.1961
42738		1035.7962	1049.1802		1054.3335
42739		1129.9573	1142.8655		1188.5195
42740		1239.6506	1259.2557		1277.7298
42741		1297.2480	1331.9751		1376.3189

42743	1401.0329	1408.6238	1413.3161		
42744	1429.9506	1443.2906	1483.2082		
42745	1494.3095	1503.1537	1870.6992		
42746	2984.4581	3075.3016	3090.8574		
42747	3103.0449	3156.3150	3158.4913		
42748	3171.8280	3701.4434	3796.4885		
42749	Zero-point correction (Hartree): 0.156317				
42750					
42751	diHPCARP_Ic.tmmmmmpu				
42752	-----				
42753	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18107284				
42754	Electronic state : 2-A				
42755	Cartesian coordinates (Angs):				
42756	O	3.019300	-0.483182	0.402971	
42757	O	1.752158	-0.232548	0.982330	
42758	C	0.897432	0.391514	0.032145	
42759	C	-0.389684	0.565904	0.875879	
42760	C	-1.116488	-0.733016	1.195782	
42761	O	-1.725837	-1.343342	0.037715	
42762	O	-2.931433	-0.911007	-0.164371	
42763	H	2.855571	-1.330583	-0.039670	
42764	C	1.435734	1.735720	-0.431436	
42765	H	2.427496	1.601041	-0.856604	
42766	H	1.502952	2.411628	0.419450	
42767	H	0.774032	2.174456	-1.174927	
42768	C	0.700394	-0.537185	-1.165524	
42769	O	1.154365	-1.649072	-1.198728	
42770	H	0.140315	-0.113965	-2.012488	
42771	H	-0.037892	0.950778	1.838184	
42772	O	-1.232588	1.595432	0.417480	
42773	O	-1.547007	1.375514	-0.952276	
42774	H	-2.429400	0.980600	-0.895933	
42775	H	-0.400179	-1.467532	1.560271	
42776	H	-1.908878	-0.558398	1.919673	
42777	Rotational constants (GHz):		1.4335500	0.7565100	0.6477000
42778	Vibrational harmonic frequencies (cm-1):				
42779	53.9055	72.3043	92.2902		
42780	134.9738	176.5696	195.6434		
42781	204.0834	220.5476	240.8009		
42782	256.8608	283.1024	319.0220		
42783	323.2674	369.2193	386.4526		
42784	449.8514	483.0516	512.6456		
42785	532.1211	542.2158	626.9700		
42786	794.6353	833.0654	854.2851		
42787	925.4832	950.9318	958.9278		
42788	1009.1401	1038.8455	1053.0892		
42789	1075.3696	1151.7965	1188.3435		
42790	1200.4853	1248.9336	1283.1780		
42791	1332.3947	1353.4376	1379.2182		
42792	1392.9981	1402.0645	1415.5790		
42793	1418.2575	1442.4479	1467.2475		
42794	1490.2778	1502.4768	1844.5313		
42795	3031.3357	3073.1418	3083.8200		
42796	3106.8608	3162.6879	3174.0473		
42797	3174.4127	3755.8105	3774.0936		
42798	Zero-point correction (Hartree): 0.156782				
42799					
42800	diHPCARP_Ic.tmmmmmtmu				
42801	-----				
42802	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18423716				
42803	Electronic state : 2-A				
42804	Cartesian coordinates (Angs):				
42805	O	3.032696	-0.072787	0.702110	
42806	O	1.671260	0.073128	1.065361	
42807	C	0.907338	0.453563	-0.065521	
42808	C	-0.495583	0.672113	0.534688	
42809	C	-1.082486	-0.568572	1.198635	
42810	O	-1.399677	-1.571858	0.215966	
42811	O	-2.531353	-1.332842	-0.376306	
42812	H	3.023970	-0.960780	0.310105	
42813	C	1.418689	1.733805	-0.716536	
42814	H	2.453733	1.602902	-1.020403	

42815	H	1.360216	2.548244	0.004293	
42816	H	0.811539	1.988868	-1.582085	
42817	C	0.895437	-0.663950	-1.102828	
42818	O	1.592768	-1.637988	-1.016909	
42819	H	0.224758	-0.506122	-1.964269	
42820	H	-0.404045	1.445304	1.304525	
42821	O	-1.296042	1.134607	-0.529031	
42822	O	-2.558865	1.504558	-0.005904	
42823	H	-3.071967	0.698897	-0.180728	
42824	H	-0.349207	-1.025132	1.858686	
42825	H	-1.995662	-0.328466	1.736969	
42826	Rotational constants (GHz):		1.4603200	0.7247100	0.6094400
42827	Vibrational harmonic frequencies (cm-1):				
42828		41.1333	82.5185		104.0594
42829		158.4969	169.3647		179.7448
42830		192.8554	221.6943		227.9670
42831		254.8367	297.5691		303.5754
42832		343.8864	363.0606		387.1780
42833		437.9117	503.5203		517.8956
42834		522.0239	559.2311		668.8506
42835		744.5166	833.5767		875.5127
42836		924.2459	933.6825		984.8815
42837		1023.2853	1035.7041		1063.5331
42838		1079.6596	1160.7011		1186.0107
42839		1216.2770	1243.4675		1287.6944
42840		1317.8831	1356.7185		1369.5165
42841		1394.4841	1402.1135		1418.1677
42842		1449.9883	1452.2046		1481.4593
42843		1489.8858	1501.1394		1851.2603
42844		3004.1378	3060.5994		3083.3653
42845		3120.5001	3161.5987		3178.1118
42846		3184.9308	3729.3638		3730.5936
42847	Zero-point correction (Hartree): 0.156893				
42848					
42849	diHPCARP_Ic.tmmmtmpu				
42850	-----				
42851	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17798279				
42852	Electronic state : 2-A				
42853	Cartesian coordinates (Angs):				
42854	O	0.346077	2.785467	-0.050294	
42855	O	-0.238804	1.596511	-0.580739	
42856	C	0.634606	0.520619	-0.253962	
42857	C	-0.066523	-0.733614	-0.869548	
42858	C	-1.576912	-0.629543	-0.874241	
42859	O	-2.002233	-0.349334	0.474739	
42860	O	-3.272137	-0.096131	0.529323	
42861	H	-0.422455	3.183970	0.376038	
42862	C	2.015448	0.756150	-0.849997	
42863	H	2.454377	1.658610	-0.432435	
42864	H	1.917840	0.875484	-1.928250	
42865	H	2.666935	-0.086667	-0.644253	
42866	C	0.702981	0.380053	1.263809	
42867	O	1.513547	-0.312933	1.815848	
42868	H	-0.048517	0.954334	1.828351	
42869	H	0.277249	-0.839678	-1.902503	
42870	O	0.196171	-1.918865	-0.154688	
42871	O	1.574075	-2.234453	-0.246661	
42872	H	1.903354	-1.866236	0.591741	
42873	H	-1.925817	0.176739	-1.512644	
42874	H	-2.014133	-1.580644	-1.172640	
42875	Rotational constants (GHz):		1.0494800	0.8975600	0.6439100
42876	Vibrational harmonic frequencies (cm-1):				
42877		34.6027	55.0658		117.2009
42878		128.6366	150.0286		171.0315
42879		178.6268	211.2752		239.9734
42880		247.4286	257.7931		293.3837
42881		320.5814	340.0895		369.7053
42882		413.6443	426.6001		471.4583
42883		539.2776	555.4470		657.1937
42884		714.5270	792.4853		898.1021
42885		909.9214	976.1958		995.8379
42886		1018.4164	1043.1382		1065.4580


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42887      1105.4016      1155.8337      1185.1448
42888      1202.0599      1229.8750      1273.7538
42889      1300.3913      1349.0192      1373.8026
42890      1395.0671      1402.9537      1411.4329
42891      1421.6668      1476.4091      1484.2981
42892      1488.4310      1501.4248      1852.5091
42893      3020.4301      3067.1473      3089.6501
42894      3110.9170      3166.4946      3179.5589
42895      3198.7349      3688.4372      3830.9078
42896      Zero-point correction (Hartree): 0.156180
42897
42898      diHPCARP_Ic.tmtmmpu
42899      -----
42900      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18219939
42901      Electronic state : 2-A
42902      Cartesian coordinates (Angs):
42903      O      2.776847      -1.319170      -0.079825
42904      O      1.369867      -1.277793      0.083564
42905      C      0.977204      0.034175      0.442726
42906      C      -0.556274      -0.098814      0.575476
42907      C      -1.164538      -0.799605      -0.635200
42908      O      -2.590273      -0.602222      -0.642614
42909      O      -3.159078      -1.206610      0.357823
42910      H      2.860876      -1.060003      -1.010360
42911      C      1.596310      0.497211      1.751867
42912      H      2.673167      0.609935      1.647875
42913      H      1.394759      -0.242502      2.524902
42914      H      1.161080      1.450325      2.048756
42915      C      1.343571      1.014124      -0.670662
42916      O      1.747963      0.651046      -1.742092
42917      H      1.251498      2.081822      -0.418927
42918      H      -0.768146      -0.676948      1.476666
42919      O      -1.168494      1.144740      0.844661
42920      O      -1.207468      1.909074      -0.353561
42921      H      -2.132205      1.802949      -0.619487
42922      H      -0.815362      -0.375309      -1.573478
42923      H      -0.958215      -1.865330      -0.604831
42924      Rotational constants (GHz):      1.4372300      0.6571500      0.6067400
42925      Vibrational harmonic frequencies (cm-1):
42926      48.0102      63.8459      90.5359
42927      112.0186      151.9914      164.6860
42928      181.0478      216.9030      240.9821
42929      276.3134      287.5217      313.0960
42930      344.0256      376.7398      378.4556
42931      404.7821      432.9152      494.3616
42932      523.4359      587.2556      672.8444
42933      715.7879      835.5375      876.0272
42934      931.5087      968.4550      980.2044
42935      994.9900      1032.6445      1047.5641
42936      1113.8281      1142.9737      1190.9902
42937      1215.6733      1246.8392      1272.9357
42938      1305.0382      1325.0742      1374.8288
42939      1400.5909      1408.1475      1414.1979
42940      1421.0352      1435.2438      1487.1188
42941      1488.6647      1501.8127      1847.3301
42942      3022.9853      3078.4189      3102.2384
42943      3124.5980      3158.2532      3165.0948
42944      3187.6069      3759.1421      3782.4265
42945      Zero-point correction (Hartree): 0.156550
42946
42947      diHPCARP_Ic.tmtmmpu
42948      -----
42949      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.21135088
42950      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.09591494
42951      T1 diagnostic: 0.020024
42952      E(MP2/Aug-CC-pVTZ) (Hartree): -721.05036068
42953      E(MP3/Aug-CC-pVTZ) (Hartree): -721.07337670
42954      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05353822
42955      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.07524219
42956      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.54227738
42957      E(UHF/Aug-CC-pVTZ) (Hartree): -718.53708637
42958      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18614857

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42959 Electronic state : 2-A
42960 Cartesian coordinates (Angs):
42961 O -2.964402 -0.957919 -0.369344
42962 O -1.595794 -0.929687 -0.733521
42963 C -1.016968 0.289183 -0.296721
42964 C 0.461984 0.106432 -0.718733
42965 C 1.095007 -1.112290 -0.056500
42966 O 2.457779 -1.249790 -0.495872
42967 O 3.261548 -0.465832 0.155990
42968 H -2.913542 -1.356423 0.512718
42969 C -1.628804 1.502582 -0.973089
42970 H -2.687824 1.567896 -0.732190
42971 H -1.517386 1.415568 -2.052565
42972 H -1.125273 2.408318 -0.639358
42973 C -1.155767 0.410621 1.222187
42974 O -1.423706 -0.531892 1.917608
42975 H -1.026572 1.419905 1.639760
42976 H 0.466630 -0.030327 -1.802826
42977 O 1.217580 1.277254 -0.538440
42978 O 1.345014 1.526413 0.854203
42979 H 2.205131 1.111104 1.034226
42980 H 1.094516 -1.046217 1.028935
42981 H 0.587450 -2.017383 -0.376563
42982 Rotational constants (GHz): 1.5270200 0.6497300 0.6102200
42983 Vibrational harmonic frequencies (cm-1):
42984 36.6409 66.5170 114.5616
42985 134.8907 171.9592 177.7288
42986 186.1317 214.2034 241.8131
42987 263.4286 306.7271 320.9665
42988 326.9893 375.4289 396.8432
42989 428.3840 478.7185 524.7143
42990 537.8407 588.5838 651.1578
42991 705.7016 837.8899 885.0331
42992 932.9605 967.9964 983.0241
42993 1000.5910 1025.5868 1048.4628
42994 1107.9646 1152.0275 1189.0139
42995 1205.0365 1255.0924 1265.2852
42996 1316.5436 1333.6655 1379.8364
42997 1405.4081 1406.1390 1421.4796
42998 1433.4307 1438.2248 1484.5764
42999 1488.6895 1500.5911 1844.8621
43000 3031.1024 3079.6899 3092.4893
43001 3124.6291 3159.7359 3165.1495
43002 3191.0199 3708.8540 3764.7138
43003 Zero-point correction (Hartree): 0.156913
43004
43005 diHPCARP_Ic.tmtmpppu
43006 -----
43007 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18033591
43008 Electronic state : 2-A
43009 Cartesian coordinates (Angs):
43010 O -2.729658 -1.331309 -0.561632
43011 O -1.389670 -1.001317 -0.880469
43012 C -1.042346 0.220293 -0.248210
43013 C 0.454100 0.347514 -0.628535
43014 C 1.323095 -0.667385 0.081437
43015 O 2.594322 -0.669418 -0.595430
43016 O 3.493798 -1.311166 0.084138
43017 H -2.606332 -1.854985 0.244337
43018 C -1.847437 1.394970 -0.772676
43019 H -2.908239 1.205053 -0.623227
43020 H -1.655833 1.524856 -1.836295
43021 H -1.565006 2.308911 -0.253018
43022 C -1.218154 0.084223 1.264787
43023 O -1.319566 -0.982365 1.807383
43024 H -1.259642 1.027265 1.831462
43025 H 0.508426 0.177431 -1.706923
43026 O 0.934787 1.665542 -0.494041
43027 O 0.833009 2.026395 0.881435
43028 H 1.751285 2.236409 1.093177
43029 H 1.496033 -0.410507 1.124442
43030 H 0.887588 -1.663006 0.014155

```

43031	Rotational constants (GHz):	1.2849100	0.6596800	0.5699800
43032	Vibrational harmonic frequencies (cm-1):			
43033		36.2254	56.1929	75.2810
43034		82.1147	126.3395	176.0510
43035		183.6677	215.1825	229.0916
43036		253.5744	277.1087	302.8801
43037		308.7722	319.4598	369.9761
43038		391.5176	395.9074	469.3943
43039		503.0072	568.6105	654.9775
43040		713.2076	840.0501	892.7599
43041		934.4476	970.4701	982.7428
43042		1007.0292	1045.2380	1049.7415
43043		1111.7464	1143.0671	1191.7131
43044		1206.2689	1254.1946	1263.7515
43045		1297.1900	1321.9606	1364.6418
43046		1403.3831	1407.4056	1419.3110
43047		1423.0486	1432.0236	1488.3653
43048		1489.0874	1500.7795	1848.6470
43049		3020.7621	3080.5759	3091.4722
43050		3107.4964	3160.5715	3166.1597
43051		3167.3176	3766.7191	3822.5851
43052	Zero-point correction (Hartree):	0.155784		
43053				
43054	diHPCARP_Ic.tpppmmmpmu			
43055	-----			
43056	E(UM062X/Aug-CC-pVTZ) (Hartree):	-722.18144356		
43057	Electronic state : 2-A			
43058	Cartesian coordinates (Angs):			
43059	O	2.235749	-0.850992	-1.406855
43060	O	1.140209	-0.023109	-1.051811
43061	C	0.555592	-0.491164	0.153702
43062	C	-0.637521	0.440543	0.428756
43063	C	-1.726318	0.415906	-0.638503
43064	O	-2.583089	-0.732839	-0.464241
43065	O	-3.222360	-0.691903	0.664042
43066	H	2.936501	-0.482096	-0.845735
43067	C	0.132646	-1.954569	0.068267
43068	H	1.006222	-2.593146	-0.031739
43069	H	-0.506870	-2.101341	-0.799466
43070	H	-0.424375	-2.242268	0.959815
43071	C	1.537132	-0.310182	1.302813
43072	O	2.669365	0.055941	1.153435
43073	H	1.141691	-0.558507	2.305099
43074	H	-1.092435	0.132662	1.373764
43075	O	-0.203899	1.761894	0.681042
43076	O	0.031439	2.423415	-0.554831
43077	H	0.893024	2.069375	-0.824219
43078	H	-2.332820	1.314130	-0.549266
43079	H	-1.329441	0.318725	-1.644718
43080	Rotational constants (GHz):	1.3188700	0.7055200	0.6083800
43081	Vibrational harmonic frequencies (cm-1):			
43082		40.9708	59.3857	92.1645
43083		142.4266	161.9521	171.2996
43084		196.3227	218.5043	228.3289
43085		229.9576	284.9366	315.6904
43086		316.4798	368.6657	405.6909
43087		412.5856	442.3959	515.4544
43088		541.5335	570.2832	622.5128
43089		737.9806	837.3915	896.3944
43090		922.9245	949.4048	978.0752
43091		1001.3290	1030.3820	1063.1270
43092		1108.4669	1146.1945	1184.2336
43093		1216.0905	1239.6581	1264.7054
43094		1305.8782	1335.0028	1382.8392
43095		1404.6448	1410.2648	1421.5778
43096		1446.7343	1454.5565	1480.2496
43097		1486.8313	1505.3529	1860.7884
43098		2970.9115	3080.6417	3088.6240
43099		3121.6556	3157.4201	3173.8861
43100		3191.2229	3737.3396	3757.2865
43101	Zero-point correction (Hartree):	0.156482		
43102				

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43103 diHPCARP_Ic.tpppppmu
43104 -----
43105 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18110884
43106 Electronic state : 2-A
43107 Cartesian coordinates (Angs):
43108 O 1.769616 -1.590895 -1.249693
43109 O 0.779848 -0.591651 -1.064257
43110 C 0.445579 -0.522849 0.310188
43111 C -0.597998 0.610441 0.445106
43112 C -1.649288 0.647052 -0.658122
43113 O -2.518318 -0.497379 -0.565045
43114 O -3.206462 -0.487660 0.536212
43115 H 2.580933 -1.073393 -1.138400
43116 C -0.063018 -1.854343 0.852239
43117 H 0.715890 -2.608992 0.776995
43118 H -0.925734 -2.183322 0.278893
43119 H -0.357627 -1.748837 1.896234
43120 C 1.658593 -0.056016 1.106827
43121 O 2.672025 0.324807 0.585279
43122 H 1.552336 -0.080087 2.205470
43123 H -1.109497 0.488721 1.402065
43124 O 0.019507 1.877965 0.571588
43125 O 0.580788 2.248629 -0.679512
43126 H 1.464447 1.847583 -0.644477
43127 H -2.248723 1.547972 -0.542303
43128 H -1.211268 0.594122 -1.648468
43129 Rotational constants (GHz): 1.3022100 0.7692500 0.6255800
43130 Vibrational harmonic frequencies (cm-1):
43131 34.1325 59.0351 108.6116
43132 135.0917 156.2863 175.9170
43133 198.7084 201.5820 218.2019
43134 249.2978 271.3825 310.2169
43135 324.2414 352.6443 390.6643
43136 408.8290 451.0351 460.5699
43137 514.0741 579.1079 626.0931
43138 722.7287 840.5565 885.9730
43139 937.9943 955.0642 982.4384
43140 1004.8195 1030.0956 1059.4987
43141 1107.6775 1145.7714 1184.4900
43142 1222.1167 1232.8329 1263.3818
43143 1304.4937 1333.0052 1378.8645
43144 1404.4574 1407.7888 1420.6930
43145 1430.8856 1457.4120 1487.0070
43146 1491.1520 1510.8401 1847.9397
43147 2990.0194 3082.1252 3103.6929
43148 3118.7439 3158.5890 3179.3827
43149 3205.1232 3734.5713 3770.8752
43150 Zero-point correction (Hartree): 0.156325
43151
43152 diHPCARP_Ic.tptmmpmu
43153 -----
43154 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.18208865
43155 Electronic state : 2-A
43156 Cartesian coordinates (Angs):
43157 O 2.353640 -1.077329 -1.233578
43158 O 1.078273 -0.476418 -1.075328
43159 C 0.700750 -0.545358 0.287791
43160 C -0.667552 0.161728 0.382933
43161 C -1.578265 -0.188973 -0.778745
43162 O -2.951261 0.060479 -0.417816
43163 O -3.352053 -0.766553 0.497586
43164 H 2.936499 -0.314663 -1.103398
43165 C 0.618370 -1.978187 0.797625
43166 H 1.547208 -2.501814 0.587851
43167 H -0.200069 -2.504612 0.309630
43168 H 0.436963 -1.987486 1.872187
43169 C 1.660972 0.279270 1.136205
43170 O 2.502635 0.991939 0.659540
43171 H 1.529582 0.197210 2.229086
43172 H -1.147136 -0.162946 1.309229
43173 O -0.538622 1.561099 0.567554
43174 O -0.037988 2.154825 -0.619774

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43175      H      0.923226      2.105850      -0.495182
43176      H      -1.376986      0.449669      -1.632916
43177      H      -1.491926      -1.236435      -1.056811
43178      Rotational constants (GHz):      1.4333500      0.6769300      0.5836800
43179      Vibrational harmonic frequencies (cm-1):
43180      42.8535      70.2507      112.7377
43181      127.8844      158.1837      160.6998
43182      187.3189      203.1592      230.4784
43183      261.8875      277.3097      307.6056
43184      325.5334      334.7333      393.5094
43185      408.9079      423.3548      456.0359
43186      525.6790      580.7002      657.8426
43187      755.9250      842.9615      872.8277
43188      944.0831      952.8993      975.5825
43189      979.7235      1014.8451      1051.2959
43190      1131.3791      1136.3470      1185.4572
43191      1217.8011      1236.2103      1256.5861
43192      1311.4295      1326.2842      1382.4358
43193      1404.6405      1411.3737      1416.9611
43194      1431.7841      1455.8733      1476.3586
43195      1488.7091      1505.8085      1848.5804
43196      2992.1566      3078.8887      3097.2656
43197      3126.5184      3150.7433      3174.4491
43198      3197.2432      3740.2825      3772.9273
43199      Zero-point correction (Hartree): 0.156262
43200
43201
43202
43203      1,4-aldehyde-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-HPCARP-
43204      Ia)
43205      =====
43206      =
43207
43208      TS.diHPCARP_I.14aldHshift.mmmmmmpu
43209      -----
43210      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14000634
43211      Electronic state : 2-A
43212      Cartesian coordinates (Angs):
43213      C      -2.030154      -0.059161      -0.085097
43214      C      -0.518993      -0.452742      -0.260483
43215      O      -0.169746      -0.770891      1.060332
43216      O      -1.224192      -1.478019      1.607838
43217      H      -2.125813      -0.684692      1.053490
43218      O      -2.774853      0.409128      -0.854258
43219      C      -0.525506      -1.648464      -1.205618
43220      H      -0.814723      -1.326312      -2.205818
43221      H      -1.235368      -2.394746      -0.856231
43222      H      0.468537      -2.089814      -1.224866
43223      C      0.351753      0.709133      -0.740724
43224      H      -0.148754      1.150452      -1.612077
43225      O      0.516408      1.690702      0.265786
43226      O      -0.768068      2.085542      0.718107
43227      H      -0.895715      2.932390      0.270331
43228      C      1.763324      0.283732      -1.147100
43229      O      2.324523      -0.712619      -0.331501
43230      H      1.728964      -0.163735      -2.140675
43231      H      2.406077      1.165608      -1.171462
43232      O      2.660809      -0.135423      0.919170
43233      H      1.855203      -0.291503      1.437652
43234      Rotational constants (GHz):      1.2894600      0.8010300      0.7088200
43235      Vibrational harmonic frequencies (cm-1):
43236      i1928.9033      83.5178      96.6603
43237      121.0383      151.2801      162.0973
43238      180.3044      219.0386      229.9054
43239      230.3576      266.8049      270.5781
43240      288.1812      325.9894      372.1662
43241      423.9363      433.4081      462.3376
43242      493.1332      597.0381      600.2451
43243      631.0923      717.8175      822.6271
43244      865.9715      896.7038      953.3772
43245      981.3270      1024.5749      1062.4453
43246      1072.6985      1088.0453      1119.4133

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43247      1151.6612      1168.6958      1196.1158
43248      1265.4347      1308.7142      1355.9956
43249      1371.6387      1394.9543      1402.1274
43250      1413.9153      1460.4071      1464.3378
43251      1482.0722      1511.7219      1814.8065
43252      1998.5599      3027.1054      3077.3867
43253      3080.5049      3135.3005      3158.8909
43254      3170.8783      3748.3459      3804.4818
43255      Zero-point correction (Hartree): 0.150833
43256
43257      TS.diHPCARP_I.14aldHshift.mmpmmpu
43258      -----
43259      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14194620
43260      Electronic state : 2-A
43261      Cartesian coordinates (Angs):
43262      C      -2.034141      -0.044653      -0.164589
43263      C      -0.522037      -0.457385      -0.232091
43264      O      -0.223050      -0.604637      1.134831
43265      O      -1.302208      -1.232520      1.735388
43266      H      -2.184598      -0.519815      1.031322
43267      O      -2.750988      0.326407      -1.007352
43268      C      -0.500595      -1.759813      -1.021181
43269      H      -0.762858      -1.560668      -2.060131
43270      H      -1.220849      -2.460022      -0.603763
43271      H      0.493713      -2.195881      -0.961993
43272      C      0.363874      0.649387      -0.806703
43273      H      -0.132424      1.030440      -1.707140
43274      O      0.538108      1.703032      0.120244
43275      O      -0.748442      2.145461      0.529884
43276      H      -0.728820      1.918719      1.470259
43277      C      1.770061      0.180179      -1.176128
43278      O      2.322208      -0.757321      -0.284631
43279      H      1.733826      -0.344271      -2.131226
43280      H      2.421254      1.050943      -1.268363
43281      O      2.669530      -0.092319      0.918671
43282      H      1.876514      -0.230560      1.458908
43283      Rotational constants (GHz): 1.3016800      0.7897400      0.7170300
43284      Vibrational harmonic frequencies (cm-1):
43285      i1833.4049      77.4175      98.3355
43286      120.1696      151.3486      160.0142
43287      176.9145      216.2501      227.8545
43288      237.8231      268.9547      289.7126
43289      328.6518      352.8291      371.8152
43290      408.6218      428.7350      461.4518
43291      494.3577      596.9852      603.1902
43292      631.7990      717.6451      815.6231
43293      866.7032      892.8595      950.0544
43294      980.7043      1027.1601      1061.3283
43295      1070.4924      1089.0372      1121.6262
43296      1147.6575      1165.3150      1194.8415
43297      1263.4559      1308.1257      1349.8313
43298      1377.8612      1394.1227      1410.5224
43299      1417.0766      1453.1306      1463.7489
43300      1481.8435      1510.3846      1816.8526
43301      2006.5897      3038.3518      3077.6618
43302      3080.8681      3135.8114      3158.1302
43303      3172.7436      3754.3237      3795.3228
43304      Zero-point correction (Hartree): 0.150977
43305
43306      TS.diHPCARP_I.14aldHshift.mmpmmpu
43307      -----
43308      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14045165
43309      Electronic state : 2-A
43310      Cartesian coordinates (Angs):
43311      C      1.994472      -0.167445      0.288167
43312      C      0.443676      -0.415442      0.284590
43313      O      0.230114      -0.742820      -1.067633
43314      O      1.274668      -1.562306      -1.470102
43315      H      2.179265      -0.833331      -0.802678
43316      O      2.687414      0.252342      1.127845
43317      C      0.242210      -1.570226      1.258219
43318      H      0.470086      -1.234660      2.269775

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43319	H	0.908540	-2.391180	1.002114	
43320	H	-0.787079	-1.915203	1.205126	
43321	C	-0.338224	0.852952	0.627086	
43322	H	0.125639	1.258553	1.535802	
43323	O	-0.284514	1.802810	-0.417425	
43324	O	1.060238	1.953366	-0.843128	
43325	H	1.010404	1.578342	-1.734146	
43326	C	-1.831094	0.691228	0.905184	
43327	O	-2.594681	0.273415	-0.198807	
43328	H	-1.991818	0.027410	1.755904	
43329	H	-2.225862	1.678650	1.146462	
43330	O	-2.487244	-1.137582	-0.320656	
43331	H	-1.843388	-1.228787	-1.038580	
43332	Rotational constants (GHz):		1.2813900	0.8091100	0.6911200
43333	Vibrational harmonic frequencies (cm-1):				
43334	i1788.5741		66.9891		105.1583
43335	117.9710		151.9100		172.6681
43336	181.2209		218.3409		230.9273
43337	238.4362		270.0048		274.5726
43338	333.3841		346.0724		383.9779
43339	439.6975		456.4439		487.2099
43340	504.2662		597.7395		605.2544
43341	635.1391		717.3113		779.6636
43342	857.8186		912.0735		958.1096
43343	974.6334		1028.8444		1061.6499
43344	1070.4744		1093.8354		1121.8435
43345	1146.2736		1162.4080		1186.8816
43346	1264.6695		1319.3623		1339.4738
43347	1388.7165		1397.3513		1413.3792
43348	1420.3749		1439.4885		1464.2406
43349	1483.0273		1515.2216		1816.5840
43350	2006.3838		3025.7287		3078.7011
43351	3082.7705		3134.7647		3157.9027
43352	3175.7848		3770.3207		3788.0038
43353	Zero-point correction (Hartree):		0.151205		
43354	-----				
43355	TS.diHPCARP_I.14aldHshift.mmppppu				
43356	-----				
43357	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13923381				
43358	Electronic state : 2-A				
43359	Cartesian coordinates (Angs):				
43360	C	1.648137	-0.388097	0.995277	
43361	C	0.546302	-0.472713	-0.119318	
43362	O	1.296465	-0.155427	-1.266370	
43363	O	2.512366	-0.811520	-1.157697	
43364	H	2.615211	-0.541015	0.143639	
43365	O	1.549662	-0.411035	2.157809	
43366	C	0.055908	-1.914174	-0.082951	
43367	H	-0.510187	-2.089369	0.830356	
43368	H	0.905017	-2.592548	-0.125854	
43369	H	-0.590973	-2.099706	-0.937608	
43370	C	-0.546854	0.577388	0.056532	
43371	H	-0.870066	0.554851	1.101593	
43372	O	-0.092309	1.870101	-0.300634	
43373	O	1.150556	2.120577	0.332123	
43374	H	1.758034	2.027458	-0.416922	
43375	C	-1.757008	0.377726	-0.855077	
43376	O	-2.620633	-0.635718	-0.391707	
43377	H	-2.288106	1.327335	-0.940598	
43378	H	-1.445560	0.050050	-1.847591	
43379	O	-3.188744	-0.184868	0.832269	
43380	H	-4.111179	-0.054720	0.579860	
43381	Rotational constants (GHz):		1.2903000	0.6826400	0.6331600
43382	Vibrational harmonic frequencies (cm-1):				
43383	i1841.4768		57.4105		61.0754
43384	113.1597		143.0052		153.6013
43385	189.9766		201.4617		215.4248
43386	232.7557		236.9769		272.4953
43387	283.1436		326.3846		380.1935
43388	412.9860		421.1079		483.0953
43389	513.2878		537.1479		606.0512
43390	641.0308		684.0429		756.4224

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43391      873.8504          927.9070          957.5498
43392      1002.4973         1044.2752         1068.5155
43393      1080.8273         1107.3109         1120.6600
43394      1145.4145         1162.1661         1182.7914
43395      1268.5412         1290.9073         1328.6350
43396      1395.6050         1399.9131         1407.1323
43397      1419.4035         1424.3227         1473.6655
43398      1484.4851         1500.9618         1814.5028
43399      2006.7933         3071.4301         3077.1019
43400      3081.3020         3135.2756         3164.8188
43401      3167.6552         3772.2524         3824.7302
43402      Zero-point correction (Hartree): 0.150599
43403
43404      TS.diHPCARP_I.14aldHshift.mpmpppu
43405      -----
43406      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13990478
43407      Electronic state : 2-A
43408      Cartesian coordinates (Angs):
43409      C      1.777421      -0.694313      0.876503
43410      C      0.653978      -0.413445      -0.188388
43411      O      1.357551      0.449942      -1.055980
43412      O      2.618358      -0.090908      -1.243568
43413      H      2.734072      -0.421965      0.044159
43414      O      1.701150      -1.115055      1.961381
43415      C      0.308741      -1.755606      -0.814276
43416      H      -0.230003      -2.371173      -0.095506
43417      H      1.215286      -2.265727      -1.131476
43418      H      -0.330452      -1.591579      -1.679328
43419      C      -0.517508      0.338944      0.435084
43420      H      -0.880929      -0.265691      1.268818
43421      O      -0.070919      1.535377      1.043584
43422      O      0.016028      2.558479      0.058563
43423      H      0.864770      2.363129      -0.366432
43424      C      -1.689793      0.596983      -0.512161
43425      O      -2.454926      -0.571241      -0.728083
43426      H      -2.303595      1.395520      -0.092963
43427      H      -1.354436      0.887439      -1.506842
43428      O      -3.035434      -0.944908      0.515803
43429      H      -3.966224      -0.738810      0.365400
43430      Rotational constants (GHz):      1.192590      0.7116300      0.6294700
43431      Vibrational harmonic frequencies (cm-1):
43432      i1856.2650      45.3808      61.3826
43433      117.6114      141.7917      164.5419
43434      186.9853      195.9062      217.6415
43435      221.8016      233.4167      270.3890
43436      300.3508      327.0825      367.2170
43437      408.4668      438.6737      485.0490
43438      516.1145      542.7658      615.2076
43439      641.6486      704.5212      772.1928
43440      866.0263      928.2783      944.5546
43441      976.2109      1030.2452      1062.9090
43442      1071.3586      1113.1503      1116.2179
43443      1118.1695      1173.1640      1178.2570
43444      1269.6388      1286.1214      1332.7151
43445      1388.0730      1395.5964      1405.8990
43446      1418.7789      1444.1033      1474.7041
43447      1480.0399      1497.8440      1822.2252
43448      2013.6939      3080.8326      3083.4196
43449      3103.0358      3148.1852      3162.8900
43450      3168.4993      3763.1687      3824.4187
43451      Zero-point correction (Hartree): 0.150629
43452
43453      TS.diHPCARP_I.14aldHshift.mtmmpu
43454      -----
43455      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14126793
43456      Electronic state : 2-A
43457      Cartesian coordinates (Angs):
43458      C      2.027441      0.702538      -0.236735
43459      C      0.867693      -0.216199      0.304058
43460      O      0.605687      -0.992812      -0.840978
43461      O      1.826074      -1.336958      -1.389946
43462      H      2.334291      -0.133912      -1.187649

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43463	O	2.478501	1.677601	0.217311		
43464	C	1.441232	-1.022963	1.457907		
43465	H	1.636707	-0.373364	2.310104		
43466	H	2.367660	-1.503071	1.151981		
43467	H	0.726860	-1.796483	1.735783		
43468	C	-0.365977	0.604840	0.656222		
43469	H	-0.081430	1.324541	1.433253		
43470	O	-0.654969	1.301683	-0.547196		
43471	O	-1.860285	2.021574	-0.400799		
43472	H	-2.494961	1.393154	-0.780639		
43473	C	-1.524119	-0.226065	1.195781		
43474	O	-1.842226	-1.358909	0.423950		
43475	H	-1.247621	-0.629157	2.170646		
43476	H	-2.398856	0.411773	1.324903		
43477	O	-2.305803	-0.908434	-0.843161		
43478	H	-1.496101	-0.976338	-1.375228		
43479	Rotational constants (GHz):			1.2779200	0.7916600	0.6634400
43480	Vibrational harmonic frequencies (cm-1):					
43481	i1946.3293		61.7856			96.9848
43482	109.6508		126.5084			138.1330
43483	207.8169		219.5612			229.8801
43484	250.3378		259.6589			308.6176
43485	330.6072		383.2463			398.1145
43486	467.0271		498.1523			500.5395
43487	539.5675		554.6636			598.7627
43488	659.5660		722.6066			822.1567
43489	851.9170		895.8462			953.6409
43490	976.3288		1034.9594			1051.1843
43491	1074.4283		1079.2651			1126.0956
43492	1132.4334		1166.1764			1208.6992
43493	1261.1462		1296.5243			1364.2186
43494	1376.6060		1398.7606			1410.7526
43495	1440.7865		1450.1609			1477.8590
43496	1485.6545		1510.4216			1817.7906
43497	2011.8689		3041.0717			3075.9836
43498	3089.3908		3133.9251			3157.3115
43499	3167.4935		3733.2415			3743.8570
43500	Zero-point correction (Hartree):			0.151452		
43501						
43502	TS.diHPCARP_I.14aldHshift.mtmtmpu					
43503	-----					
43504	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13969286					
43505	Electronic state : 2-A					
43506	Cartesian coordinates (Angs):					
43507	C	1.964446	0.945757	0.307869		
43508	C	1.049055	-0.333117	0.212049		
43509	O	1.432225	-0.829329	-1.045659		
43510	O	2.808400	-0.728624	-1.113479		
43511	H	2.816066	0.471699	-0.560078		
43512	O	1.910473	1.849627	1.042785		
43513	C	1.446405	-1.234914	1.373002		
43514	H	1.195518	-0.758531	2.319416		
43515	H	2.516051	-1.426958	1.337591		
43516	H	0.921923	-2.185633	1.294763		
43517	C	-0.425221	0.027334	0.171312		
43518	H	-0.695919	0.435544	1.147836		
43519	O	-0.549003	1.055184	-0.801136		
43520	O	-1.748051	1.771696	-0.541273		
43521	H	-2.330812	1.416285	-1.227329		
43522	C	-1.296095	-1.173926	-0.183306		
43523	O	-2.643717	-0.804971	-0.384323		
43524	H	-0.979868	-1.585981	-1.141907		
43525	H	-1.234473	-1.939946	0.592031		
43526	O	-3.163671	-0.364295	0.860963		
43527	H	-3.013270	0.592416	0.809093		
43528	Rotational constants (GHz):			1.4814500	0.6262800	0.5598000
43529	Vibrational harmonic frequencies (cm-1):					
43530	i1941.3836		47.7105			87.4701
43531	103.7624		136.4784			165.4359
43532	174.2679		194.7583			215.6581
43533	251.5348		258.7636			268.8290
43534	325.4285		365.9015			391.5000

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43535      406.0708      470.4298      496.1433
43536      517.2554      563.9638      568.3195
43537      622.5967      703.0537      820.4662
43538      889.7945      899.8458      962.6654
43539      991.1986      1035.5923     1054.1060
43540     1077.4815     1107.6241     1117.3598
43541     1141.8991     1158.3796     1194.7951
43542     1274.1514     1303.0559     1337.4525
43543     1383.1863     1401.2609     1416.8854
43544     1426.2362     1440.6900     1472.0475
43545     1482.6434     1503.5151     1820.1127
43546     2012.5594     3072.4876     3080.6632
43547     3085.6277     3139.6417     3160.2026
43548     3170.4295     3745.6400     3790.1733
43549 Zero-point correction (Hartree): 0.151054
43550
43551 TS.diHPCARP_I.14aldHshift.mtppppu
43552 -----
43553 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13705569
43554 Electronic state : 2-A
43555 Cartesian coordinates (Angs):
43556 C      1.983733      0.358632      0.639969
43557 C      0.741355     -0.430591      0.079030
43558 O      1.189971     -0.712220     -1.223386
43559 O      2.504917     -1.119757     -1.117156
43560 H      2.794037     -0.192667     -0.225964
43561 O      2.072745      1.046266      1.579878
43562 C      0.585942     -1.662564      0.960930
43563 H      0.324619     -1.360282      1.974020
43564 H      1.518347     -2.221862      0.976666
43565 H     -0.208143     -2.288628      0.561377
43566 C     -0.490851      0.453553      0.002279
43567 H     -0.838849      0.641428      1.019545
43568 O     -0.060301      1.674380     -0.586409
43569 O     -1.031358      2.662530     -0.278670
43570 H     -0.563237      3.192995      0.379019
43571 C     -1.623736     -0.116469     -0.847998
43572 O     -2.221846     -1.262757     -0.281860
43573 H     -2.363582      0.670827     -1.002594
43574 H     -1.236571     -0.451640     -1.810087
43575 O     -2.810868     -0.870609      0.953888
43576 H     -3.751357     -0.948201      0.752477
43577 Rotational constants (GHz):      1.1285900      0.7415400      0.5981900
43578 Vibrational harmonic frequencies (cm-1):
43579 i1971.1687      21.8975      57.9048
43580      77.3261      122.7409      148.1743
43581      156.6068      186.7649      206.0714
43582      218.1373      229.0039      247.9989
43583      267.9961      309.1177      328.4699
43584      376.4668      393.2169      445.8271
43585      496.5010      564.6502      581.5742
43586      633.5074      694.4304      756.8277
43587      878.5082      931.9005      955.5199
43588      1027.2884     1031.8378     1064.3136
43589      1078.7951     1101.8122     1113.3230
43590      1127.3859     1165.2587     1191.7853
43591      1276.6848     1288.9227     1338.8035
43592      1392.2848     1394.3762     1403.5263
43593      1414.1412     1426.1040     1482.7032
43594      1484.9449     1498.5919     1816.1002
43595      2002.3995     3078.6290     3082.3687
43596      3099.6634     3144.5083     3163.9024
43597      3175.4812     3809.4751     3826.6840
43598 Zero-point correction (Hartree): 0.149879
43599
43600 TS.diHPCARP_I.14aldHshift.tmmmpu
43601 -----
43602 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13980278
43603 Electronic state : 2-A
43604 Cartesian coordinates (Angs):
43605 C      -0.849694     -0.658476      1.039509
43606 C      -0.851181      0.372362     -0.143731

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43607	O	-1.669014	-0.296137	-1.072452			
43608	O	-2.723837	-0.847153	-0.368654			
43609	H	-1.943422	-1.233270	0.625467			
43610	O	-0.212473	-0.694204	2.022198			
43611	C	-1.479824	1.640550	0.416281			
43612	H	-0.872608	2.032833	1.228405			
43613	H	-2.482035	1.417882	0.775473			
43614	H	-1.536150	2.386003	-0.375447			
43615	C	0.512860	0.566976	-0.817050			
43616	H	0.383465	1.246447	-1.664454			
43617	O	1.447317	1.127518	0.085007			
43618	O	1.250021	2.540194	0.111197			
43619	H	2.130542	2.847973	-0.136911			
43620	C	1.079856	-0.749285	-1.337694			
43621	O	1.017917	-1.797211	-0.396874			
43622	H	0.461514	-1.088543	-2.167214			
43623	H	2.108221	-0.605650	-1.668552			
43624	O	2.091430	-1.637626	0.515622			
43625	H	1.667483	-1.199503	1.271001			
43626	Rotational constants (GHz):				1.0831700	0.9226200	0.7119600
43627	Vibrational harmonic frequencies (cm-1):						
43628	i1954.2124			58.6403		98.0243	
43629	131.6452			141.5194		182.8393	
43630	189.7068			209.4981		224.7974	
43631	242.4648			270.9678		282.5157	
43632	296.4770			337.8994		369.1063	
43633	384.8120			435.4515		465.7056	
43634	482.4115			508.6508		618.6898	
43635	644.1068			722.7004		780.7613	
43636	872.1228			914.9300		949.4674	
43637	987.9733			1022.2665		1062.2560	
43638	1065.9693			1101.2514		1121.0428	
43639	1139.1397			1151.4566		1193.4193	
43640	1262.7903			1305.7164		1344.0458	
43641	1367.3671			1401.3076		1405.7479	
43642	1413.8015			1460.1710		1463.4632	
43643	1486.0143			1498.8990		1818.2523	
43644	1980.4793			3064.5293		3080.9656	
43645	3094.7690			3154.7175		3162.6155	
43646	3176.8628			3736.5958		3827.5040	
43647	Zero-point correction (Hartree):				0.150740		
43648							
43649	TS.diHPCARP_I.14aldHshift.tmmppmu						
43650	-----						
43651	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.14153543		
43652	Electronic state : 2-A						
43653	Cartesian coordinates (Angs):						
43654	C	0.752097	-1.009256	1.100227			
43655	C	-0.116954	-0.721852	-0.170409			
43656	O	0.876471	-0.760522	-1.176327			
43657	O	1.736217	-1.807130	-0.886000			
43658	H	1.709202	-1.553408	0.428195			
43659	O	0.495960	-0.896296	2.234135			
43660	C	-1.112598	-1.865982	-0.272379			
43661	H	-1.820804	-1.811727	0.551425			
43662	H	-0.582779	-2.815571	-0.245622			
43663	H	-1.654302	-1.779354	-1.211614			
43664	C	-0.725241	0.689448	-0.222986			
43665	H	-0.781456	0.971586	-1.276674			
43666	O	-2.009709	0.752650	0.354164			
43667	O	-2.965893	0.311726	-0.604168			
43668	H	-3.500686	1.108173	-0.712435			
43669	C	0.093609	1.716584	0.568632			
43670	O	1.476796	1.502661	0.442539			
43671	H	-0.169768	2.726253	0.255603			
43672	H	-0.114496	1.597638	1.632529			
43673	O	1.850324	1.861076	-0.881004			
43674	H	1.888280	0.989442	-1.306631			
43675	Rotational constants (GHz):				1.0646600	0.8709300	0.7005100
43676	Vibrational harmonic frequencies (cm-1):						
43677	i1797.6434			65.2860		88.2728	
43678	131.4006			143.1357		168.4932	

43679	202.0168	219.0448	230.1383			
43680	251.0519	262.8654	272.3882			
43681	291.6855	350.1169	386.3366			
43682	431.6758	470.6430	494.8818			
43683	499.4120	516.6638	608.9901			
43684	634.8104	691.8628	738.2642			
43685	877.8707	936.2009	956.5294			
43686	1016.2656	1021.0467	1064.5588			
43687	1088.5398	1097.8503	1127.7869			
43688	1133.7014	1176.1168	1185.3349			
43689	1260.7951	1286.4595	1332.1236			
43690	1379.5493	1399.9199	1409.9368			
43691	1417.2077	1454.6828	1484.1116			
43692	1486.9388	1495.1239	1826.4206			
43693	2003.2461	3084.9038	3085.4039			
43694	3088.5353	3145.2325	3170.4346			
43695	3174.9685	3737.6754	3822.7825			
43696	Zero-point correction (Hartree): 0.151220					
43697						
43698	TS.diHPCARP_I.14aldHshift.tpmmpu					
43699	-----					
43700	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13919448					
43701	Electronic state : 2-A					
43702	Cartesian coordinates (Angs):					
43703	C	-0.712958	-0.337340	1.178963		
43704	C	-0.981672	0.302338	-0.232124		
43705	O	-1.668928	-0.745372	-0.869931		
43706	O	-2.522733	-1.306722	0.060969		
43707	H	-1.625326	-1.253566	1.015368		
43708	O	-0.136126	0.082838	2.109270		
43709	C	-1.843934	1.530720	0.019621		
43710	H	-1.301962	2.260109	0.619137		
43711	H	-2.755101	1.241511	0.538384		
43712	H	-2.102829	1.983776	-0.936511		
43713	C	0.247224	0.581962	-1.110065		
43714	H	-0.134673	0.909764	-2.081434		
43715	O	0.965750	1.721882	-0.683411		
43716	O	1.710283	1.417414	0.487359		
43717	H	1.106789	1.651644	1.208393		
43718	C	1.080649	-0.681282	-1.328391		
43719	O	1.151116	-1.493947	-0.171506		
43720	H	0.582033	-1.289108	-2.082107		
43721	H	2.083546	-0.425288	-1.667484		
43722	O	2.387961	-1.308158	0.490845		
43723	H	2.313091	-0.400702	0.829474		
43724	Rotational constants (GHz):			1.2482700	0.8556200	0.7671600
43725	Vibrational harmonic frequencies (cm-1):					
43726	i1985.4832		44.3310			65.2751
43727	147.3949		158.0713			188.2903
43728	201.6003		209.8888			224.0193
43729	244.8781		264.7958			292.4958
43730	314.1043		355.5570			373.7496
43731	466.8671		491.8604			495.5827
43732	512.0421		541.7298			607.0638
43733	644.1797		723.1206			787.4031
43734	834.9388		934.3390			954.5427
43735	968.5253		1024.8268			1053.4711
43736	1064.6602		1107.2479			1122.5801
43737	1137.9489		1150.1796			1194.6813
43738	1253.2650		1297.3415			1336.6471
43739	1374.4988		1396.6389			1404.0224
43740	1428.0547		1464.7301			1477.9056
43741	1478.5764		1497.0842			1811.2836
43742	1975.7657		3075.2932			3076.7680
43743	3095.1827		3151.5186			3155.6352
43744	3168.6087		3713.1402			3764.1629
43745	Zero-point correction (Hartree): 0.151039					
43746						
43747	TS.diHPCARP_I.14aldHshift.tpmmpu					
43748	-----					
43749	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13966797					
43750	Electronic state : 2-A					

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43751 Cartesian coordinates (Angs):
43752 C 0.523751 -0.772512 1.162661
43753 C 0.056902 -0.758154 -0.337068
43754 O 1.303695 -0.660929 -0.999839
43755 O 2.206574 -1.477860 -0.336274
43756 H 1.710210 -1.171614 0.871637
43757 O -0.060182 -0.623516 2.160881
43758 C -0.630468 -2.092041 -0.586026
43759 H -1.502875 -2.193293 0.054385
43760 H 0.072208 -2.899495 -0.393193
43761 H -0.946941 -2.130066 -1.627361
43762 C -0.753618 0.464204 -0.797930
43763 H -0.528290 0.581987 -1.861945
43764 O -2.141308 0.209869 -0.788585
43765 O -2.521121 -0.040375 0.564045
43766 H -3.138848 0.681719 0.732271
43767 C -0.440462 1.783887 -0.091128
43768 O 0.853513 2.265791 -0.367661
43769 H -1.111768 2.541934 -0.497143
43770 H -0.589579 1.710743 0.986455
43771 O 1.767361 1.590579 0.488983
43772 H 2.231001 1.017303 -0.140551
43773 Rotational constants (GHz): 1.0958700 0.9470800 0.7310500
43774 Vibrational harmonic frequencies (cm-1):
43775 i1728.1067 86.3959 102.6074
43776 115.0259 144.5087 162.2035
43777 184.7449 210.5060 221.9866
43778 234.8470 260.5731 288.3068
43779 307.3534 347.9167 358.3625
43780 409.0165 468.4722 493.4896
43781 518.5777 535.9095 603.7698
43782 619.0821 714.8566 752.7236
43783 884.1698 935.7661 957.3564
43784 969.1992 1029.4032 1063.1286
43785 1092.2270 1105.0619 1123.8675
43786 1131.4470 1156.0935 1187.1308
43787 1258.1645 1289.5103 1325.4609
43788 1368.1292 1395.0044 1401.1644
43789 1413.1815 1425.6948 1485.8275
43790 1491.9141 1495.7006 1828.4613
43791 2012.5675 3077.7195 3082.3432
43792 3082.7130 3137.5049 3163.4336
43793 3180.9337 3763.7777 3828.5100
43794 Zero-point correction (Hartree): 0.151006
43795
43796 TS.diHPCARP_I.14aldHshift.tppppmu
43797 -----
43798 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13966797
43799 Electronic state : 2-A
43800 Cartesian coordinates (Angs):
43801 C 0.524251 -0.772331 1.162623
43802 C 0.057328 -0.758162 -0.337044
43803 O 1.304013 -0.660353 -0.999944
43804 O 2.207395 -1.476703 -0.336347
43805 H 1.711007 -1.170552 0.871534
43806 O -0.059908 -0.624105 2.160830
43807 C -0.629467 -2.092363 -0.585926
43808 H -1.501922 -2.193852 0.054379
43809 H 0.073485 -2.899529 -0.392882
43810 H -0.945787 -2.130646 -1.627297
43811 C -0.753784 0.463864 -0.797810
43812 H -0.528330 0.581946 -1.861764
43813 O -2.141325 0.208792 -0.788759
43814 O -2.521401 -0.040843 0.563933
43815 H -3.140527 0.680289 0.731104
43816 C -0.441304 1.783587 -0.090768
43817 O 0.852360 2.266249 -0.367466
43818 H -1.113124 2.541332 -0.496497
43819 H -0.590151 1.710157 0.986821
43820 O 1.766710 1.591332 0.488876
43821 H 2.230456 1.018329 -0.140826
43822 Rotational constants (GHz): 1.0958800 0.9470200 0.7310000

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43823 Vibrational harmonic frequencies (cm-1):
43824 i1728.1948 86.1946 102.4938
43825 114.6565 144.4331 161.7750
43826 184.6807 207.8103 221.9238
43827 234.8792 260.4779 288.3076
43828 307.3475 347.8745 358.3219
43829 409.0230 468.4906 493.4859
43830 518.5622 535.9160 603.7811
43831 619.1104 714.8733 752.7131
43832 884.1808 935.7579 957.3497
43833 969.1766 1029.3918 1063.1342
43834 1092.2150 1105.0492 1123.8821
43835 1131.4227 1156.0909 1187.1254
43836 1258.1408 1289.4489 1325.4253
43837 1368.0797 1394.9588 1401.1754
43838 1413.1748 1425.6822 1485.8097
43839 1491.8970 1495.7140 1828.4440
43840 2012.5599 3077.7271 3082.3707
43841 3082.7168 3137.5599 3163.4343
43842 3180.9568 3763.8037 3828.7290
43843 Zero-point correction (Hartree): 0.150996
43844
43845 TS.diHPCARP_I.14aldHshift.tppppmu
43846 -----
43847 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14229927
43848 Electronic state : 2-A
43849 Cartesian coordinates (Angs):
43850 C 0.289963 -0.939944 1.198343
43851 C -0.023849 -0.748916 -0.325968
43852 O 1.289005 -0.808962 -0.859342
43853 O 1.973120 -1.813867 -0.197034
43854 H 1.434474 -1.491547 0.983714
43855 O -0.367772 -0.768658 2.146995
43856 C -0.883969 -1.922002 -0.763775
43857 H -1.819677 -1.931090 -0.210850
43858 H -0.339708 -2.848328 -0.594994
43859 H -1.101177 -1.817365 -1.825691
43860 C -0.567282 0.633525 -0.726923
43861 H -0.150929 0.838301 -1.716536
43862 O -1.955130 0.636422 -0.968036
43863 O -2.615025 0.301296 0.252152
43864 H -3.169474 1.078557 0.392351
43865 C -0.163302 1.742397 0.246353
43866 O 1.168680 1.599527 0.677643
43867 H -0.315465 2.718965 -0.214753
43868 H -0.754279 1.664333 1.158249
43869 O 2.014796 1.880951 -0.429726
43870 H 2.245474 0.984142 -0.720892
43871 Rotational constants (GHz): 1.0838800 0.9356000 0.7250500
43872 Vibrational harmonic frequencies (cm-1):
43873 i1781.6597 81.2274 95.5703
43874 118.7934 153.7235 168.7586
43875 197.8965 216.7266 229.9966
43876 245.8230 264.6799 276.2606
43877 297.2794 330.0639 370.8051
43878 429.7216 480.6237 496.2074
43879 507.4586 548.2100 612.3053
43880 638.9408 710.7006 735.8728
43881 877.4024 933.5197 958.9290
43882 976.3494 1019.9415 1064.1913
43883 1094.9291 1104.0432 1124.6175
43884 1135.4215 1162.6386 1184.3390
43885 1256.0360 1285.6797 1336.2343
43886 1364.2288 1393.1150 1400.8476
43887 1423.0383 1450.9823 1486.2695
43888 1490.6685 1494.4539 1826.8886
43889 2008.5335 3083.9060 3084.5344
43890 3089.2056 3149.4654 3164.4549
43891 3181.8500 3736.9140 3829.4432
43892 Zero-point correction (Hartree): 0.151226
43893
43894 TS.diHPCARP_I.14aldHshift.tpptmmu

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43895 -----
43896 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13758262
43897 Electronic state : 2-A
43898 Cartesian coordinates (Angs):
43899   C      -1.589405      0.133967      1.081192
43900   C      -0.990132     -0.116820     -0.356567
43901   O      -1.272602     -1.493510     -0.488346
43902   O      -2.559946     -1.701649     -0.034215
43903   H      -2.406378     -0.872750      0.985745
43904   O      -1.402415      0.978191      1.865718
43905   C      -1.778275      0.763649     -1.311849
43906   H      -1.623519      1.811928     -1.067253
43907   H      -2.834862      0.514654     -1.250046
43908   H      -1.420691      0.581360     -2.324365
43909   C       0.534049      0.006517     -0.506881
43910   H       0.818770     -0.693290     -1.296345
43911   O       0.929449      1.249863     -1.032696
43912   O       0.614954      2.257322     -0.077084
43913   H       1.495953      2.545801      0.193839
43914   C       1.273839     -0.363604      0.768754
43915   O       2.671322     -0.353649      0.595225
43916   H       1.095785      0.378550      1.546391
43917   H       0.926943     -1.342705      1.113017
43918   O       2.993325     -1.368749     -0.348182
43919   H       3.454844     -2.008355      0.207746
43920 Rotational constants (GHz):      1.2408300      0.6987400      0.6010000
43921 Vibrational harmonic frequencies (cm-1):
43922   i1903.6194      36.5110      54.2947
43923      100.6240      134.3265      146.3960
43924      149.6595      205.6094      225.1534
43925      232.0678      255.9368      285.5050
43926      295.4972      315.6421      329.3456
43927      354.7558      394.5978      480.4785
43928      507.3383      543.1705      590.2381
43929      669.3838      710.5450      755.7846
43930      885.6190      915.7191      957.6468
43931      978.7071      995.1102     1065.6248
43932     1081.3910     1094.1315     1129.0695
43933     1144.5316     1167.2556     1195.4951
43934     1259.5945     1298.7485     1319.3223
43935     1379.3434     1395.9747     1401.1161
43936     1409.9272     1425.1056     1483.3791
43937     1485.4025     1495.4637     1821.3175
43938     2003.9280     3056.9604     3081.8738
43939     3097.1471     3141.3362     3162.9566
43940     3179.1203     3816.2130     3826.4769
43941 Zero-point correction (Hartree): 0.150186
43942
43943 TS.diHPCARP_I.14aldHshift.tpptpmu
43944 -----
43945 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14095553
43946 Electronic state : 2-A
43947 Cartesian coordinates (Angs):
43948   C      -1.476173      0.153954      1.181504
43949   C      -1.086936      0.046568     -0.344549
43950   O      -1.763607     -1.147856     -0.672833
43951   O      -3.017873     -1.089164     -0.098150
43952   H      -2.554174     -0.553733      1.020082
43953   O      -0.997382      0.738934      2.070495
43954   C      -1.657571      1.281482     -1.021410
43955   H      -1.186679      2.176579     -0.622093
43956   H      -2.732589      1.319536     -0.863151
43957   H      -1.451088      1.218782     -2.089098
43958   C       0.387796     -0.221706     -0.679037
43959   H       0.389206     -0.770979     -1.625048
43960   O       1.096043      0.955622     -0.998317
43961   O       1.154493      1.772941      0.161141
43962   H       1.965990      1.452737      0.587541
43963   C       1.094162     -1.065756      0.373446
43964   O       2.409185     -1.400673     -0.014144
43965   H       1.114133     -0.573254      1.346117
43966   H       0.571836     -2.018914      0.469894

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43967      O      3.237210      -0.265524      0.225368
43968      H      3.371148      0.067750      -0.672454
43969      Rotational constants (GHz):      1.4912200      0.6486100      0.6067300
43970      Vibrational harmonic frequencies (cm-1):
43971      i1899.0654      59.7286      82.3333
43972      121.6743      131.5452      164.1557
43973      177.3610      215.2333      225.9868
43974      258.6976      275.9198      303.0390
43975      323.4098      346.6941      379.2089
43976      415.1967      480.9140      511.1311
43977      525.8667      553.1418      586.1513
43978      647.8889      710.3838      759.4632
43979      892.4079      912.6030      951.6738
43980      977.6590      1005.5141      1066.4045
43981      1084.0568      1095.8038      1120.9804
43982      1148.9900      1151.4190      1196.1646
43983      1258.4742      1303.8823      1317.1148
43984      1382.3215      1401.6423      1411.1809
43985      1421.4773      1436.1876      1485.1987
43986      1485.9779      1496.6121      1820.7972
43987      2006.6236      3076.1428      3081.8807
43988      3087.4039      3140.5545      3162.8424
43989      3180.0694      3720.0695      3800.5528
43990      Zero-point correction (Hartree): 0.151124
43991
43992      TS.diHPCARP_I.14aldHshift.tpptppu
43993      -----
43994      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13925361
43995      Electronic state : 2-A
43996      Cartesian coordinates (Angs):
43997      C      -1.452322      0.085615      1.209356
43998      C      -1.106384      0.061618      -0.329994
43999      O      -1.787498      -1.117562      -0.702283
44000      O      -3.024527      -1.099070      -0.088732
44001      H      -2.530029      -0.620845      1.042565
44002      O      -0.954110      0.629430      2.114215
44003      C      -1.701905      1.329613      -0.918313
44004      H      -1.213781      2.201456      -0.488764
44005      H      -2.770535      1.359185      -0.719804
44006      H      -1.532212      1.324965      -1.994189
44007      C      0.361038      -0.173357      -0.725149
44008      H      0.334912      -0.684699      -1.691538
44009      O      1.041877      1.018613      -1.021138
44010      O      1.186779      1.764810      0.178249
44011      H      2.081741      1.502607      0.444793
44012      C      1.097122      -1.059302      0.271551
44013      O      2.409310      -1.358102      -0.157359
44014      H      1.128002      -0.611002      1.264449
44015      H      0.585052      -2.021679      0.327117
44016      O      3.237439      -0.245784      0.174460
44017      H      3.857388      -0.653801      0.791368
44018      Rotational constants (GHz):      1.4907200      0.6422800      0.6036000
44019      Vibrational harmonic frequencies (cm-1):
44020      i1896.1536      57.9096      77.1231
44021      115.5423      132.7099      157.3701
44022      170.1371      206.2902      226.5158
44023      256.2934      277.4017      292.1986
44024      301.3752      328.5989      345.8624
44025      396.3935      475.2133      490.6217
44026      509.8497      549.0497      586.1413
44027      648.8746      710.4363      754.8312
44028      890.2974      910.5666      951.0910
44029      976.9533      1005.1887      1065.5403
44030      1082.1717      1094.4843      1118.3216
44031      1150.8769      1156.2799      1198.5665
44032      1256.8365      1305.5172      1321.0731
44033      1383.2814      1397.4175      1401.1806
44034      1429.8534      1437.8726      1481.1394
44035      1484.6523      1494.2792      1820.8544
44036      2004.6881      3080.2798      3081.3501
44037      3085.3561      3141.8486      3161.4317
44038      3177.7439      3737.7359      3821.9726

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44039 Zero-point correction (Hartree): 0.150754
44040
44041 TS.diHPCARP_I.14aldHshift.tptmmpu
44042 -----
44043 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14084393
44044 Electronic state : 2-A
44045 Cartesian coordinates (Angs):
44046 C -0.740239 -0.698712 1.032809
44047 C -0.931151 0.349079 -0.130531
44048 O -1.777473 -0.387857 -0.986658
44049 O -2.708426 -1.037621 -0.200784
44050 H -1.811078 -1.358158 0.706609
44051 O -0.042739 -0.725329 1.973448
44052 C -1.602200 1.558601 0.502432
44053 H -0.942853 2.000827 1.245013
44054 H -2.539044 1.256413 0.964904
44055 H -1.805708 2.291009 -0.277753
44056 C 0.273436 0.705875 -1.011846
44057 H -0.156788 1.131094 -1.924639
44058 O 1.028950 1.785202 -0.518699
44059 O 1.453856 1.511116 0.806102
44060 H 2.217435 0.929197 0.668021
44061 C 1.088262 -0.512810 -1.456009
44062 O 1.261733 -1.532718 -0.496640
44063 H 0.540875 -1.017572 -2.251625
44064 H 2.057515 -0.185294 -1.836896
44065 O 2.294841 -1.147144 0.402464
44066 H 1.825063 -1.184897 1.251369
44067 Rotational constants (GHz): 1.2401800 0.8576800 0.7711100
44068 Vibrational harmonic frequencies (cm-1):
44069 i1922.6592 83.6485 109.5117
44070 145.5591 164.9634 190.1451
44071 202.7904 219.1509 229.6652
44072 245.5403 259.6656 266.3953
44073 302.7570 319.2608 373.2330
44074 431.4362 478.9616 500.5148
44075 565.9800 567.5458 592.7586
44076 636.1662 715.0995 779.2025
44077 833.9200 933.4307 949.9300
44078 974.9928 1023.9295 1052.3052
44079 1069.3816 1101.5192 1118.4394
44080 1137.3815 1157.4098 1204.0486
44081 1253.3607 1302.6947 1353.4455
44082 1383.8629 1397.9740 1407.6225
44083 1445.3860 1457.3278 1477.4031
44084 1485.3683 1495.0448 1816.0898
44085 1981.3663 3063.9461 3079.8026
44086 3080.7345 3140.7100 3161.4097
44087 3180.6904 3733.6531 3745.5592
44088 Zero-point correction (Hartree): 0.151225
44089
44090 TS.diHPCARP_I.14aldHshift.ttmmmmu
44091 -----
44092 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13908580
44093 Electronic state : 2-A
44094 Cartesian coordinates (Angs):
44095 C -1.040892 -0.623109 1.028828
44096 C -1.014930 0.443468 -0.132221
44097 O -1.748846 -0.226187 -1.125433
44098 O -2.816881 -0.844960 -0.499700
44099 H -2.054943 -1.246788 0.524756
44100 O -0.505085 -0.649713 2.063700
44101 C -1.712503 1.680523 0.413881
44102 H -1.154223 2.077633 1.258255
44103 H -2.723250 1.425362 0.723530
44104 H -1.758063 2.431889 -0.374023
44105 C 0.370743 0.728226 -0.714546
44106 H 0.263497 1.471674 -1.514619
44107 O 1.088493 1.286619 0.367422
44108 O 2.409505 1.560912 -0.057008
44109 H 2.869543 0.777914 0.281883
44110 C 1.015502 -0.512020 -1.313680

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44111	O	1.108076	-1.580690	-0.393991	
44112	H	0.373669	-0.889719	-2.108168	
44113	H	1.998619	-0.277817	-1.719679	
44114	O	2.190359	-1.289497	0.491367	
44115	H	2.672656	-2.124562	0.463635	
44116	Rotational constants (GHz):		1.3363600	0.7723000	0.6997300
44117	Vibrational harmonic frequencies (cm-1):				
44118	i1813.1004		56.0337		75.4710
44119	125.8247		141.5948		166.8550
44120	183.5534		187.0330		205.8003
44121	211.1883		251.3961		253.9897
44122	293.4905		319.7079		374.2798
44123	396.2514		453.2970		478.6367
44124	495.4881		550.1466		604.5275
44125	671.3250		716.8306		775.7382
44126	867.6776		906.9473		944.7071
44127	980.4670		1034.6435		1044.8840
44128	1067.9635		1106.0012		1120.5676
44129	1135.6950		1164.9689		1211.4278
44130	1258.6723		1295.9668		1366.7648
44131	1378.9718		1394.9477		1399.9028
44132	1423.8748		1445.5866		1468.6122
44133	1486.1540		1495.5743		1819.0180
44134	2012.6970		3031.2468		3077.3009
44135	3100.5917		3155.6984		3158.1830
44136	3177.2842		3757.8555		3835.8752
44137	Zero-point correction (Hartree): 0.150621				
44138					
44139	TS.diHPCARP_I.14aldHshift.ttmmpu				
44140	-----				
44141	IRC pathway available				
44142	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17127064				
44143	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.04878054				
44144	T1 diagnostic: 0.022885				
44145	E(MP2/Aug-CC-pVTZ) (Hartree): -721.01012094				
44146	E(MP3/Aug-CC-pVTZ) (Hartree): -721.02344516				
44147	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01800818				
44148	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02821673				
44149	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47279052				
44150	E(UHF/Aug-CC-pVTZ) (Hartree): -718.46181440				
44151	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14444663				
44152	Electronic state : 2-A				
44153	Cartesian coordinates (Angs):				
44154	C	-1.022852	-0.701833	0.954829	
44155	C	-0.989144	0.473537	-0.091697	
44156	O	-1.782110	-0.071058	-1.115667	
44157	O	-2.863459	-0.682468	-0.510278	
44158	H	-2.119766	-1.196503	0.451119	
44159	O	-0.394432	-0.888773	1.924701	
44160	C	-1.621327	1.673999	0.598625	
44161	H	-1.023762	1.967818	1.458054	
44162	H	-2.632399	1.427801	0.913899	
44163	H	-1.658624	2.500016	-0.110973	
44164	C	0.390806	0.759003	-0.685807	
44165	H	0.290429	1.557355	-1.431013	
44166	O	1.145426	1.227861	0.419029	
44167	O	2.466341	1.489709	-0.010773	
44168	H	2.895489	0.639598	0.179641	
44169	C	0.994518	-0.459053	-1.368607	
44170	O	1.059861	-1.592802	-0.528670	
44171	H	0.342415	-0.763422	-2.186105	
44172	H	1.981677	-0.226603	-1.766516	
44173	O	2.096453	-1.380925	0.423941	
44174	H	1.587904	-1.192334	1.229561	
44175	Rotational constants (GHz):		1.3570600	0.7861000	0.7095600
44176	Vibrational harmonic frequencies (cm-1):				
44177	i1969.2033		70.7045		108.2919
44178	149.0691		155.5853		177.5678
44179	200.0525		209.9005		230.4947
44180	257.5168		266.7874		300.7681
44181	332.0892		373.8545		399.1703
44182	440.8417		465.8605		489.7251

44183	533.2087	554.9786	603.1278
44184	673.4571	723.6222	781.4755
44185	868.5427	908.2102	947.6838
44186	977.5586	1032.9679	1046.6308
44187	1068.8328	1100.2393	1123.9542
44188	1132.5477	1158.3590	1209.4840
44189	1258.1725	1292.4939	1363.1974
44190	1379.2743	1397.3709	1406.0574
44191	1444.1533	1455.0658	1478.4460
44192	1485.5378	1495.5953	1816.4847
44193	1985.9653	3038.7986	3079.3854
44194	3099.6249	3152.2027	3160.1978
44195	3178.9615	3729.1309	3739.2900

44196 Zero-point correction (Hartree): 0.151518

44197
44198 TS.diHPCARP_I.14aldHshift.ttmppmu
44199 -----

44200 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13945876
44201 Electronic state : 2-A

44202 Cartesian coordinates (Angs):

44203	C	1.141528	-0.572971	1.120119
44204	C	0.440156	-0.722139	-0.271544
44205	O	1.346643	-0.013466	-1.095829
44206	O	2.629048	-0.335425	-0.685339
44207	H	2.298182	-0.316211	0.607424
44208	O	0.738545	-0.789927	2.194573
44209	C	0.397740	-2.207621	-0.592630
44210	H	-0.173853	-2.741550	0.162659
44211	H	1.413980	-2.593076	-0.632296
44212	H	-0.082863	-2.344148	-1.559893
44213	C	-0.902005	0.006210	-0.392200
44214	H	-1.005315	0.296713	-1.442185
44215	O	-1.909074	-0.935035	-0.074255
44216	O	-3.145800	-0.335262	-0.447274
44217	H	-3.629650	-0.360142	0.387340
44218	C	-0.999209	1.230453	0.526483
44219	O	0.225279	1.918448	0.633360
44220	H	-1.782775	1.905937	0.187861
44221	H	-1.215921	0.889292	1.540539
44222	O	0.446479	2.599180	-0.594651
44223	H	1.060000	1.991486	-1.037495

44224 Rotational constants (GHz): 1.0911300 0.8544700 0.6756600

44225 Vibrational harmonic frequencies (cm-1):

44226	i1826.3722	57.5477	81.2765
44227	109.8691	131.3191	164.8591
44228	173.0495	197.1505	213.6570
44229	239.9568	248.2464	268.3839
44230	308.2955	336.8637	372.9146
44231	434.6549	445.5947	491.0993
44232	507.0558	523.7356	593.9143
44233	629.2785	705.2415	752.8600
44234	883.2782	935.7113	960.8583
44235	1012.4425	1031.6407	1066.5049
44236	1094.4284	1104.8075	1123.1745
44237	1130.8337	1163.6906	1195.5489
44238	1260.4951	1291.2670	1341.6111
44239	1371.9936	1401.3417	1408.8249
44240	1417.6674	1451.3364	1485.0589
44241	1490.7524	1494.2498	1828.0873
44242	2004.6164	3064.2343	3082.6038
44243	3084.9520	3144.9673	3164.8433
44244	3176.2923	3736.0047	3830.9128

44245 Zero-point correction (Hartree): 0.150864

44246
44247 TS.diHPCARP_I.14aldHshift.ttmtpmu
44248 -----

44249 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13825307
44250 Electronic state : 2-A

44251 Cartesian coordinates (Angs):

44252	C	-1.797467	0.201409	1.042906
44253	C	-1.098501	0.081697	-0.363753
44254	O	-1.500877	-1.217684	-0.724162

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44255      O      -2.842853      -1.327978      -0.415444
44256      H      -2.702475      -0.682978      0.733880
44257      O      -1.585986      0.912300      1.944043
44258      C      -1.693208      1.173893      -1.239172
44259      H      -1.484425      2.152594      -0.814799
44260      H      -2.766479      1.025201      -1.327636
44261      H      -1.238300      1.111893      -2.227464
44262      C      0.430032      0.075835      -0.335245
44263      H      0.761542      -0.175698      -1.346920
44264      O      0.821385      1.404916      -0.040154
44265      O      2.157681      1.587413      -0.488013
44266      H      2.652514      1.463388      0.334932
44267      C      0.996661      -0.917473      0.671753
44268      O      2.402358      -0.814158      0.779662
44269      H      0.642175      -0.678824      1.676202
44270      H      0.708293      -1.934854      0.404334
44271      O      2.966584      -1.241024      -0.451034
44272      H      3.055722      -0.403162      -0.930656
44273      Rotational constants (GHz):      1.4214800      0.6286800      0.5763700
44274      Vibrational harmonic frequencies (cm-1):
44275      i1930.0704      32.5632      83.6009
44276      119.5964      122.6285      154.5129
44277      177.3108      184.5362      206.7255
44278      246.5720      269.9326      317.4126
44279      326.8357      364.9316      388.9056
44280      414.0332      454.2135      483.4692
44281      507.9636      527.0406      565.1748
44282      621.5149      710.4444      778.4843
44283      899.3645      913.4331      964.8181
44284      988.1043      1030.9248      1067.3047
44285      1082.7434      1098.2137      1126.1637
44286      1145.7024      1153.4495      1208.4674
44287      1267.4315      1305.3264      1334.3627
44288      1371.4043      1399.0624      1422.4866
44289      1430.8670      1441.1452      1475.7380
44290      1486.0289      1493.9978      1820.7268
44291      2006.8810      3066.9979      3078.5586
44292      3080.3486      3136.9571      3161.0651
44293      3181.4153      3746.0225      3781.6394
44294      Zero-point correction (Hartree): 0.150873
44295
44296      TS.diHPCARP_I.14aldHshift.ttmtpu
44297      -----
44298      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13759803
44299      Electronic state : 2-A
44300      Cartesian coordinates (Angs):
44301      C      -1.646085      -0.313893      1.143589
44302      C      -1.145427      0.237380      -0.242904
44303      O      -1.702730      -0.728841      -1.102707
44304      O      -2.997148      -0.959843      -0.677934
44305      H      -2.654166      -0.934717      0.603977
44306      O      -1.261400      -0.120564      2.228790
44307      C      -1.748759      1.623271      -0.406660
44308      H      -1.415696      2.275822      0.395857
44309      H      -2.833490      1.549929      -0.407692
44310      H      -1.411837      2.035657      -1.357434
44311      C      0.371773      0.198235      -0.452283
44312      H      0.555167      0.401090      -1.511160
44313      O      0.915195      1.253007      0.314384
44314      O      2.022533      1.801317      -0.378665
44315      H      2.750621      1.241282      -0.065347
44316      C      0.957759      -1.159071      -0.084947
44317      O      2.288251      -1.332171      -0.534927
44318      H      0.909948      -1.317406      0.994725
44319      H      0.399631      -1.941908      -0.600153
44320      O      3.147943      -0.602676      0.333828
44321      H      3.663100      -1.307117      0.744300
44322      Rotational constants (GHz):      1.4426500      0.6163600      0.5725400
44323      Vibrational harmonic frequencies (cm-1):
44324      i1912.8456      27.9596      43.7644
44325      88.4396      104.5495      127.9929
44326      147.7772      185.1666      203.2002

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44327      236.7145      242.0934      273.2141
44328      313.9632      339.6903      364.5413
44329      405.7308      436.7007      488.7671
44330      520.0711      537.3086      551.8642
44331      610.9078      710.0408      770.1387
44332      887.8778      929.4841      967.2216
44333      978.2016      1041.4599     1068.6399
44334      1088.1316     1094.3982     1117.3144
44335      1134.8045     1157.5174     1204.4684
44336      1257.7146     1313.7122     1319.4730
44337      1370.5757     1385.3866     1397.4153
44338      1433.4908     1464.8389     1468.4452
44339      1486.1583     1492.7577     1821.8649
44340      2005.0158     3068.4332     3076.8554
44341      3079.9724     3136.1666     3160.7290
44342      3182.4651     3741.5860     3836.5245
44343      Zero-point correction (Hartree): 0.150131
44344
44345      TS.diHPCARP_I.14aldHshift.ttpmmpu
44346      -----
44347      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13966615
44348      Electronic state : 2-A
44349      Cartesian coordinates (Angs):
44350      C      -1.037901     -0.628717      0.967611
44351      C      -0.925001      0.520534     -0.099935
44352      O      -1.714374     -0.003168     -1.136255
44353      O      -2.831985     -0.567387     -0.548824
44354      H      -2.125720     -1.103198      0.432716
44355      O      -0.468457     -0.790499      1.977208
44356      C      -1.515563      1.765282      0.546117
44357      H      -0.940995      2.038088      1.428178
44358      H      -2.549767      1.577209      0.824706
44359      H      -1.484209      2.582283     -0.174330
44360      C      0.481532      0.717376     -0.668574
44361      H      0.446193      1.524702     -1.409034
44362      O      1.260932      1.129081      0.443012
44363      O      2.545031      1.479548     -0.053456
44364      H      2.591405      2.412427      0.189965
44365      C      1.013893     -0.547499     -1.325337
44366      O      0.821605     -1.687629     -0.512932
44367      H      0.442836     -0.744785     -2.231528
44368      H      2.069558     -0.434419     -1.566271
44369      O      1.877584     -1.754594      0.431242
44370      H      1.526250     -1.256979      1.186331
44371      Rotational constants (GHz): 1.2669100  0.8117600  0.7072100
44372      Vibrational harmonic frequencies (cm-1):
44373      i1942.1288      69.4977      83.4883
44374      115.9007      153.3011      179.7612
44375      189.0059      201.3650      205.7894
44376      218.5788      256.9684      265.1133
44377      295.9313      325.0989      367.6802
44378      376.8761      396.0244      468.9601
44379      488.8984      546.3480      607.6776
44380      666.1868      721.8709      785.2581
44381      866.6414      915.7143      950.5361
44382      986.4841      1031.4291     1046.9353
44383      1066.3032     1103.3647     1125.9769
44384      1133.7854     1154.2374     1206.4908
44385      1255.1082     1297.2611     1364.0259
44386      1369.6342     1395.3447     1403.2706
44387      1417.7628     1462.3117     1464.5695
44388      1486.9316     1496.5758     1816.6393
44389      1987.0285     3040.9268     3077.4634
44390      3103.4409     3158.0213     3159.1149
44391      3175.9456     3750.2158     3825.4727
44392      Zero-point correction (Hartree): 0.150543
44393
44394      TS.diHPCARP_I.14aldHshift.ttpppmu
44395      -----
44396      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13949407
44397      Electronic state : 2-A
44398      Cartesian coordinates (Angs):

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44399      C      1.164448      -0.548598      1.111168
44400      C      0.438221      -0.721233      -0.266037
44401      O      1.328289      -0.025032      -1.117908
44402      O      2.618943      -0.337541      -0.725127
44403      H      2.309120      -0.294018      0.574785
44404      O      0.787465      -0.758966      2.195696
44405      C      0.396245      -2.212721      -0.558602
44406      H      -0.174458      -2.731330      0.208045
44407      H      1.412207      -2.599545      -0.591823
44408      H      -0.081634      -2.369049      -1.524445
44409      C      -0.907257      0.003267      -0.380201
44410      H      -1.014675      0.297460      -1.429451
44411      O      -1.910801      -0.938442      -0.048403
44412      O      -3.159414      -0.293713      -0.267197
44413      H      -3.524774      -0.823317      -0.986625
44414      C      -1.000423      1.226317      0.540640
44415      O      0.223739      1.919618      0.621922
44416      H      -1.794901      1.894961      0.216329
44417      H      -1.201145      0.883847      1.556583
44418      O      0.422249      2.592697      -0.614763
44419      H      1.039112      1.989836      -1.058969
44420      Rotational constants (GHz):      1.0940300      0.8539100      0.6760400
44421      Vibrational harmonic frequencies (cm-1):
44422      i1802.9625      61.2606      83.8484
44423      116.2790      134.0909      166.1597
44424      194.0842      202.6514      215.7252
44425      242.9166      251.2467      268.3763
44426      308.7851      336.8530      372.3241
44427      434.9411      446.4047      486.2683
44428      507.2479      525.0889      593.0605
44429      629.8168      703.9627      751.5515
44430      882.3620      935.4957      958.8024
44431      1011.0910      1030.3154      1065.0915
44432      1095.3110      1105.5331      1120.8562
44433      1131.2028      1163.7796      1197.6063
44434      1259.4714      1290.2478      1343.9172
44435      1371.5705      1399.8008      1410.2556
44436      1418.5744      1450.1317      1485.5011
44437      1489.8218      1495.6079      1827.7134
44438      2007.3022      3054.0552      3081.3007
44439      3095.6307      3155.2383      3162.7069
44440      3176.1141      3741.9788      3821.8479
44441      Zero-point correction (Hartree): 0.150972
44442
44443
44444
44445      1,5-aldehyde-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-HPCARP-
44446      Ib)
44447      =====
44448      =
44449
44450      TS.diHPCARP_Ib.15aldHshift.umdmudd
44451      -----
44452      IRC pathway available
44453      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17292453
44454      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05078752
44455      T1 diagnostic: 0.023684
44456      E(MP2/Aug-CC-pVTZ) (Hartree): -721.00667826
44457      E(MP3/Aug-CC-pVTZ) (Hartree): -721.02462160
44458      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01325899
44459      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02883297
44460      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47791843
44461      E(UHF/Aug-CC-pVTZ) (Hartree): -718.46871743
44462      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14630065
44463      Electronic state : 2-A
44464      Cartesian coordinates (Angs):
44465      O      1.028411      1.779450      -0.127831
44466      O      1.578151      1.205329      1.003651
44467      H      0.496643      0.587452      1.531223
44468      C      -0.514844      -0.076627      1.219669
44469      C      -0.908787      0.376333      -0.193786
44470      C      0.375245      0.803729      -0.934557

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44471 O -1.014129 -0.907989 1.888375
44472 C -1.883657 1.538693 -0.062439
44473 O -1.425783 -0.714139 -0.925380
44474 H -1.382254 2.388538 0.396953
44475 H -2.743439 1.254194 0.537425
44476 H -2.223659 1.817064 -1.059380
44477 O -2.681155 -1.093448 -0.393358
44478 H -2.425470 -1.720891 0.299634
44479 H 0.088371 1.362655 -1.826575
44480 C 1.239074 -0.380419 -1.348754
44481 O 1.405866 -1.318282 -0.301499
44482 H 0.729666 -0.902578 -2.158794
44483 H 2.212980 -0.036789 -1.694522
44484 O 2.706371 -1.194326 0.247476
44485 H 2.623109 -0.372660 0.761771
44486 Rotational constants (GHz): 1.3324700 0.7937200 0.7222900
44487 Vibrational harmonic frequencies (cm-1):
44488 i1679.4544 69.5720 78.1194
44489 148.8300 160.6653 175.3957
44490 197.0381 214.6501 245.9684
44491 267.1856 302.6650 323.1497
44492 330.9786 354.9818 380.0259
44493 394.0831 493.9615 510.9511
44494 545.8077 577.0637 586.0115
44495 618.5772 785.3427 831.4126
44496 839.4621 933.1929 957.9466
44497 972.2636 1028.3783 1050.7495
44498 1052.7827 1088.6887 1136.0004
44499 1142.9941 1160.3369 1221.4439
44500 1245.0727 1294.7807 1348.6689
44501 1365.6773 1398.2574 1403.4510
44502 1443.5166 1465.6196 1469.3141
44503 1487.0249 1501.2111 1685.4699
44504 1939.3749 3079.6482 3089.2035
44505 3107.6446 3146.2459 3159.1017
44506 3178.0613 3673.6556 3765.8038
44507 Zero-point correction (Hartree): 0.151324
44508
44509 TS.diHPCARP_Ib.15aldHshift.umdpudd
44510 -----
44511 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14149046
44512 Electronic state : 2-A
44513 Cartesian coordinates (Angs):
44514 O -1.132278 -1.940251 -0.246985
44515 O -1.613450 -1.527946 0.983330
44516 H -0.525020 -0.979833 1.495075
44517 C 0.486439 -0.266458 1.215964
44518 C 0.746403 -0.470281 -0.285595
44519 C -0.603783 -0.819563 -0.939637
44520 O 1.058382 0.442665 1.965513
44521 C 1.755906 -1.596208 -0.450563
44522 O 1.149318 0.738250 -0.892645
44523 H 1.342227 -2.523786 -0.059515
44524 H 2.677773 -1.358617 0.073194
44525 H 1.971478 -1.717342 -1.511708
44526 O 2.427673 1.113891 -0.415718
44527 H 2.204938 1.598997 0.393237
44528 H -0.426406 -1.180471 -1.953510
44529 C -1.556281 0.368187 -0.979162
44530 O -1.501802 1.090078 0.245607
44531 H -1.261733 1.037281 -1.783616
44532 H -2.573254 0.007309 -1.141050
44533 O -1.190109 2.449166 -0.039549
44534 H -1.963968 2.895586 0.325428
44535 Rotational constants (GHz): 1.0946100 0.9743200 0.7449700
44536 Vibrational harmonic frequencies (cm-1):
44537 i1880.2936 24.6972 82.8049
44538 140.2912 143.7844 164.0224
44539 175.9475 212.9866 224.3903
44540 240.4109 265.1237 302.8239
44541 317.5004 341.7582 366.5374
44542 381.5403 401.0268 454.7266

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44543      525.4479      547.1038      584.1933
44544      611.4654      777.3188      830.2226
44545      882.6417      931.9926      936.3557
44546      995.1625      1011.7338     1049.7563
44547      1072.5488     1083.5340     1120.9330
44548      1143.9807     1157.9030     1217.7109
44549      1246.0037     1285.0186     1349.0847
44550      1362.4137     1398.0385     1404.9947
44551      1411.8072     1447.4564     1474.7227
44552      1486.7331     1499.8663     1671.3673
44553      1930.8172     3079.0648     3084.1181
44554      3110.1369     3158.2728     3158.7090
44555      3176.1061     3764.5309     3826.1080
44556      Zero-point correction (Hartree): 0.150463
44557
44558      TS.diHPCARP_Ib.15aldHshift.umdmtddd
44559      -----
44560      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14398286
44561      Electronic state : 2-A
44562      Cartesian coordinates (Angs):
44563      O      -1.570922      -1.605718      -0.295615
44564      O      -1.928186      -1.172368      0.967705
44565      H      -0.758330      -0.947239      1.476799
44566      C      0.405667      -0.491281      1.203930
44567      C      0.572549      -0.591316      -0.321748
44568      C      -0.835460      -0.577885      -0.948854
44569      O      1.170114      -0.012640      1.966763
44570      C      1.314634      -1.874061      -0.661556
44571      O      1.232689      0.577141      -0.786316
44572      H      0.686909      -2.728557      -0.416703
44573      H      2.249619      -1.942593      -0.112847
44574      H      1.530661      -1.877622      -1.729397
44575      O      2.597085      0.556004      -0.401911
44576      H      2.552426      0.771663      0.544359
44577      H      -0.769786      -0.906594      -1.986502
44578      C      -1.524626      0.780716      -0.864190
44579      O      -1.180410      1.454821      0.338241
44580      H      -1.233209      1.402216      -1.707717
44581      H      -2.603559      0.624206      -0.881922
44582      O      -0.523666      2.672816      0.028306
44583      H      0.375058      2.367036      -0.168945
44584      Rotational constants (GHz):      1.1090100      0.9768300      0.7496200
44585      Vibrational harmonic frequencies (cm-1):
44586      i2017.0291      79.7741      109.1730
44587      136.2427      163.3540      167.2463
44588      188.8428      214.7538      235.9781
44589      282.3889      310.8965      323.1555
44590      340.5563      375.6414      386.6708
44591      437.7418      480.7776      487.3583
44592      530.7552      549.9760      583.2473
44593      608.9987      778.7267      826.6144
44594      879.1068      930.3820      937.4343
44595      990.0695      1015.1023     1045.5419
44596      1072.4757     1081.8520     1123.0097
44597      1136.2706     1157.6706     1208.2725
44598      1243.0603     1284.2295     1346.3555
44599      1358.9311     1393.1273     1405.9598
44600      1444.9449     1459.9521     1476.0642
44601      1488.6389     1500.2464     1668.3321
44602      1923.2823     3079.7552     3090.3022
44603      3110.4336     3152.4678     3159.9718
44604      3177.2069     3723.9520     3750.8873
44605      Zero-point correction (Hartree): 0.151303
44606
44607      TS.diHPCARP_Ib.15aldHshift.umdppduu
44608      -----
44609      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14200010
44610      Electronic state : 2-A
44611      Cartesian coordinates (Angs):
44612      O      0.156195      1.777760      -0.240593
44613      O      -1.087115      2.374724      -0.303565
44614      H      -1.816524      1.354813      -0.633921

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44615	C	-2.025631	0.142476	-0.306177		
44616	C	-0.677198	-0.412976	0.237988		
44617	C	0.128936	0.777879	0.775275		
44618	O	-3.069496	-0.395163	-0.305918		
44619	C	-0.956016	-1.485437	1.266561		
44620	O	-0.075662	-0.883683	-0.980464		
44621	H	-1.547252	-2.279899	0.819038		
44622	H	-1.522097	-1.045316	2.086807		
44623	H	-0.032506	-1.907958	1.654016		
44624	O	0.544151	-2.143150	-0.814239		
44625	H	1.420591	-1.879214	-0.481280		
44626	H	-0.383923	1.196749	1.647387		
44627	C	1.563529	0.468999	1.180418		
44628	O	2.275466	-0.358158	0.284684		
44629	H	2.100476	1.408946	1.314459		
44630	H	1.562168	-0.086081	2.118945		
44631	O	2.546432	0.373000	-0.899424		
44632	H	1.697584	0.329662	-1.373686		
44633	Rotational constants (GHz):			1.2659000	0.8641900	0.6581900
44634	Vibrational harmonic frequencies (cm-1):					
44635	i1905.1025		43.6647			77.4883
44636	141.1516		173.1945			198.1290
44637	221.0185		248.0295			268.2040
44638	280.1944		301.0181			304.9125
44639	339.9797		379.0301			409.1004
44640	448.8331		466.0401			489.2666
44641	549.5621		567.6050			617.7103
44642	651.1713		760.5953			818.2747
44643	851.8924		895.2550			931.9347
44644	984.7670		1023.8785			1054.9883
44645	1081.1659		1117.1766			1131.3194
44646	1138.9686		1167.9756			1221.1472
44647	1245.3223		1308.5269			1353.7938
44648	1370.4965		1406.5799			1414.0450
44649	1461.9716		1468.9052			1482.3774
44650	1483.5821		1493.8944			1657.2438
44651	1957.3342		3054.2748			3083.5749
44652	3086.0586		3138.5976			3161.3620
44653	3179.4999		3664.3479			3709.9858
44654	Zero-point correction (Hartree):			0.151581		
44655	TS.diHPCARP_Ib.15aldHshift.umdtmddd					
44656	-----					
44657	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14207612					
44658	Electronic state : 2-A					
44659	Cartesian coordinates (Angs):					
44660	O	-0.872941	1.393366	0.851353		
44661	O	-0.548108	2.249044	-0.181282		
44662	H	0.705940	1.984097	-0.319966		
44663	C	1.476269	0.971075	-0.461364		
44664	C	0.877248	-0.163177	0.384099		
44665	C	-0.652740	0.043056	0.457464		
44666	O	2.364112	0.894023	-1.236722		
44667	C	1.492509	-0.104823	1.775821		
44668	O	1.082519	-1.397238	-0.275382		
44669	H	1.158713	0.800516	2.279664		
44670	H	2.577667	-0.116401	1.726988		
44671	H	1.153850	-0.975541	2.335934		
44672	O	2.455625	-1.742161	-0.225311		
44673	H	2.809681	-1.270196	-0.994211		
44674	H	-1.043514	-0.543602	1.288508		
44675	C	-1.397037	-0.330857	-0.814620		
44676	O	-2.788610	-0.182643	-0.647798		
44677	H	-1.145362	0.352154	-1.625658		
44678	H	-1.148960	-1.352769	-1.101319		
44679	O	-3.202686	-1.169484	0.292409		
44680	H	-3.764794	-1.729164	-0.256498		
44681	Rotational constants (GHz):			1.3586800	0.6681700	0.5683500
44682	Vibrational harmonic frequencies (cm-1):					
44683	i2045.3493		39.3410			51.7428
44684	129.5292		144.0697			158.5025
44685	179.7833		212.4778			223.1269

44687	227.9997	259.7210	303.3924		
44688	313.5799	351.0732	367.1340		
44689	374.2262	403.0075	443.8384		
44690	501.1692	559.5312	599.7511		
44691	667.5517	738.5375	819.1475		
44692	877.7352	923.2291	959.3963		
44693	987.7771	1015.2529	1043.3926		
44694	1085.0348	1119.4701	1130.2077		
44695	1142.4494	1179.8247	1219.6215		
44696	1248.7283	1308.7986	1328.8066		
44697	1374.5941	1395.4932	1401.8939		
44698	1429.7728	1441.9551	1467.9706		
44699	1486.5976	1500.5766	1658.0025		
44700	1922.8063	3079.8889	3089.5328		
44701	3124.2063	3148.2873	3159.7426		
44702	3176.8910	3764.3546	3827.3185		
44703	Zero-point correction (Hartree): 0.150559				
44704					
44705	TS.diHPCARP_Ib.15aldHshift.umdtmudd				
44706	-----				
44707	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14298506				
44708	Electronic state : 2-A				
44709	Cartesian coordinates (Angs):				
44710	O	-1.068378	1.115086	0.861826	
44711	O	-0.896382	2.001418	-0.184122	
44712	H	0.394713	1.945225	-0.323648	
44713	C	1.316629	1.075616	-0.458411	
44714	C	0.919257	-0.135627	0.401405	
44715	C	-0.620539	-0.178185	0.475735	
44716	O	2.201445	1.142521	-1.237212	
44717	C	1.530971	0.028125	1.784985	
44718	O	1.304289	-1.326114	-0.255377	
44719	H	1.072085	0.879931	2.284203	
44720	H	2.605274	0.177302	1.723774	
44721	H	1.331291	-0.876626	2.357870	
44722	O	2.714946	-1.450193	-0.230454	
44723	H	2.976063	-0.947237	-1.016560	
44724	H	-0.910928	-0.816811	1.308715	
44725	C	-1.278168	-0.667042	-0.811729	
44726	O	-2.650277	-0.362314	-0.845116	
44727	H	-0.874020	-0.159781	-1.687854	
44728	H	-1.111765	-1.740702	-0.910757	
44729	O	-3.255151	-0.992287	0.278018	
44730	H	-3.495540	-0.223558	0.811834	
44731	Rotational constants (GHz): 1.4860800			0.6490700	0.5826900
44732	Vibrational harmonic frequencies (cm-1):				
44733	i1992.6194		49.0728		58.3178
44734	127.1210		140.6274		163.3192
44735	176.6715		207.5316		228.4467
44736	260.9264		297.6157		307.5345
44737	313.8033		347.2958		366.7169
44738	369.0407		402.0381		446.0638
44739	492.5577		559.8086		602.0046
44740	702.7560		735.3213		818.3013
44741	872.7435		922.5399		962.6856
44742	992.1907		1016.7678		1044.3369
44743	1079.9347		1123.0984		1137.8864
44744	1145.2802		1183.4075		1224.5802
44745	1251.7663		1299.3985		1329.7150
44746	1375.2275		1402.5874		1407.7268
44747	1423.8608		1442.9248		1475.8019
44748	1486.9566		1500.8366		1659.6277
44749	1926.3819		3079.2757		3083.2015
44750	3121.6912		3140.1310		3158.2660
44751	3177.3751		3767.3437		3808.4931
44752	Zero-point correction (Hartree): 0.150808				
44753					
44754	TS.diHPCARP_Ib.15aldHshift.umdtppdd				
44755	-----				
44756	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14291807				
44757	Electronic state : 2-A				
44758	Cartesian coordinates (Angs):				

44759	O	-1.088788	1.012813	0.924969		
44760	O	-1.108263	1.785562	-0.222991		
44761	H	0.174034	1.844059	-0.502159		
44762	C	1.150510	1.056166	-0.650916		
44763	C	0.988853	-0.057661	0.392405		
44764	C	-0.518502	-0.268289	0.650207		
44765	O	1.929446	1.107187	-1.535860		
44766	C	1.700426	0.373569	1.668027		
44767	O	1.464459	-1.276969	-0.139811		
44768	H	1.180697	1.226004	2.102227		
44769	H	2.734543	0.640095	1.469119		
44770	H	1.678363	-0.458679	2.370458		
44771	O	2.875675	-1.230141	-0.247554		
44772	H	2.997620	-0.834447	-1.123687		
44773	H	-0.635441	-0.805463	1.592324		
44774	C	-1.256527	-1.026639	-0.443745		
44775	O	-2.594275	-1.257574	-0.062024		
44776	H	-1.225345	-0.501882	-1.399085		
44777	H	-0.803765	-2.010749	-0.555549		
44778	O	-3.383807	-0.146445	-0.456100		
44779	H	-3.244829	0.482722	0.265454		
44780	Rotational constants (GHz):			1.5492300	0.6339600	0.5760900
44781	Vibrational harmonic frequencies (cm-1):					
44782	i1907.7198		53.9834			75.2545
44783	131.0745		144.0451			160.2976
44784	174.2377		217.0415			233.0388
44785	258.8723		291.8742			312.1601
44786	330.1369		367.5748			376.9285
44787	388.1795		408.3123			445.0465
44788	502.6149		559.6989			598.1360
44789	646.3171		743.3000			820.4119
44790	875.0663		927.7807			959.6534
44791	987.5947		1016.7899			1043.9033
44792	1095.5109		1115.8085			1132.9841
44793	1141.9667		1176.2889			1221.9515
44794	1251.8983		1305.7117			1326.4352
44795	1369.6334		1401.3474			1414.4108
44796	1430.4720		1440.2690			1463.2799
44797	1485.9244		1500.9719			1666.8285
44798	1928.8406		3079.5229			3091.0207
44799	3109.1653		3151.0937			3158.9747
44800	3177.2509		3769.2140			3791.9645
44801	Zero-point correction (Hartree):			0.150924		
44802	-----					
44803	TS.diHPCARP_Ib.15aldHshift.updmmudd					
44804	-----					
44805	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14285764		
44806	Electronic state : 2-A					
44807	Cartesian coordinates (Angs):					
44808	O	-0.725341	-0.772946	-1.658167		
44809	O	-1.570500	-1.382723	-0.748798		
44810	H	-0.733772	-1.618752	0.269241		
44811	C	0.252163	-1.176243	0.906293		
44812	C	0.979873	-0.241437	-0.062707		
44813	C	-0.043015	0.330066	-1.066696		
44814	O	0.537783	-1.461484	2.008738		
44815	C	2.048192	-1.081220	-0.753961		
44816	O	1.524156	0.774010	0.755530		
44817	H	1.586233	-1.890539	-1.316368		
44818	H	2.724890	-1.499093	-0.010288		
44819	H	2.605255	-0.451119	-1.444841		
44820	O	2.158553	1.712367	-0.111641		
44821	H	3.062440	1.696575	0.226142		
44822	H	0.495112	0.771122	-1.906045		
44823	C	-0.930808	1.394676	-0.437827		
44824	O	-1.454990	0.993198	0.814676		
44825	H	-0.314319	2.274711	-0.252430		
44826	H	-1.746158	1.657806	-1.110122		
44827	O	-2.816870	0.630182	0.665093		
44828	H	-2.740441	-0.236591	0.230648		
44829	Rotational constants (GHz):			1.2178400	0.8127400	0.7600100
44830	Vibrational harmonic frequencies (cm-1):					

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44831      i1683.2010          70.6917          74.9705
44832      132.0327           158.2959         180.7074
44833      200.7773           216.5745         219.9661
44834      235.8456           262.7191         294.6682
44835      319.1226           338.2718         380.7300
44836      408.5540           497.2102         514.2249
44837      528.8105           559.6320         588.3845
44838      636.0602           772.0710         803.0225
44839      852.5752           944.3509         964.0294
44840      972.8654           1024.9564        1043.8263
44841      1050.0589          1070.5058        1129.8083
44842      1143.1216          1165.0098        1214.5646
44843      1231.7549          1297.2915        1350.4103
44844      1369.3969          1395.0099        1398.5282
44845      1400.9447          1468.1446        1469.3504
44846      1491.2601          1499.5209        1678.2474
44847      1958.7669          3076.4643        3090.1587
44848      3114.9378          3146.2841        3160.0681
44849      3161.9374          3682.7605        3829.4328
44850      Zero-point correction (Hartree): 0.150905
44851
44852      TS.diHPCARP_Ib.15aldHshift.updmtddd
44853      -----
44854      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14190324
44855      Electronic state : 2-A
44856      Cartesian coordinates (Angs):
44857      O      -1.123120          1.590186          -1.003494
44858      O      -0.708967          2.344865           0.078416
44859      H      -0.820705          1.475031           1.029274
44860      C      -0.695502          0.238368           1.334334
44861      C      -0.727920          -0.524250           0.001872
44862      C      -0.290834          0.441827          -1.115372
44863      O      -0.561865          -0.210154           2.413331
44864      C      -2.145047          -1.037422          -0.202812
44865      O      0.203902           -1.582926           0.180610
44866      H      -2.838113          -0.201664          -0.276558
44867      H      -2.432558          -1.670297           0.635428
44868      H      -2.192871          -1.608030          -1.129301
44869      O      0.347256           -2.252516          -1.067826
44870      H      -0.031627          -3.118023          -0.867840
44871      H      -0.543107           0.019128          -2.087394
44872      C      1.196414           0.772143          -1.055219
44873      O      1.652058           0.857792           0.288752
44874      H      1.767233           0.001074          -1.567748
44875      H      1.360308           1.735325          -1.539335
44876      O      2.641901           -0.131756           0.519425
44877      H      2.099434           -0.900471           0.752940
44878      Rotational constants (GHz):      1.0160700      0.9851900      0.8203900
44879      Vibrational harmonic frequencies (cm-1):
44880      i1971.3119          71.1920          106.5125
44881      124.4296           156.3942          176.4481
44882      186.5363           220.4610          227.5651
44883      244.9933           263.6914          294.6533
44884      320.8997           339.2242          383.3512
44885      408.6008           432.1501          478.7736
44886      524.5142           534.7622          579.9415
44887      634.2004           771.9008          795.8205
44888      887.1621           931.9755          950.9987
44889      988.8932           1016.9837         1032.6127
44890      1060.6194          1071.0049         1119.6418
44891      1136.2079          1165.8941         1199.9730
44892      1234.2298          1287.9685         1348.9407
44893      1360.7277          1391.7985         1400.0839
44894      1402.0179          1451.8737         1474.4621
44895      1493.3930          1499.4540         1667.5534
44896      1947.5031          3073.8477         3090.6911
44897      3119.8544          3154.3569         3154.5778
44898      3162.3876          3757.3829         3818.5428
44899      Zero-point correction (Hartree): 0.150657
44900
44901      TS.diHPCARP_Ib.15aldHshift.upumpddd
44902      -----

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44903 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14181934
44904 Electronic state : 2-A
44905 Cartesian coordinates (Angs):
44906 O 1.627708 -1.118272 -0.951449
44907 O 1.685808 -1.780370 0.259047
44908 H 1.556448 -0.770836 1.069897
44909 C 0.939647 0.327423 1.242747
44910 C 0.467375 0.786848 -0.144266
44911 C 0.370908 -0.454196 -1.059999
44912 O 0.721757 0.838872 2.279518
44913 C 1.475964 1.789040 -0.691091
44914 O -0.777058 1.417372 0.111517
44915 H 1.603152 2.603917 0.018859
44916 H 2.435132 1.309402 -0.875213
44917 H 1.087753 2.188993 -1.627271
44918 O -1.480802 1.544230 -1.116275
44919 H -2.210692 0.922496 -0.963014
44920 H 0.335354 -0.125718 -2.097724
44921 C -0.790046 -1.408938 -0.772772
44922 O -1.247336 -1.385983 0.568046
44923 H -0.431668 -2.421948 -0.952851
44924 H -1.631117 -1.212202 -1.434584
44925 O -2.450835 -0.624200 0.630960
44926 H -2.161390 0.131651 1.163281
44927 Rotational constants (GHz): 1.0687400 0.9601500 0.8150400
44928 Vibrational harmonic frequencies (cm-1):
44929 i1910.4942 60.3742 105.3507
44930 140.1260 151.5024 177.5520
44931 212.4358 218.4943 233.3668
44932 253.8167 297.4174 318.1914
44933 325.9044 371.7545 407.1527
44934 430.1183 487.7944 513.6274
44935 528.2073 540.7862 589.8137
44936 626.7168 769.8922 792.4590
44937 884.4162 929.1020 952.3459
44938 983.5759 1016.6907 1037.4754
44939 1065.6503 1078.4728 1123.9022
44940 1137.4437 1161.8870 1207.3770
44941 1236.0556 1303.9492 1344.8471
44942 1365.2267 1397.3782 1406.5328
44943 1434.2901 1449.9652 1472.5521
44944 1492.7894 1496.5850 1669.2610
44945 1947.0233 3075.1455 3098.0448
44946 3123.8129 3150.9430 3156.3524
44947 3167.7409 3734.9342 3774.2627
44948 Zero-point correction (Hartree): 0.151336
44949
44950 TS.diHPCARP_Ib.15aldHshift.upupmudd
44951 -----
44952 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14329995
44953 Electronic state : 2-A
44954 Cartesian coordinates (Angs):
44955 O 1.460834 -1.382340 -0.959634
44956 O 1.874848 -1.781130 0.299832
44957 H 1.944703 -0.627925 0.909304
44958 C 1.292464 0.450897 1.089258
44959 C 0.527331 0.691254 -0.212078
44960 C 0.229824 -0.682141 -0.852969
44961 O 1.233358 1.050413 2.098882
44962 C 1.414410 1.551740 -1.102759
44963 O -0.657994 1.371452 0.170506
44964 H 2.336387 1.023812 -1.338712
44965 H 1.646692 2.485621 -0.594284
44966 H 0.879619 1.769919 -2.024565
44967 O -1.418385 1.641644 -0.999368
44968 H -2.005311 0.863927 -1.026054
44969 H -0.079558 -0.522657 -1.886782
44970 C -0.817901 -1.524983 -0.124291
44971 O -2.101271 -0.916374 -0.217488
44972 H -0.867772 -2.501302 -0.607750
44973 H -0.570846 -1.669675 0.924462
44974 O -2.529172 -0.495142 1.068131

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44975      H      -2.058435      0.349491      1.174531
44976 Rotational constants (GHz):      1.1100100      0.8718100      0.7360000
44977 Vibrational harmonic frequencies (cm-1):
44978      i1919.5760      48.6994      87.1618
44979      143.1698      175.8361      196.2027
44980      203.2450      210.7534      242.5535
44981      246.1969      283.0336      316.4233
44982      360.5942      374.0928      407.2000
44983      483.4648      503.0554      513.9936
44984      533.3134      576.8642      622.2355
44985      646.5710      720.6794      772.4322
44986      900.3589      951.7204      964.5106
44987      989.7751      1033.9811      1038.6541
44988      1081.2930      1110.0941      1114.5613
44989      1130.6106      1190.2422      1213.1567
44990      1228.8634      1281.6099      1337.1050
44991      1371.7108      1399.3975      1405.1319
44992      1461.5586      1484.2981      1488.2259
44993      1495.0167      1498.8867      1662.6417
44994      1951.4503      3080.6472      3091.6608
44995      3105.8973      3159.2080      3164.5278
44996      3168.5359      3654.0590      3723.5970
44997 Zero-point correction (Hartree): 0.151728
44998
44999 TS.diHPCARP_Ib.15aldHshift.upuppudd
45000 -----
45001 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14567427
45002 Electronic state : 2-A
45003 Cartesian coordinates (Angs):
45004      O      0.402719      1.744911      0.984839
45005      O      1.057965      2.327372      -0.085791
45006      H      1.863747      1.344617      -0.410814
45007      C      1.903568      0.090081      -0.587954
45008      C      0.774000      -0.509926      0.259952
45009      C      -0.279110      0.587127      0.525782
45010      O      2.631893      -0.464490      -1.325473
45011      C      1.405367      -1.012803      1.552100
45012      O      0.255001      -1.556111      -0.536098
45013      H      1.822304      -0.180218      2.116448
45014      H      2.191536      -1.729224      1.321616
45015      H      0.636755      -1.501567      2.146904
45016      O      -0.779333      -2.192778      0.202675
45017      H      -1.564460      -1.785829      -0.199154
45018      H      -0.912296      0.286886      1.360111
45019      C      -1.153976      0.909715      -0.684244
45020      O      -2.218452      -0.018380      -0.827346
45021      H      -1.545174      1.922392      -0.581123
45022      H      -0.608669      0.826108      -1.623725
45023      O      -3.089248      0.146362      0.287953
45024      H      -3.867208      0.536582      -0.130145
45025 Rotational constants (GHz):      1.2057100      0.8181900      0.6332900
45026 Vibrational harmonic frequencies (cm-1):
45027      i1854.7696      53.9371      85.3675
45028      133.5249      156.5320      183.8690
45029      197.3911      207.9942      229.8114
45030      246.5839      255.8912      281.3056
45031      323.2136      344.4111      382.9875
45032      406.8384      497.5781      511.1998
45033      517.8649      548.7458      576.0797
45034      631.0515      728.5100      778.0462
45035      900.2783      952.6884      965.2290
45036      995.2984      1031.2855      1039.7214
45037      1073.2671      1099.5826      1115.3993
45038      1135.6242      1183.4652      1217.1217
45039      1238.0234      1295.1019      1334.2946
45040      1367.0122      1396.7222      1399.6808
45041      1425.1606      1447.7723      1472.6427
45042      1489.3504      1499.7402      1661.8929
45043      1951.9329      3078.7963      3086.6600
45044      3123.5778      3148.1789      3161.8658
45045      3167.4314      3719.7331      3818.3626
45046 Zero-point correction (Hartree): 0.150978

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45047
45048 TS.diHPCARP_Ib.15aldHshift.upuptddd
45049 -----
45050 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14330609
45051 Electronic state : 2-A
45052 Cartesian coordinates (Angs):
45053 O -0.670581 1.707894 -1.078965
45054 O -0.990104 2.350536 0.103425
45055 H -1.684292 1.399226 0.689431
45056 C -1.702961 0.154133 0.915366
45057 C -0.864654 -0.508514 -0.187158
45058 C 0.092351 0.551007 -0.775334
45059 O -2.219982 -0.356261 1.839032
45060 C -1.837786 -1.036454 -1.233353
45061 O -0.163402 -1.539236 0.476754
45062 H -2.381193 -0.212443 -1.692904
45063 H -2.540977 -1.722560 -0.765279
45064 H -1.273888 -1.567018 -1.997567
45065 O 0.611107 -2.234702 -0.492061
45066 H 1.481679 -1.824926 -0.356472
45067 H 0.466195 0.201613 -1.738641
45068 C 1.267353 0.888890 0.139034
45069 O 2.296995 -0.033479 -0.192754
45070 H 1.593689 1.911196 -0.057724
45071 H 1.018316 0.780601 1.194659
45072 O 3.334380 0.123962 0.760253
45073 H 4.007343 0.590228 0.247694
45074 Rotational constants (GHz): 1.1524700 0.7752800 0.6212800
45075 Vibrational harmonic frequencies (cm-1):
45076 i1832.1035 50.8479 82.8131
45077 129.8631 151.3384 174.7652
45078 188.4622 212.1103 230.5893
45079 250.3199 252.0744 264.6651
45080 323.7549 334.0026 354.1185
45081 379.3017 434.4637 510.3398
45082 541.4897 555.3013 570.8687
45083 643.8650 732.4332 781.2128
45084 915.3964 960.6324 983.6699
45085 1024.2311 1033.2993 1037.7935
45086 1075.8791 1102.3394 1132.9532
45087 1134.8564 1184.6409 1215.7861
45088 1229.8620 1265.0980 1339.8785
45089 1360.8646 1400.2993 1412.5485
45090 1428.5014 1464.6349 1489.2796
45091 1500.5325 1513.0584 1662.7081
45092 1954.1007 3075.9142 3078.1366
45093 3108.7079 3133.5719 3161.6357
45094 3166.4079 3702.9912 3812.1405
45095 Zero-point correction (Hartree): 0.150841
45096
45097 TS.diHPCARP_Ib.15aldHshift.uputmudd
45098 -----
45099 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14137791
45100 Electronic state : 2-A
45101 Cartesian coordinates (Angs):
45102 O 0.419699 1.678217 1.060377
45103 O 1.134083 2.297380 0.051206
45104 H 1.893400 1.313263 -0.361948
45105 C 1.863699 0.080914 -0.674770
45106 C 0.786061 -0.534193 0.215698
45107 C -0.270077 0.552789 0.524635
45108 O 2.491816 -0.418773 -1.533692
45109 C 1.492606 -1.007131 1.482570
45110 O 0.238329 -1.600469 -0.531063
45111 H 1.955760 -0.165474 1.993720
45112 H 2.252397 -1.741598 1.221981
45113 H 0.760245 -1.468390 2.141169
45114 O -0.721605 -2.258091 0.285540
45115 H -1.548767 -1.832798 0.004443
45116 H -0.894588 0.200613 1.345837
45117 C -1.159408 0.928575 -0.663260
45118 O -2.529621 0.943851 -0.328406

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45119	H	-0.942750	1.951935	-0.962371		
45120	H	-1.003983	0.263832	-1.515397		
45121	O	-2.914291	-0.429779	-0.196296		
45122	H	-3.696266	-0.345797	0.361989		
45123	Rotational constants (GHz):			1.1587600	0.8219500	0.6226600
45124	Vibrational harmonic frequencies (cm-1):					
45125	i1888.5266		29.6614			66.9441
45126	120.3352		127.4581			148.9651
45127	188.0118		203.6594			213.5400
45128	236.3346		251.4543			307.7952
45129	320.4276		323.3156			356.1470
45130	412.0922		473.3717			490.4304
45131	518.5499		554.6487			563.7755
45132	639.6687		749.7996			799.4692
45133	914.3437		936.5089			961.3189
45134	979.6481		1025.6207			1037.9338
45135	1080.8016		1104.0346			1110.1587
45136	1127.1109		1169.5307			1217.6951
45137	1230.4845		1288.1987			1320.0486
45138	1363.6690		1398.8753			1418.5684
45139	1432.9074		1473.3677			1487.4215
45140	1491.0173		1500.0447			1666.1885
45141	1952.0737		3079.7976			3081.0439
45142	3118.4844		3157.3263			3164.2014
45143	3169.4944		3707.7122			3847.0980
45144	Zero-point correction (Hartree):			0.150606		
45145						
45146	TS.diHPCARP_Ib.15aldHshift.utdmmudd					
45147	-----					
45148	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.14427094		
45149	Electronic state : 2-A					
45150	Cartesian coordinates (Angs):					
45151	O	0.446329	1.435625	-1.068498		
45152	O	0.661775	1.805697	0.241258		
45153	H	-0.583755	1.557058	0.717535		
45154	C	-1.552437	0.825169	0.484812		
45155	C	-1.020253	-0.388305	-0.340403		
45156	C	0.232023	0.025030	-1.161149		
45157	O	-2.659555	1.021668	0.815670		
45158	C	-2.119783	-0.920141	-1.240173		
45159	O	-0.771653	-1.414820	0.604147		
45160	H	-2.999969	-1.150049	-0.645740		
45161	H	-2.376636	-0.177946	-1.994445		
45162	H	-1.771165	-1.825504	-1.737431		
45163	O	-0.234255	-0.854216	1.794566		
45164	H	0.723120	-0.871043	1.598869		
45165	H	-0.018507	-0.087573	-2.218351		
45166	C	1.480736	-0.824340	-0.955034		
45167	O	2.036507	-0.823208	0.345465		
45168	H	2.248957	-0.508715	-1.661058		
45169	H	1.215393	-1.865238	-1.148149		
45170	O	2.914416	0.280491	0.482351		
45171	H	2.292338	1.014635	0.640780		
45172	Rotational constants (GHz):			1.4007800	0.7778700	0.7332100
45173	Vibrational harmonic frequencies (cm-1):					
45174	i1555.0321		53.6647			100.4691
45175	123.9677		166.4364			200.8767
45176	235.4884		251.3499			264.3142
45177	272.6118		295.7949			317.6370
45178	356.9105		392.8106			463.5341
45179	488.7502		509.7820			540.1763
45180	564.8532		587.0986			622.4107
45181	648.5833		761.9853			825.4524
45182	846.7031		933.2068			944.9417
45183	970.1773		1037.1659			1055.5954
45184	1067.4882		1085.5346			1129.8545
45185	1147.0517		1183.1672			1200.0597
45186	1237.8375		1326.7699			1363.9823
45187	1384.5478		1406.4799			1414.8737
45188	1455.1075		1479.7297			1485.0341
45189	1492.9760		1496.3053			1718.6435
45190	1966.3682		3072.2419			3078.0284


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45191          3089.8423          3136.0612          3148.5282
45192          3175.4864          3582.3557          3634.9417
45193 Zero-point correction (Hartree): 0.152163
45194
45195 TS.diHPCARP_Ib.15aldHshift.utdppddd
45196 -----
45197 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14297624
45198 Electronic state : 2-A
45199 Cartesian coordinates (Angs):
45200 O          0.562097          1.996708          0.505421
45201 O          1.120595          2.124209         -0.753286
45202 H          1.805760          1.002041         -0.793562
45203 C          1.801539         -0.200291         -0.420316
45204 C          0.573119         -0.400080          0.501776
45205 C         -0.308434          0.869791          0.528414
45206 O          2.595571         -1.012008         -0.717349
45207 C          1.106184         -0.681971          1.900379
45208 O         -0.111181         -1.576743          0.114713
45209 H          1.585032          0.211355          2.298388
45210 H          1.821248         -1.500273          1.866120
45211 H          0.273301         -0.954251          2.548991
45212 O         -0.229248         -1.611377         -1.301953
45213 H         -1.143326         -1.296880         -1.416099
45214 H         -0.771007          0.925310          1.513404
45215 C         -1.404898          1.051970         -0.521048
45216 O         -2.290225         -0.048486         -0.633113
45217 H         -1.960021          1.955034         -0.261640
45218 H         -0.983150          1.163709         -1.517930
45219 O         -2.772926         -0.393579          0.656788
45220 H         -2.230355         -1.172346          0.857330
45221 Rotational constants (GHz):          1.2028500          0.8646700          0.6975900
45222 Vibrational harmonic frequencies (cm-1):
45223 i1784.6655          45.1350          95.6101
45224          133.1351          162.6117          207.7065
45225          231.0051          238.7642          250.9714
45226          269.4122          288.7198          323.7572
45227          347.0657          384.1550          406.5245
45228          430.2923          458.7077          505.5644
45229          550.0226          568.6836          619.4877
45230          644.8709          695.5013          802.5483
45231          897.9394          937.4400          958.4728
45232          998.7224          1025.5745          1053.4371
45233          1058.0798          1106.9165          1115.1395
45234          1134.1996          1197.2873          1205.2659
45235          1243.1863          1288.0843          1343.7133
45236          1398.2607          1407.9072          1413.1432
45237          1439.8720          1466.2930          1489.1398
45238          1498.0778          1503.3022          1673.4058
45239          1961.1403          3070.3724          3082.1341
45240          3114.2668          3148.7644          3156.8628
45241          3171.9118          3671.4797          3746.7588
45242 Zero-point correction (Hartree): 0.151810
45243
45244 TS.diHPCARP_Ib.15aldHshift.utdppudd
45245 -----
45246 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14313487
45247 Electronic state : 2-A
45248 Cartesian coordinates (Angs):
45249 O          0.251669          2.010644          0.402198
45250 O          0.806639          2.193152         -0.854152
45251 H          1.668142          1.179651         -0.865088
45252 C          1.828044         -0.016311         -0.507771
45253 C          0.741767         -0.318718          0.541885
45254 C         -0.381490          0.735122          0.440619
45255 O          2.650163         -0.742277         -0.927905
45256 C          1.414065         -0.230469          1.908416
45257 O          0.310026         -1.654257          0.441976
45258 H          1.736093          0.790400          2.102126
45259 H          2.269765         -0.901027          1.939983
45260 H          0.694104         -0.531007          2.668745
45261 O         -0.045586         -1.950390         -0.900831
45262 H         -1.013669         -1.918287         -0.843781

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45263	H	-0.940203	0.727850	1.376884	
45264	C	-1.374082	0.628221	-0.715517	
45265	O	-2.290265	-0.440450	-0.547239	
45266	H	-1.908967	1.576800	-0.788645	
45267	H	-0.885922	0.418770	-1.664150	
45268	O	-3.065230	-0.184538	0.615505	
45269	H	-3.928496	0.014707	0.231709	
45270	Rotational constants (GHz):		1.2105500	0.8099100	0.6562100
45271	Vibrational harmonic frequencies (cm-1):				
45272	i1778.2306		46.8084		82.2428
45273	143.8768		154.0333		191.4663
45274	202.6108		216.7642		228.2233
45275	238.6465		250.1296		283.8319
45276	317.7163		350.6816		387.8952
45277	417.2567		447.0093		505.7190
45278	517.7164		547.4855		583.9203
45279	617.9309		714.1348		811.6189
45280	894.1401		943.8213		962.3614
45281	989.8382		1028.2263		1046.9049
45282	1067.6676		1104.2293		1110.7710
45283	1129.7618		1197.2263		1209.9980
45284	1247.1934		1297.4800		1326.8065
45285	1381.4091		1402.7557		1406.3981
45286	1424.5111		1451.8723		1480.8727
45287	1490.1007		1500.0545		1671.9147
45288	1958.9060		3076.8418		3084.5615
45289	3113.6386		3158.0613		3164.3506
45290	3172.6501		3729.4694		3819.4318
45291	Zero-point correction (Hartree): 0.151047				
45292					
45293	TS.diHPCARP_Ib.15aldHshift.utdtpduu				
45294	-----				
45295	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14287385				
45296	Electronic state : 2-A				
45297	Cartesian coordinates (Angs):				
45298	O	0.339918	1.326799	-0.832506	
45299	O	-0.255160	2.381828	-0.168943	
45300	H	-1.363114	1.831482	0.149707	
45301	C	-1.925433	0.671747	0.234308	
45302	C	-0.790728	-0.340328	0.520273	
45303	C	0.556864	0.287974	0.118188	
45304	O	-3.052146	0.413296	0.015233	
45305	C	-0.834503	-0.681843	2.002250	
45306	O	-1.084548	-1.551994	-0.145628	
45307	H	-0.755532	0.228170	2.595094	
45308	H	-1.765193	-1.192355	2.239531	
45309	H	0.008505	-1.328893	2.244527	
45310	O	-1.170462	-1.298588	-1.540077	
45311	H	-2.128282	-1.269736	-1.674569	
45312	H	1.015791	0.738290	0.999858	
45313	C	1.513328	-0.718136	-0.489237	
45314	O	2.822506	-0.210958	-0.591225	
45315	H	1.221348	-0.948268	-1.512440	
45316	H	1.510485	-1.638780	0.097273	
45317	O	3.333500	-0.124818	0.738113	
45318	H	3.669971	0.779085	0.746590	
45319	Rotational constants (GHz):		1.3910900	0.6644900	0.6026800
45320	Vibrational harmonic frequencies (cm-1):				
45321	i2058.5110		37.4347		47.5955
45322	119.8939		145.8071		152.4949
45323	165.3987		219.6248		224.6654
45324	237.7714		255.4259		275.7260
45325	300.8193		331.5473		362.4603
45326	396.9840		450.2514		464.5373
45327	493.9793		531.4904		586.7543
45328	598.7044		744.6795		827.3869
45329	870.8109		911.0438		959.7951
45330	981.7741		1043.1537		1056.3326
45331	1079.7256		1114.7465		1119.5420
45332	1155.1444		1183.0555		1188.6480
45333	1265.5066		1300.7002		1335.6887
45334	1391.8959		1405.1350		1411.6808

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45335      1414.2589      1432.0095      1466.8313
45336      1487.7148      1496.8579      1675.8394
45337      1947.2297      3071.0596      3081.8158
45338      3096.2109      3149.0316      3155.5288
45339      3166.7348      3791.2615      3837.1931
45340      Zero-point correction (Hartree): 0.150394
45341
45342      TS.diHPCARP_Ib.15aldHshift.utdttudd
45343      -----
45344      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14340170
45345      Electronic state : 2-A
45346      Cartesian coordinates (Angs):
45347      O      0.312641      1.743631      0.646626
45348      O      1.104315      2.358619      -0.304767
45349      H      1.839687      1.357572      -0.643042
45350      C      1.916793      0.079395      -0.542869
45351      C      0.466951      -0.443589      -0.398203
45352      C      -0.446492      0.734812      -0.009650
45353      O      2.902559      -0.557488      -0.457292
45354      C      0.061339      -1.067912      -1.725820
45355      O      0.466172      -1.507085      0.530967
45356      H      0.147291      -0.330504      -2.522821
45357      H      0.704404      -1.917342      -1.945812
45358      H      -0.975921      -1.392053      -1.657428
45359      O      0.966288      -1.027848      1.771831
45360      H      1.870032      -1.372713      1.763517
45361      H      -0.867672      1.171047      -0.916537
45362      C      -1.576236      0.343135      0.929164
45363      O      -2.428971      -0.606743      0.325009
45364      H      -2.130824      1.239560      1.212039
45365      H      -1.195552      -0.153091      1.819449
45366      O      -3.065624      0.031344      -0.779701
45367      H      -3.984633      0.047043      -0.486482
45368      Rotational constants (GHz):      1.2967100      0.7427300      0.6586300
45369      Vibrational harmonic frequencies (cm-1):
45370      i2009.4646      55.1165      62.5664
45371      120.4763      154.7133      158.0250
45372      180.4353      201.0797      213.1118
45373      232.7106      263.2735      277.5790
45374      319.4956      365.2820      375.6334
45375      400.5607      423.6530      468.0864
45376      493.6200      532.0297      581.2084
45377      624.4422      679.6804      821.8271
45378      878.7110      938.6641      954.1661
45379      1035.8469      1040.9830      1050.4270
45380      1072.3497      1109.6938      1117.0338
45381      1147.0888      1185.3505      1194.5030
45382      1265.2969      1287.4180      1345.6890
45383      1392.7859      1398.0439      1410.1209
45384      1411.9576      1424.1679      1486.9898
45385      1493.9152      1500.1136      1676.2971
45386      1946.3265      3075.5198      3081.0100
45387      3099.0270      3156.9792      3161.1533
45388      3168.4083      3794.5575      3830.8513
45389      Zero-point correction (Hartree): 0.150669
45390
45391      TS.diHPCARP_Ib.15aldHshift.utummduu
45392      -----
45393      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14206051
45394      Electronic state : 2-A
45395      Cartesian coordinates (Angs):
45396      O      0.233946      1.771367      -0.098016
45397      O      1.115736      1.920791      -1.154073
45398      H      1.811531      0.797510      -1.052990
45399      C      1.746835      -0.425004      -0.760019
45400      C      0.452861      -0.606026      0.086565
45401      C      -0.489951      0.551132      -0.263177
45402      O      2.478984      -1.257945      -1.143594
45403      C      -0.140575      -1.981845      -0.134008
45404      O      0.841260      -0.536558      1.454292
45405      H      0.651667      -2.725091      -0.088093
45406      H      -0.633302      -2.030149      -1.104044

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45407	H	-0.882392	-2.181962	0.635285	
45408	O	1.917209	0.381765	1.612682	
45409	H	1.478959	1.244189	1.540470	
45410	H	-0.817110	0.474606	-1.302124	
45411	C	-1.697820	0.676566	0.655953	
45412	O	-2.620106	-0.374239	0.477974	
45413	H	-1.396866	0.599072	1.701102	
45414	H	-2.171287	1.644141	0.478690	
45415	O	-3.119494	-0.283897	-0.852545	
45416	H	-4.049586	-0.081527	-0.693942	
45417	Rotational constants (GHz):		1.3073900	0.7029500	0.6379500
45418	Vibrational harmonic frequencies (cm-1):				
45419	i1706.1816		23.9047		58.1421
45420	116.9648		135.1339		167.9584
45421	188.5069		210.3576		222.3842
45422	255.3254		274.2611		294.6705
45423	317.4779		335.8214		389.7898
45424	419.1815		449.7771		464.2592
45425	481.3607		518.7900		589.1044
45426	621.6539		697.8858		805.1199
45427	879.0050		927.4078		955.6458
45428	1025.5726		1046.9681		1049.4650
45429	1074.7560		1102.3830		1123.0844
45430	1135.4212		1185.0339		1204.8360
45431	1257.6873		1292.0553		1329.1400
45432	1392.2063		1397.5216		1413.8258
45433	1426.5878		1441.0129		1483.6723
45434	1485.5241		1492.9403		1677.7266
45435	1963.2090		3073.8215		3084.2618
45436	3095.7082		3137.9599		3164.3462
45437	3176.8307		3748.3961		3828.4477
45438	Zero-point correction (Hartree): 0.150610				
45439					
45440	TS.diHPCARP_Ib.15aldHshift.utummudd				
45441	-----				
45442	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14461922				
45443	Electronic state : 2-A				
45444	Cartesian coordinates (Angs):				
45445	O	0.735132	1.806862	-0.481615	
45446	O	1.259804	1.566443	0.778070	
45447	H	0.245698	0.963311	1.401839	
45448	C	-0.705586	0.155377	1.234640	
45449	C	-1.090575	0.286682	-0.234326	
45450	C	0.179624	0.615186	-1.047737	
45451	O	-1.155550	-0.564066	2.051043	
45452	C	-2.100174	1.428511	-0.326092	
45453	O	-1.798946	-0.846643	-0.688584	
45454	H	-1.638896	2.366525	-0.027395	
45455	H	-2.955819	1.216130	0.311262	
45456	H	-2.437389	1.508179	-1.358706	
45457	O	-1.078712	-2.038154	-0.428204	
45458	H	-1.377326	-2.268163	0.464092	
45459	H	-0.136526	0.937318	-2.041704	
45460	C	1.169474	-0.529445	-1.206101	
45461	O	1.518254	-1.140184	0.023303	
45462	H	0.706264	-1.298278	-1.822939	
45463	H	2.072313	-0.166898	-1.696188	
45464	O	2.797992	-0.682548	0.427370	
45465	H	2.581312	0.190337	0.796370	
45466	Rotational constants (GHz):		1.2202200	0.8875000	0.7618800
45467	Vibrational harmonic frequencies (cm-1):				
45468	i1809.1775		59.8998		106.4922
45469	156.2557		173.1668		184.1335
45470	209.9786		231.3467		240.4391
45471	256.7681		285.7601		312.9448
45472	337.7621		371.5781		403.7374
45473	427.1970		455.4235		514.3708
45474	535.5394		572.1176		602.6051
45475	626.2777		800.0775		819.4910
45476	850.9307		943.2685		949.3488
45477	972.9540		1020.4896		1045.0900
45478	1055.7711		1068.6230		1113.8997

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45479      1139.6557      1173.3759      1211.8010
45480      1236.3670      1298.0575      1354.4836
45481      1358.9867      1398.8552      1405.5618
45482      1428.5703      1460.4243      1474.6393
45483      1490.5958      1499.3663      1682.0864
45484      1943.4211      3079.3527      3091.2772
45485      3102.9058      3147.4164      3159.0748
45486      3175.8247      3685.6352      3776.5265
45487      Zero-point correction (Hartree): 0.151448
45488
45489      TS.diHPCARP_Ib.15aldHshift.utupmuuu
45490      -----
45491      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14497167
45492      Electronic state : 2-A
45493      Cartesian coordinates (Angs):
45494      O      0.219850      1.815035      0.241074
45495      O      1.548645      2.151124      0.084627
45496      H      2.098585      1.003401      0.317951
45497      C      1.979155      -0.248505      0.124773
45498      C      0.534284      -0.503069      -0.404748
45499      C      -0.125205      0.843658      -0.742162
45500      O      2.817448      -1.058153      0.263712
45501      C      0.586198      -1.441600      -1.595716
45502      O      -0.130533      -1.233884      0.615616
45503      H      1.089734      -2.360680      -1.305463
45504      H      1.133597      -0.980691      -2.415816
45505      H      -0.425504      -1.672827      -1.929040
45506      O      -0.048822      -0.533162      1.846071
45507      H      -0.788598      0.095914      1.772495
45508      H      0.274113      1.185156      -1.702690
45509      C      -1.643262      0.849067      -0.836287
45510      O      -2.288918      0.400400      0.344177
45511      H      -1.953959      1.884325      -0.982627
45512      H      -1.987775      0.251372      -1.678464
45513      O      -2.791878      -0.909821      0.135372
45514      H      -2.033541      -1.455586      0.403291
45515      Rotational constants (GHz):      1.3070700      0.8210900      0.6877800
45516      Vibrational harmonic frequencies (cm-1):
45517      i1904.3681      48.9320      70.8740
45518      137.8361      175.6613      204.2971
45519      217.7095      225.6215      244.2053
45520      253.2522      292.4720      323.5668
45521      337.9030      396.9575      419.9686
45522      439.9954      479.6929      497.6319
45523      514.7286      574.7551      585.0442
45524      619.1701      761.2419      835.2276
45525      857.7091      919.8721      942.2697
45526      963.6540      1034.8920      1053.4510
45527      1065.0625      1098.1880      1130.1203
45528      1145.0042      1160.3067      1201.3593
45529      1261.5531      1309.8875      1349.8733
45530      1377.5446      1404.1295      1411.6804
45531      1459.9925      1464.9426      1472.6854
45532      1487.0279      1499.0709      1660.0840
45533      1961.3883      3055.8477      3075.1061
45534      3088.4510      3144.9610      3153.0638
45535      3169.8525      3693.3539      3712.9738
45536      Zero-point correction (Hartree): 0.151366
45537
45538      TS.diHPCARP_Ib.15aldHshift.utuppduu
45539      -----
45540      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14568596
45541      Electronic state : 2-A
45542      Cartesian coordinates (Angs):
45543      O      0.659274      1.420821      0.062173
45544      O      -0.309335      2.397561      0.153142
45545      H      -1.338027      1.712445      -0.322897
45546      C      -1.856806      0.569591      -0.374413
45547      C      -0.916669      -0.416465      0.377813
45548      C      0.311140      0.339144      0.923854
45549      O      -2.890958      0.310368      -0.863899
45550      C      -1.710593      -1.071048      1.496731

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45551	O	-0.592234	-1.460239	-0.511511		
45552	H	-2.545187	-1.620073	1.067719		
45553	H	-2.089597	-0.317163	2.184690		
45554	H	-1.071321	-1.761405	2.047161		
45555	O	-0.105474	-0.898290	-1.721829		
45556	H	0.854241	-0.934004	-1.563828		
45557	H	0.056613	0.760452	1.900072		
45558	C	1.553329	-0.533103	1.064326		
45559	O	2.162692	-0.821896	-0.182660		
45560	H	2.288684	-0.047379	1.703733		
45561	H	1.279165	-1.499423	1.487949		
45562	O	3.054716	0.230804	-0.516725		
45563	H	2.453562	0.944792	-0.783985		
45564	Rotational constants (GHz):			1.3771400	0.7651300	0.6834800
45565	Vibrational harmonic frequencies (cm-1):					
45566	i1713.8276		52.7420			90.8545
45567	144.9717		166.9625			175.7133
45568	198.9936		218.0696			240.2868
45569	252.7144		281.5270			321.3281
45570	333.4602		406.8799			417.1945
45571	447.6191		457.5593			486.9280
45572	531.3227		580.5631			581.4728
45573	619.3066		753.5847			831.0259
45574	868.9569		911.3355			944.8133
45575	1005.8947		1015.9861			1048.4440
45576	1062.7986		1108.1913			1128.8340
45577	1137.5857		1164.0347			1196.6802
45578	1264.5864		1317.4770			1349.0744
45579	1389.8163		1398.2275			1408.7013
45580	1463.2344		1466.5426			1472.4795
45581	1485.7058		1496.4474			1670.9663
45582	1964.5706		3068.7571			3074.5554
45583	3093.5252		3147.7175			3150.3565
45584	3171.6914		3669.1847			3736.3508
45585	Zero-point correction (Hartree):			0.151372		
45586	TS.diHPCARP_Ib.15aldHshift.utuppuuu					
45587	-----					
45588	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14271962					
45589	Electronic state : 2-A					
45590	Cartesian coordinates (Angs):					
45591	O	-0.189329	1.655352	-0.291971		
45592	O	1.063465	2.190387	-0.548579		
45593	H	1.852143	1.211840	-0.142493		
45594	C	1.978535	-0.044206	-0.066238		
45595	C	0.539423	-0.623050	-0.176703		
45596	C	-0.287375	0.398219	-0.966931		
45597	O	2.991826	-0.634578	-0.024183		
45598	C	0.543199	-2.002635	-0.796876		
45599	O	0.067967	-0.775051	1.159508		
45600	H	1.275653	-2.626876	-0.291059		
45601	H	0.801153	-1.939500	-1.853471		
45602	H	-0.447450	-2.442427	-0.692970		
45603	O	0.511653	0.308992	1.970737		
45604	H	-0.011415	1.058313	1.634436		
45605	H	0.173041	0.532165	-1.951453		
45606	C	-1.755597	0.046126	-1.189602		
45607	O	-2.384407	-0.697480	-0.180489		
45608	H	-2.302237	0.971802	-1.382901		
45609	H	-1.830063	-0.598786	-2.066170		
45610	O	-2.524515	0.138271	0.959364		
45611	H	-1.913217	-0.300403	1.569097		
45612	Rotational constants (GHz):			1.3217400	0.8032300	0.7304900
45613	Vibrational harmonic frequencies (cm-1):					
45614	i1785.6383		60.3490			89.9584
45615	107.8938		165.3291			183.7936
45616	207.4255		217.2136			248.5386
45617	276.7898		294.2508			324.0226
45618	343.6446		380.3614			408.2646
45619	422.7956		453.9187			466.8992
45620	508.9089		588.0793			591.4294
45621	627.7810		767.6058			846.6144

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45623      860.1872          894.1261          944.3618
45624      981.8982          1037.3671         1046.5750
45625      1069.2512         1084.2339         1133.4531
45626      1141.0358         1173.1932         1215.6143
45627      1262.2710         1311.9164         1362.6216
45628      1374.2393         1404.6036         1415.5172
45629      1433.7870         1461.8315         1462.5045
45630      1486.2723         1498.4627         1675.9062
45631      1963.3052         3051.0594         3070.8695
45632      3077.9405         3125.9411         3156.3322
45633      3171.5838         3687.0123         3777.9465
45634      Zero-point correction (Hartree): 0.151259
45635
45636
45637
45638      1,6-aldehyde-H-shift in (2R,3S)-2-Me-2,3-diOOH-butanal-4-peroxyl (C', R,S-di-HPCARP-
45639      Ic)
45640      =====
45641      =
45642
45643      TS.diHPCARP_Ic.16aldHshift.a.mpmud
45644      -----
45645      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14712225
45646      Electronic state : 2-A
45647      Cartesian coordinates (Angs):
45648      O      0.678033      2.617410      0.376001
45649      H      -0.426433      2.080446      0.060750
45650      C      -1.176213      1.113764      -0.322961
45651      O      1.555554      1.930864      -0.431221
45652      C      -0.625908      -0.222265      0.215951
45653      C      1.831730      0.666056      0.138462
45654      C      0.823111      -0.405087      -0.282235
45655      O      -2.137121      1.245572      -0.994724
45656      C      -0.744768      -0.215616      1.735208
45657      O      -1.321378      -1.288247      -0.398324
45658      H      -1.791722      -0.185188      2.023023
45659      H      -0.235884      0.653996      2.147424
45660      H      -0.290248      -1.122442      2.127939
45661      O      -2.669998      -1.294167      0.030554
45662      H      -3.087205      -0.728833      -0.636411
45663      O      1.246307      -1.644952      0.260662
45664      H      0.795751      -0.477493      -1.372625
45665      O      2.362523      -2.081312      -0.500274
45666      H      1.986033      -2.836803      -0.969726
45667      H      2.802627      0.364276      -0.251693
45668      H      1.888007      0.749585      1.223379
45669      Rotational constants (GHz):      1.0425800      0.8917900      0.5744200
45670      Vibrational harmonic frequencies (cm-1):
45671      i2032.2121          61.8176          84.5579
45672      101.5618          126.1146          176.1568
45673      203.9548          213.6479          231.3601
45674      240.9464          263.0613          294.2487
45675      326.8984          349.8264          399.7999
45676      408.2255          453.3298          457.9219
45677      473.9760          523.1073          560.9147
45678      619.1975          716.6456          828.0108
45679      888.1310          928.7347          990.3948
45680      1026.5996         1037.1892         1054.0392
45681      1096.8835         1120.6905         1141.0445
45682      1159.1073         1174.1612         1207.8938
45683      1257.0397         1291.7896         1338.2316
45684      1381.1508         1401.7850         1407.7539
45685      1415.6441         1435.6722         1480.4355
45686      1494.0710         1505.7678         1515.1748
45687      1929.3964         3073.6219         3088.0767
45688      3096.2308         3154.4694         3167.6939
45689      3181.5041         3770.3941         3814.5943
45690      Zero-point correction (Hartree): 0.150679
45691
45692      TS.diHPCARP_Ic.16aldHshift.a.mpmdu
45693      -----
45694      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14621967

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45695 Electronic state : 2-A
45696 Cartesian coordinates (Angs):
45697 O 1.397886 -1.576543 1.033857
45698 H 0.337263 -0.875288 1.285991
45699 C -0.720654 -0.199133 1.154579
45700 O 2.130193 -0.781652 0.181156
45701 C -0.896216 0.338453 -0.290779
45702 C 1.451301 -0.642297 -1.061164
45703 C 0.443499 0.509236 -1.040262
45704 O -1.515159 -0.092072 2.016997
45705 C -1.684758 1.635157 -0.276510
45706 O -1.734650 -0.578037 -0.979846
45707 H -1.138537 2.395483 0.273890
45708 H -2.648249 1.463311 0.195691
45709 H -1.835277 1.974955 -1.300467
45710 O -1.243532 -1.903859 -0.789877
45711 H -1.988678 -2.316230 -0.333892
45712 O 1.094132 1.698939 -0.617945
45713 H 0.168964 0.716914 -2.078695
45714 O 1.167053 1.686385 0.804590
45715 H 1.945571 1.128684 0.963196
45716 H 2.234667 -0.371766 -1.769133
45717 H 0.997862 -1.589854 -1.343233
45718 Rotational constants (GHz): 1.1195300 0.9346100 0.8062900
45719 Vibrational harmonic frequencies (cm-1):
45720 i1882.4431 64.1258 88.8494
45721 131.3973 158.7467 197.1448
45722 210.5523 234.0335 258.7678
45723 272.1221 277.3760 304.7839
45724 339.7078 350.3145 359.6717
45725 396.7763 466.5173 492.4974
45726 506.3283 536.9523 603.1244
45727 616.9061 776.4230 841.1605
45728 878.7648 929.9820 940.4459
45729 993.1573 1003.3621 1043.6440
45730 1064.5223 1105.3470 1121.9755
45731 1139.7800 1196.8552 1205.2527
45732 1241.7125 1305.4761 1358.5318
45733 1369.7318 1400.1187 1406.7142
45734 1414.1351 1432.5844 1473.4219
45735 1488.1517 1495.6061 1509.3108
45736 1941.9302 3073.6584 3087.1340
45737 3098.2023 3165.0283 3167.5061
45738 3189.1597 3736.0964 3815.2909
45739 Zero-point correction (Hartree): 0.150990
45740
45741 TS.diHPCARP_Ic.16aldHshift.a.mptmud
45742 -----
45743 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15062696
45744 Electronic state : 2-A
45745 Cartesian coordinates (Angs):
45746 O -2.599082 -0.949296 0.296611
45747 H -1.519951 -1.530275 -0.027984
45748 C -0.276723 -1.548430 -0.357970
45749 O -2.564389 0.168549 -0.504280
45750 C 0.405211 -0.311152 0.242588
45751 C -1.740308 1.158366 0.079986
45752 C -0.269013 0.977229 -0.302530
45753 O 0.236872 -2.379584 -1.019480
45754 C 0.354013 -0.404596 1.760789
45755 O 1.729631 -0.216861 -0.258290
45756 H 0.993540 -1.212612 2.104292
45757 H -0.665166 -0.590411 2.093750
45758 H 0.705626 0.536972 2.178804
45759 O 2.513885 -1.294773 0.217833
45760 H 2.367434 -1.957395 -0.474314
45761 O 0.394614 2.103839 0.227751
45762 H -0.178722 0.989531 -1.390387
45763 O 1.446738 2.492852 -0.638490
45764 H 2.142512 1.856738 -0.413092
45765 H -2.067634 2.106935 -0.341715
45766 H -1.882861 1.174195 1.160222

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45767 Rotational constants (GHz): 1.0748000 0.9144100 0.5984700
45768 Vibrational harmonic frequencies (cm-1):
45769 i2034.6029 76.4745 93.1034
45770 133.2516 153.9480 179.8919
45771 209.0426 215.9760 230.5924
45772 264.2467 300.3281 344.6620
45773 360.7275 373.1044 413.6846
45774 428.4427 440.5951 467.0217
45775 509.8635 527.5356 554.2696
45776 613.5768 702.8840 824.3090
45777 891.0038 932.2712 980.2666
45778 1023.8620 1040.3673 1047.1045
45779 1111.8766 1123.0837 1141.9864
45780 1162.6110 1169.7013 1204.5490
45781 1249.5978 1289.1424 1331.8700
45782 1378.0616 1397.8500 1406.7825
45783 1438.1401 1457.1250 1481.2743
45784 1497.5800 1504.2779 1519.5072
45785 1929.8998 3086.9892 3091.0162
45786 3097.1026 3155.5544 3167.0655
45787 3179.4028 3762.6945 3764.8174
45788 Zero-point correction (Hartree): 0.151343
45789
45790 TS.diHPCARP_Ic.16aldHshift.a.pmmdu
45791 -----
45792 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14403555
45793 Electronic state : 2-A
45794 Cartesian coordinates (Angs):
45795 O -0.467347 2.185734 0.706355
45796 H 0.210420 1.215587 1.171112
45797 C 0.599499 -0.007276 1.148621
45798 O -1.608485 1.536477 0.291554
45799 C 0.683317 -0.438817 -0.334527
45800 C -1.408654 0.978776 -0.994947
45801 C -0.698624 -0.376132 -1.032131
45802 O 0.820281 -0.670414 2.094653
45803 C 1.338592 -1.798546 -0.459761
45804 O 1.406273 0.563286 -1.024433
45805 H 0.779194 -2.544920 0.099721
45806 H 2.350300 -1.754287 -0.063322
45807 H 1.371088 -2.088038 -1.509054
45808 O 2.624043 0.787822 -0.324608
45809 H 2.531145 1.723027 -0.097607
45810 O -1.519855 -1.455407 -0.654043
45811 H -0.501455 -0.590369 -2.087775
45812 O -1.883093 -1.268142 0.712036
45813 H -1.525410 -2.067440 1.119981
45814 H -2.411235 0.830667 -1.396852
45815 H -0.863361 1.692894 -1.611850
45816 Rotational constants (GHz): 1.1282900 0.9234700 0.7740400
45817 Vibrational harmonic frequencies (cm-1):
45818 i2035.3082 49.4236 63.7235
45819 101.6302 127.9634 166.0009
45820 176.5763 213.5242 216.3099
45821 250.5962 262.3556 288.7434
45822 308.1526 310.5713 334.4713
45823 431.2859 449.4104 467.0395
45824 483.8464 532.8112 587.6467
45825 611.8287 764.3610 841.9255
45826 863.6104 933.4648 941.3119
45827 991.6966 999.5231 1044.7390
45828 1070.0430 1133.6020 1154.1361
45829 1164.1158 1177.1640 1228.2241
45830 1238.4090 1316.2853 1354.8150
45831 1367.3949 1401.6840 1412.4067
45832 1412.7650 1419.4116 1460.1301
45833 1477.7255 1493.7258 1526.4324
45834 1949.4208 3066.3669 3083.0129
45835 3087.4692 3143.8742 3163.5602
45836 3172.7275 3804.7663 3813.7999
45837 Zero-point correction (Hartree): 0.150149
45838

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45839 TS.diHPCARP_Ic.16aldHshift.a.pmmud
45840 -----
45841 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14953492
45842 Electronic state : 2-A
45843 Cartesian coordinates (Angs):
45844 O -1.395508 2.347806 0.023492
45845 H -1.817140 1.162656 -0.082605
45846 C -1.708239 -0.118390 -0.170360
45847 O -0.267786 2.320084 -0.763557
45848 C -0.381918 -0.560997 0.477094
45849 C 0.793329 1.713775 -0.050834
45850 C 0.792015 0.189443 -0.188404
45851 O -2.508047 -0.830187 -0.664853
45852 C -0.488853 -0.314110 1.976947
45853 O -0.236571 -1.956428 0.345707
45854 H -1.258240 -0.960438 2.394737
45855 H -0.750532 0.724051 2.170477
45856 H 0.466224 -0.542920 2.444218
45857 O -0.117842 -2.296139 -1.025571
45858 H -1.039045 -2.485958 -1.256815
45859 O 1.952240 -0.319456 0.445668
45860 H 0.811169 -0.077475 -1.245601
45861 O 3.054778 -0.069076 -0.411666
45862 H 3.222784 -0.951776 -0.766978
45863 H 1.710641 2.077961 -0.511718
45864 H 0.766022 2.022728 0.993864
45865 Rotational constants (GHz): 1.0014800 0.9471000 0.6219100
45866 Vibrational harmonic frequencies (cm-1):
45867 i2054.2180 53.8985 80.6724
45868 102.8069 137.3064 170.1816
45869 196.1584 218.0187 236.5155
45870 247.0003 289.4935 307.9672
45871 326.4761 361.7247 376.1622
45872 420.8861 452.3737 461.0394
45873 484.5357 517.6890 580.8205
45874 613.0211 717.8616 827.2454
45875 873.2452 943.5173 987.3768
45876 1028.8534 1032.7233 1061.6134
45877 1092.7675 1120.4544 1140.7418
45878 1160.0556 1171.9786 1219.1887
45879 1256.2253 1287.9846 1344.4334
45880 1380.7869 1400.9275 1408.4519
45881 1418.1439 1427.1424 1481.2164
45882 1494.8053 1502.1645 1513.4734
45883 1931.9168 3084.0668 3092.0808
45884 3105.0967 3151.2625 3165.4863
45885 3174.3944 3776.7037 3805.5992
45886 Zero-point correction (Hartree): 0.150848
45887 -----
45888 TS.diHPCARP_Ic.16aldHshift.a.pmpdu
45889 -----
45890 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14861530
45891 Electronic state : 2-A
45892 Cartesian coordinates (Angs):
45893 O 1.234367 -1.893139 0.788367
45894 H 0.276816 -1.081897 1.184045
45895 C -0.579702 -0.165266 1.153041
45896 O 2.089182 -1.060078 0.102254
45897 C -0.761188 0.321399 -0.305983
45898 C 1.509140 -0.696079 -1.142445
45899 C 0.587901 0.517086 -1.034815
45900 O -1.199296 0.172723 2.093454
45901 C -1.615669 1.568265 -0.355044
45902 O -1.324404 -0.769931 -1.021277
45903 H -1.113543 2.371104 0.180440
45904 H -2.578548 1.379254 0.110241
45905 H -1.762895 1.862179 -1.393699
45906 O -2.609843 -1.052122 -0.486695
45907 H -2.482019 -1.947090 -0.146290
45908 O 1.281485 1.641117 -0.530944
45909 H 0.331266 0.811308 -2.056922
45910 O 1.402619 1.511897 0.880082

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45911	H	2.146455	0.896093	0.974967	
45912	H	2.352758	-0.412529	-1.772141	
45913	H	0.993936	-1.554583	-1.571089	
45914	Rotational constants (GHz):		1.1988600	0.8516300	0.7689300
45915	Vibrational harmonic frequencies (cm-1):				
45916	i1744.5514		53.1112		94.5191
45917	123.3872		148.6211		160.9263
45918	202.5029		210.8115		252.8381
45919	261.7129		280.5394		300.6995
45920	312.8521		337.4552		403.0290
45921	424.2960		456.6265		471.1660
45922	490.4152		524.7641		592.8452
45923	605.3960		775.3556		848.8048
45924	870.0289		930.3406		941.2447
45925	993.1549		1004.7786		1045.7603
45926	1083.1229		1109.3522		1136.5462
45927	1155.4798		1174.8192		1212.7550
45928	1249.7107		1307.2331		1364.7873
45929	1371.6931		1399.4481		1408.3430
45930	1417.1116		1438.2792		1468.4544
45931	1480.7561		1493.2181		1507.1093
45932	1949.5690		3072.9026		3083.6467
45933	3089.5656		3148.2786		3163.7560
45934	3185.1826		3745.4604		3814.9152
45935	Zero-point correction (Hartree): 0.150700				
45936					
45937	TS.diHPCARP_Ic.16aldHshift.a.pmpmdu				
45938	-----				
45939	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14627425				
45940	Electronic state : 2-A				
45941	Cartesian coordinates (Angs):				
45942	O	-0.158455	2.295201	0.550258	
45943	H	0.506901	1.306726	1.049282	
45944	C	0.832232	0.080294	1.147160	
45945	O	-1.372532	1.710772	0.264494	
45946	C	0.708022	-0.555403	-0.260405	
45947	C	-1.283754	0.968599	-0.938897	
45948	C	-0.763898	-0.449520	-0.719263	
45949	O	1.120060	-0.460314	2.149161	
45950	C	1.224522	-1.978387	-0.261798	
45951	O	1.401782	0.272663	-1.170526	
45952	H	0.650712	-2.580227	0.438553	
45953	H	2.270896	-1.992548	0.032919	
45954	H	1.125651	-2.390134	-1.265305	
45955	O	2.737905	0.401899	-0.699462	
45956	H	2.799139	1.360762	-0.594935	
45957	O	-1.468775	-1.129309	0.302615	
45958	H	-0.858309	-0.997873	-1.663367	
45959	O	-2.833682	-1.203392	-0.070754	
45960	H	-3.238419	-0.601424	0.568159	
45961	H	-2.305068	0.903803	-1.310792	
45962	H	-0.664673	1.497262	-1.661577	
45963	Rotational constants (GHz):		1.1844400	0.8252500	0.6953400
45964	Vibrational harmonic frequencies (cm-1):				
45965	i1930.4275		38.4250		62.6820
45966	99.9374		114.8979		161.5844
45967	172.8037		204.6176		247.5107
45968	275.5836		284.7712		294.5799
45969	305.5712		322.7402		376.9962
45970	381.2643		435.3292		452.1585
45971	485.2219		515.5903		608.6849
45972	646.9924		761.4929		784.3374
45973	873.1781		933.6772		956.0655
45974	987.4329		1037.7091		1059.7404
45975	1071.3111		1130.3095		1153.2523
45976	1158.8223		1182.4584		1229.7599
45977	1241.0368		1298.2493		1360.4624
45978	1378.4977		1401.4043		1406.8659
45979	1415.6919		1421.4803		1473.6052
45980	1482.2906		1492.7224		1519.7351
45981	1960.2231		3049.3204		3083.9166
45982	3104.3428		3157.7503		3165.9743

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45983          3179.6979          3802.3091          3811.1157
45984 Zero-point correction (Hartree): 0.150391
45985
45986 TS.diHPCARP_Ic.16aldHshift.a.pmpmud
45987 -----
45988 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14671638
45989 Electronic state : 2-A
45990 Cartesian coordinates (Angs):
45991 O      0.329264      2.646793      0.331222
45992 H     -0.725133      1.936173      0.392835
45993 C     -1.422064      0.873072      0.241914
45994 O      0.937960      2.132694     -0.790097
45995 C     -0.516421     -0.368105      0.391757
45996 C      1.599849      0.926787     -0.457608
45997 C      0.666658     -0.279078     -0.608903
45998 O     -2.582704      0.863538      0.032156
45999 C     -0.118990     -0.443306      1.861119
46000 O     -1.276422     -1.530573      0.163940
46001 H     -1.016984     -0.468236      2.476287
46002 H      0.480270      0.421645      2.137578
46003 H      0.455971     -1.349763      2.025962
46004 O     -1.752840     -1.533123     -1.171708
46005 H     -2.625947     -1.128456     -1.063001
46006 O      1.396558     -1.485360     -0.630741
46007 H      0.233437     -0.250047     -1.609712
46008 O      2.252940     -1.522965      0.516708
46009 H      3.078500     -1.807690      0.107584
46010 H      2.401570      0.812162     -1.187737
46011 H      2.026077      1.009966      0.538698
46012 Rotational constants (GHz):      1.0164000      0.9746800      0.6453600
46013 Vibrational harmonic frequencies (cm-1):
46014 i1978.3164          44.9116          91.1371
46015      119.5585          143.2969          171.3968
46016      187.5444          200.3418          236.7817
46017      252.6154          279.5811          304.6320
46018      316.4989          355.5365          364.7056
46019      395.3781          427.3095          473.4809
46020      513.0958          556.0023          569.9867
46021      605.5519          750.7266          825.8780
46022      864.0590          944.9879          952.4771
46023      986.4178          1029.8297          1057.7224
46024      1099.7716          1111.5512          1140.6096
46025      1155.2516          1169.9098          1216.9396
46026      1251.2744          1289.0434          1334.7357
46027      1379.5844          1392.7704          1408.3172
46028      1424.9313          1428.0825          1482.6015
46029      1494.7717          1504.3122          1520.4910
46030      1930.1391          3085.1737          3095.6455
46031      3110.5921          3160.3934          3164.4611
46032      3185.9044          3775.7876          3839.1934
46033 Zero-point correction (Hartree): 0.150755
46034
46035 TS.diHPCARP_Ic.16aldHshift.a.pmpmud
46036 -----
46037 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14459675
46038 Electronic state : 2-A
46039 Cartesian coordinates (Angs):
46040 O      0.318107      2.326473      0.439301
46041 H      0.844268      1.286784      0.969533
46042 C      0.902416      0.020060      1.127263
46043 O     -0.999137      1.935219      0.337085
46044 C      0.593514     -0.632562     -0.241613
46045 C     -1.190098      1.162757     -0.834888
46046 C     -0.863682     -0.316318     -0.646966
46047 O      1.087013     -0.530219      2.148373
46048 C      0.890417     -2.117325     -0.207193
46049 O      1.349574      0.040286     -1.227563
46050 H      0.311438     -2.594824      0.579191
46051 H      1.948323     -2.273751     -0.009218
46052 H      0.636298     -2.555257     -1.171699
46053 O      2.706941      0.040793     -0.804440
46054 H      2.873977      0.990974     -0.739914

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46055      O      -1.648177      -0.903231      0.371565
46056      H      -1.051076      -0.829345      -1.597372
46057      O      -2.997878      -0.876515      -0.075061
46058      H      -3.229393      -1.811096      -0.013495
46059      H      -2.253520      1.243397      -1.056335
46060      H      -0.607255      1.580983      -1.654392
46061      Rotational constants (GHz):      1.1580100      0.8355400      0.6908100
46062      Vibrational harmonic frequencies (cm-1):
46063      i1995.9221      60.3384      74.0917
46064      98.4110      116.9735      153.0605
46065      166.5859      176.6723      210.7613
46066      246.4952      272.6558      281.0667
46067      288.4368      313.7017      373.9056
46068      382.3707      442.9037      452.8938
46069      491.2946      511.7851      611.4512
46070      644.0280      758.7008      794.3600
46071      875.1767      934.1231      953.4368
46072      988.1352      1037.3055      1056.0242
46073      1067.3254      1131.0094      1154.8076
46074      1164.0756      1183.8617      1233.5943
46075      1240.2174      1305.1360      1366.3873
46076      1370.4203      1402.5970      1405.7033
46077      1414.5158      1421.3197      1469.6526
46078      1482.8998      1493.9729      1531.7671
46079      1958.6704      3039.9383      3081.8023
46080      3099.6900      3155.7720      3163.0238
46081      3177.3031      3804.7197      3832.1427
46082      Zero-point correction (Hartree): 0.150176
46083
46084      TS.diHPCARP_Ic.16aldHshift.a.pmppud
46085      -----
46086      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14754758
46087      Electronic state : 2-A
46088      Cartesian coordinates (Angs):
46089      O      2.642238      0.460045      0.272961
46090      H      1.682996      1.277908      0.133507
46091      C      0.434439      1.630877      0.044770
46092      O      2.415187      -0.466035      -0.717398
46093      C      -0.403994      0.388762      0.405993
46094      C      1.384387      -1.357415      -0.329799
46095      C      0.010133      -0.730411      -0.593679
46096      O      0.028566      2.701099      -0.236258
46097      C      -0.149849      0.131157      1.889726
46098      O      -1.779779      0.667591      0.311290
46099      H      -0.549039      0.968901      2.459781
46100      H      0.917451      0.052575      2.080248
46101      H      -0.634214      -0.786291      2.205738
46102      O      -2.102577      0.987804      -1.032870
46103      H      -2.025104      1.953379      -1.021985
46104      O      -0.989891      -1.704863      -0.747473
46105      H      0.045418      -0.292024      -1.593424
46106      O      -1.214509      -2.353080      0.498874
46107      H      -2.087363      -2.004245      0.725671
46108      H      1.481850      -2.219043      -0.988778
46109      H      1.523425      -1.669463      0.704163
46110      Rotational constants (GHz):      1.0626000      0.9645200      0.6535000
46111      Vibrational harmonic frequencies (cm-1):
46112      i2077.7561      52.8795      93.8046
46113      121.2223      154.8849      168.7778
46114      187.5193      218.6286      239.8800
46115      286.4519      308.8108      325.8454
46116      353.7363      369.3721      372.7283
46117      406.0385      409.2016      451.6395
46118      507.9155      544.8946      565.5527
46119      611.1128      770.6849      829.0499
46120      861.5209      950.1962      960.9731
46121      984.7956      1026.4199      1060.0345
46122      1081.1667      1120.8396      1137.0519
46123      1156.7805      1189.1293      1232.7913
46124      1258.1367      1279.6906      1331.0531
46125      1379.9456      1399.7834      1409.9062
46126      1426.1232      1430.0121      1484.2534

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46127      1492.1068      1504.4226      1514.6214
46128      1934.9406      3091.2561      3093.2548
46129      3098.2475      3155.1978      3168.7478
46130      3199.2220      3774.5464      3797.7578
46131 Zero-point correction (Hartree): 0.151124
46132
46133 TS.diHPCARP_Ic.16aldHshift.a.pmtmud
46134 -----
46135 IRC pathway available
46136 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17791662
46137 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05638515
46138 T1 diagnostic: 0.021591
46139 E(MP2/Aug-CC-pVTZ) (Hartree): -721.01460258
46140 E(MP3/Aug-CC-pVTZ) (Hartree): -721.03160618
46141 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.02194556
46142 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03608307
46143 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48412950
46144 E(UHF/Aug-CC-pVTZ) (Hartree): -718.47375750
46145 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15232754
46146 Electronic state : 2-A
46147 Cartesian coordinates (Angs):
46148 O      2.780333      -0.074702      0.034528
46149 H      1.984933      0.902932      -0.035620
46150 C      0.820980      1.457323      -0.090156
46151 O      2.207553      -0.971232      -0.836831
46152 C      -0.206942      0.466599      0.471468
46153 C      1.150538      -1.659462      -0.196450
46154 C      -0.167704      -0.886242      -0.284953
46155 O      0.604012      2.547345      -0.485880
46156 C      0.069194      0.316450      1.962025
46157 O      -1.507411      1.025597      0.397539
46158 H      -0.136950      1.257939      2.467243
46159 H      1.109183      0.042830      2.126515
46160 H      -0.578355      -0.460105      2.363748
46161 O      -1.840614      1.279957      -0.960101
46162 H      -1.546441      2.197626      -1.061750
46163 O      -1.140463      -1.738026      0.283708
46164 H      -0.411410      -0.715778      -1.333397
46165 O      -2.369366      -1.585648      -0.405296
46166 H      -2.735497      -0.783578      -0.003695
46167 H      1.021161      -2.588116      -0.749408
46168 H      1.424641      -1.888083      0.833423
46169 Rotational constants (GHz): 1.1279800      0.9034700      0.6368900
46170 Vibrational harmonic frequencies (cm-1):
46171 i2035.9610      77.9861      96.3514
46172 131.3049      149.8514      181.2628
46173 206.4909      216.9456      248.3060
46174 273.0431      295.4988      336.3283
46175 351.5022      382.0554      413.4501
46176 429.2314      430.6162      473.6193
46177 510.1304      525.3416      559.7662
46178 619.2934      704.4811      821.8480
46179 879.3700      941.2149      977.3167
46180 1026.8487      1032.9245      1052.7880
46181 1107.2214      1122.2759      1138.6774
46182 1157.5861      1173.8379      1214.6878
46183 1248.8501      1287.6277      1334.5467
46184 1377.7493      1397.8409      1406.7198
46185 1426.4178      1435.8366      1482.7787
46186 1496.9287      1502.4892      1520.9029
46187 1931.0847      3083.7761      3092.8294
46188 3115.0236      3154.4244      3165.7888
46189 3172.4747      3769.4692      3771.8098
46190 Zero-point correction (Hartree): 0.151350
46191
46192 TS.diHPCARP_Ic.16aldHshift.a.pmpmdu
46193 -----
46194 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14774006
46195 Electronic state : 2-A
46196 Cartesian coordinates (Angs):
46197 O      1.308101      -1.890502      0.766120
46198 H      0.308270      -1.138141      1.150662

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46199	C	-0.560399	-0.229362	1.153038		
46200	O	2.114541	-1.016099	0.071464		
46201	C	-0.770861	0.304509	-0.286831		
46202	C	1.499555	-0.675065	-1.162791		
46203	C	0.562106	0.524121	-1.038482		
46204	O	-1.149683	0.100948	2.114649		
46205	C	-1.622106	1.555090	-0.271303		
46206	O	-1.350417	-0.759057	-1.031608		
46207	H	-1.103826	2.340461	0.274255		
46208	H	-2.568479	1.359951	0.226922		
46209	H	-1.798152	1.887575	-1.294528		
46210	O	-2.552717	-1.167128	-0.400167		
46211	H	-3.225918	-0.776949	-0.972073		
46212	O	1.247167	1.657342	-0.543726		
46213	H	0.284412	0.817208	-2.055759		
46214	O	1.385246	1.530885	0.865976		
46215	H	2.127711	0.911667	0.952467		
46216	H	2.321133	-0.382377	-1.817020		
46217	H	0.987178	-1.546271	-1.568385		
46218	Rotational constants (GHz):			1.1987400	0.8500200	0.7684300
46219	Vibrational harmonic frequencies (cm-1):					
46220	i1786.1985		65.4730			96.2872
46221	120.3053		154.3512			162.0033
46222	207.4571		213.8972			249.5261
46223	275.2687		285.0581			300.9061
46224	313.7125		339.3647			400.8386
46225	433.0276		457.4390			472.6269
46226	494.8701		524.6396			595.2000
46227	598.8557		779.6224			848.2015
46228	869.1325		930.3360			942.5047
46229	993.9262		1004.4323			1046.8913
46230	1084.3443		1098.2942			1132.8067
46231	1155.2637		1172.5036			1208.4380
46232	1252.3543		1308.1135			1363.7331
46233	1372.8826		1399.7068			1405.5737
46234	1410.3878		1442.0604			1467.6868
46235	1482.1193		1497.2728			1510.6208
46236	1953.2401		3069.0613			3077.5198
46237	3088.8046		3148.8618			3159.9221
46238	3174.3874		3739.8393			3816.8687
46239	Zero-point correction (Hartree):			0.150744		
46240						
46241	TS.diHPCARP_Ic.16aldHshift.a.pppmdu					
46242	-----					
46243	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14500009					
46244	Electronic state : 2-A					
46245	Cartesian coordinates (Angs):					
46246	O	-0.650363	2.224335	0.569255		
46247	H	0.173727	1.357571	1.042214		
46248	C	0.767734	0.236146	1.159781		
46249	O	-1.704088	1.449505	0.138065		
46250	C	0.797522	-0.460346	-0.226426		
46251	C	-1.343945	0.768728	-1.050561		
46252	C	-0.651490	-0.560486	-0.750646		
46253	O	1.186592	-0.193465	2.169747		
46254	C	1.473585	-1.812797	-0.142944		
46255	O	1.431078	0.419620	-1.135823		
46256	H	0.902036	-2.468226	0.509904		
46257	H	2.476052	-1.712664	0.265940		
46258	H	1.519837	-2.250770	-1.140205		
46259	O	2.730479	0.706658	-0.643701		
46260	H	3.292301	0.189069	-1.234497		
46261	O	-1.303348	-1.276452	0.285079		
46262	H	-0.637395	-1.155403	-1.671157		
46263	O	-2.683673	-1.366979	-0.009848		
46264	H	-3.042448	-0.658566	0.544701		
46265	H	-2.281853	0.561786	-1.561987		
46266	H	-0.716096	1.403956	-1.672320		
46267	Rotational constants (GHz):			1.2259700	0.7988500	0.6950800
46268	Vibrational harmonic frequencies (cm-1):					
46269	i1962.2821		49.3545			65.5460
46270	101.8557		108.4235			159.1028

46271	162.8356	203.9152	238.9827			
46272	265.1086	280.6242	296.2869			
46273	314.6145	380.7949	383.2233			
46274	408.7151	419.6289	447.3826			
46275	482.4359	520.4395	603.5796			
46276	647.7393	763.3420	783.9850			
46277	871.1390	936.6873	957.3407			
46278	988.0422	1036.8710	1060.5022			
46279	1075.7186	1121.6727	1133.1839			
46280	1157.3161	1180.5882	1219.0407			
46281	1244.7787	1295.0564	1352.0449			
46282	1382.9634	1400.3686	1403.4062			
46283	1408.0207	1427.5943	1478.2727			
46284	1485.0305	1496.4852	1508.2646			
46285	1958.1062	3040.6593	3077.2514			
46286	3108.7865	3159.9819	3163.5829			
46287	3174.9723	3772.3346	3816.1289			
46288	Zero-point correction (Hartree): 0.150314					
46289						
46290	TS.diHPCARP_Ic.16aldHshift.a.pptmud					
46291	-----					
46292	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14901999					
46293	Electronic state : 2-A					
46294	Cartesian coordinates (Angs):					
46295	O	2.793211	-0.123381	0.016869		
46296	H	1.978760	0.884172	-0.107167		
46297	C	0.856138	1.465714	-0.127261		
46298	O	2.209628	-1.054552	-0.809025		
46299	C	-0.202291	0.496693	0.438573		
46300	C	1.133896	-1.677441	-0.141583		
46301	C	-0.161734	-0.870875	-0.287120		
46302	O	0.695626	2.584457	-0.446056		
46303	C	0.069665	0.377419	1.933144		
46304	O	-1.490677	1.066388	0.345677		
46305	H	-0.171699	1.322549	2.415146		
46306	H	1.117593	0.143709	2.110040		
46307	H	-0.550299	-0.412622	2.353093		
46308	O	-1.810266	1.286771	-1.018940		
46309	H	-2.286032	0.470548	-1.240119		
46310	O	-1.155363	-1.727482	0.250935		
46311	H	-0.349344	-0.725712	-1.352051		
46312	O	-2.422407	-1.407870	-0.309350		
46313	H	-2.844485	-0.940727	0.425719		
46314	H	0.980824	-2.631894	-0.642494		
46315	H	1.392634	-1.853729	0.902435		
46316	Rotational constants (GHz):			1.1461500	0.8947700	0.6333200
46317	Vibrational harmonic frequencies (cm-1):					
46318	i1824.1786		78.4275			98.3514
46319	140.1477		158.6219			185.6948
46320	205.5312		222.4694			254.6523
46321	269.5994		280.5718			326.7284
46322	353.2608		385.3545			388.6247
46323	412.2289		463.7391			510.4102
46324	530.1147		552.5304			558.0026
46325	616.6938		706.6669			817.2304
46326	878.4047		945.8400			976.6850
46327	1024.0208		1036.2802			1057.9568
46328	1103.2254		1117.5116			1136.5310
46329	1162.7190		1172.0833			1222.4775
46330	1257.0405		1290.0662			1337.9147
46331	1382.5629		1401.3560			1408.5866
46332	1419.0772		1451.0484			1484.8244
46333	1495.0024		1504.2570			1518.4668
46334	1958.4789		3081.5129			3091.6590
46335	3099.2307		3152.2327			3164.0185
46336	3168.4529		3738.1812			3788.0695
46337	Zero-point correction (Hartree): 0.151593					
46338						
46339	TS.diHPCARP_Ic.16aldHshift.a.pptpud					
46340	-----					
46341	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14724390					
46342	Electronic state : 2-A					


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46343 Cartesian coordinates (Angs):
46344 O 2.787609 -0.273899 -0.030461
46345 H 2.023128 0.785366 -0.161672
46346 C 0.937965 1.422630 -0.183152
46347 O 2.123064 -1.187903 -0.813206
46348 C -0.160594 0.542701 0.452280
46349 C 1.028494 -1.722043 -0.101457
46350 C -0.219751 -0.841771 -0.241174
46351 O 0.831630 2.529571 -0.560931
46352 C 0.157716 0.440946 1.939259
46353 O -1.404829 1.190938 0.396198
46354 H -0.002198 1.412593 2.402051
46355 H 1.191981 0.138974 2.090091
46356 H -0.508832 -0.288029 2.396028
46357 O -1.793571 1.352831 -0.958737
46358 H -2.432329 0.629245 -1.044045
46359 O -1.259386 -1.613146 0.342024
46360 H -0.424123 -0.705760 -1.303496
46361 O -2.496480 -1.289782 -0.281034
46362 H -2.725121 -2.131167 -0.695330
46363 H 0.807834 -2.680220 -0.569889
46364 H 1.302370 -1.884661 0.940897
46365 Rotational constants (GHz): 1.1368300 0.8913800 0.6305900
46366 Vibrational harmonic frequencies (cm-1):
46367 i1761.6336 77.3679 92.9265
46368 136.0315 147.2608 183.6419
46369 209.9503 222.3055 251.4776
46370 267.7499 277.2724 296.2126
46371 330.2831 350.7496 384.6700
46372 410.4861 464.6160 476.3777
46373 511.7057 526.3145 558.6010
46374 614.9547 705.9003 817.2406
46375 874.4672 949.0125 979.7969
46376 1021.9850 1036.2359 1061.4044
46377 1098.3795 1113.8968 1136.2133
46378 1160.9661 1170.2888 1227.0100
46379 1258.7112 1288.6516 1339.3540
46380 1379.0520 1398.4718 1404.3152
46381 1411.7641 1451.4452 1482.5511
46382 1497.6291 1504.0964 1521.2173
46383 1957.3798 3082.5009 3090.1608
46384 3105.2353 3148.2297 3165.6886
46385 3170.0516 3766.5669 3823.2884
46386 Zero-point correction (Hartree): 0.151248
46387
46388 TS.diHPCARP_Ic.16aldHshift.a.ttmpdu
46389 -----
46390 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14701083
46391 Electronic state : 2-A
46392 Cartesian coordinates (Angs):
46393 O -1.776322 -0.514236 -1.627560
46394 H -0.866186 0.385580 -1.491568
46395 C 0.140077 1.020544 -1.050871
46396 O -2.162094 -0.786522 -0.333713
46397 C 0.874646 0.179345 0.025658
46398 C -1.122204 -1.480683 0.344345
46399 C -0.106625 -0.535006 0.980058
46400 O 0.492908 2.057630 -1.476563
46401 C 1.877213 1.032117 0.771446
46402 O 1.487735 -0.792700 -0.819921
46403 H 1.358803 1.838964 1.284947
46404 H 2.589002 1.462095 0.069860
46405 H 2.400504 0.427086 1.510187
46406 O 2.174339 -1.732075 -0.000847
46407 H 3.094654 -1.539340 -0.219181
46408 O -0.737835 0.390475 1.845599
46409 H 0.508547 -1.134388 1.654992
46410 O -1.310369 1.431500 1.062710
46411 H -2.141194 1.032267 0.759185
46412 H -1.625015 -2.018972 1.147603
46413 H -0.644657 -2.183773 -0.337470
46414 Rotational constants (GHz): 1.1071700 0.8673300 0.8071900

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46415 Vibrational harmonic frequencies (cm-1):
46416 i1915.6632 58.7123 101.8364
46417 128.3141 147.5094 176.2101
46418 210.6119 220.1942 240.2833
46419 260.4200 275.4824 306.2690
46420 316.5777 335.1181 379.4774
46421 422.4856 480.0461 490.0589
46422 498.4594 531.0575 577.2877
46423 636.9061 760.1922 835.2720
46424 888.3624 920.5537 939.5383
46425 995.0625 998.6923 1028.4361
46426 1077.5173 1107.9422 1130.5252
46427 1149.5950 1173.8471 1207.7383
46428 1246.6502 1309.2326 1370.8297
46429 1372.7685 1399.4716 1401.5579
46430 1407.7158 1436.3634 1467.6463
46431 1488.4134 1491.6668 1504.5277
46432 1952.4917 3080.8432 3087.9865
46433 3097.6606 3150.1210 3161.3028
46434 3169.7429 3743.8508 3822.2475
46435 Zero-point correction (Hartree): 0.150746
46436
46437 TS.diHPCARP_Ic.16aldHshift.b.mppud
46438 -----
46439 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14644410
46440 Electronic state : 2-A
46441 Cartesian coordinates (Angs):
46442 O -2.127832 -1.693324 -0.330884
46443 H -0.877004 -1.928024 -0.261219
46444 C 0.376620 -1.604630 -0.241283
46445 O -2.271779 -0.717315 0.626198
46446 C 0.507473 -0.110054 0.144555
46447 C -1.987094 0.555374 0.069547
46448 C -0.629625 0.606932 -0.635287
46449 O 1.256872 -2.316230 -0.573263
46450 C 0.474070 -0.000747 1.665791
46451 O 1.695161 0.415937 -0.421235
46452 H 1.333385 -0.518700 2.082662
46453 H -0.434345 -0.452199 2.055970
46454 H 0.508940 1.045183 1.957893
46455 O 2.830930 -0.136138 0.219983
46456 H 2.968504 -0.949535 -0.288644
46457 O -0.319084 1.932159 -0.992083
46458 H -0.716811 0.128077 -1.613013
46459 O 0.004344 2.673307 0.175120
46460 H 0.971903 2.642686 0.143132
46461 H -2.761143 0.842200 -0.642729
46462 H -1.990994 1.241899 0.915322
46463 Rotational constants (GHz): 1.0981500 0.9543300 0.6220700
46464 Vibrational harmonic frequencies (cm-1):
46465 i2079.7496 75.5943 109.0090
46466 142.4432 146.2771 168.7039
46467 204.6292 224.5628 255.8505
46468 274.5824 292.8829 312.5903
46469 344.0938 368.7268 380.5061
46470 399.0536 409.5724 448.0693
46471 503.6114 536.1224 589.9757
46472 633.3059 727.9497 819.0303
46473 868.3638 931.1045 975.4994
46474 992.4678 1027.4704 1044.9018
46475 1080.9496 1125.6900 1135.2591
46476 1162.2200 1176.1456 1212.7851
46477 1242.4343 1281.0637 1346.3515
46478 1386.2136 1402.3059 1423.0938
46479 1428.9429 1442.5554 1490.3901
46480 1498.2641 1505.8026 1564.3582
46481 1929.7779 3086.7851 3088.3791
46482 3099.6345 3151.8589 3180.6292
46483 3184.7572 3764.8830 3772.7431
46484 Zero-point correction (Hartree): 0.151205
46485
46486 TS.diHPCARP_Ic.16aldHshift.b.mptmud

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46487 -----
46488 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14927485
46489 Electronic state : 2-A
46490 Cartesian coordinates (Angs):
46491 O -2.443155 -1.076843 -0.710270
46492 H -1.275306 -1.588738 -0.659277
46493 C -0.012439 -1.571801 -0.452366
46494 O -2.445414 -0.379939 0.473386
46495 C 0.415620 -0.260603 0.249089
46496 C -1.893657 0.905490 0.270302
46497 C -0.464022 0.895259 -0.288288
46498 O 0.724628 -2.407471 -0.843394
46499 C 0.358438 -0.407715 1.761160
46500 O 1.718285 0.066945 -0.218059
46501 H 1.072354 -1.154964 2.093694
46502 H -0.640489 -0.702054 2.073767
46503 H 0.615377 0.553210 2.206010
46504 O 2.688225 -0.803981 0.330945
46505 H 2.647044 -1.554552 -0.281690
46506 O 0.058450 2.141313 0.119098
46507 H -0.474033 0.859850 -1.378433
46508 O 0.981276 2.615658 -0.844832
46509 H 1.783030 2.122496 -0.614634
46510 H -2.527612 1.492455 -0.393350
46511 H -1.882365 1.363052 1.259541
46512 Rotational constants (GHz): 1.0698200 0.9204000 0.6116000
46513 Vibrational harmonic frequencies (cm-1):
46514 i2032.0345 62.9977 96.2189
46515 156.8085 178.6747 187.8268
46516 193.9543 221.1889 249.2329
46517 263.3524 309.9406 317.8891
46518 354.9124 365.4150 389.5798
46519 428.6632 439.1814 448.0644
46520 495.7604 513.8056 563.5404
46521 639.7424 713.7815 818.3733
46522 886.3043 934.4547 971.5337
46523 1014.9711 1034.6663 1046.9739
46524 1078.2945 1107.1359 1144.4454
46525 1168.3662 1182.9451 1204.5717
46526 1247.2427 1291.6192 1339.1726
46527 1385.8219 1401.6652 1413.6028
46528 1444.6703 1454.8818 1485.0622
46529 1499.0775 1502.3517 1565.6390
46530 1925.1305 3085.1639 3090.4414
46531 3098.1777 3148.0176 3166.6803
46532 3184.3697 3756.2014 3769.8528
46533 Zero-point correction (Hartree): 0.151358
46534
46535 TS.diHPCARP_Ic.16aldHshift.b.pmppud
46536 -----
46537 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14910691
46538 Electronic state : 2-A
46539 Cartesian coordinates (Angs):
46540 O 2.504898 0.704183 -0.653197
46541 H 1.529076 1.435578 -0.297808
46542 C 0.297736 1.678246 0.034592
46543 O 2.406268 -0.333819 0.243465
46544 C -0.383174 0.339478 0.409594
46545 C 1.495764 -1.308076 -0.239587
46546 C 0.134754 -0.711300 -0.608315
46547 O -0.228852 2.730152 -0.027717
46548 C -0.097366 0.081605 1.886930
46549 O -1.784257 0.473050 0.332462
46550 H -0.552580 0.878598 2.472623
46551 H 0.973488 0.072471 2.070733
46552 H -0.519501 -0.873460 2.185092
46553 O -2.146931 0.827306 -0.993422
46554 H -2.243402 1.787417 -0.911722
46555 O -0.796838 -1.732763 -0.863264
46556 H 0.209079 -0.229053 -1.584030
46557 O -1.127997 -2.386017 0.355215
46558 H -1.982662 -1.975626 0.549649

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46559      H      1.908753      -1.815274      -1.111762
46560      H      1.381141      -2.017105      0.579601
46561      Rotational constants (GHz):      1.0710600      0.9953900      0.6648200
46562      Vibrational harmonic frequencies (cm-1):
46563      i2067.8612      81.2493      112.9203
46564      149.3649      157.0044      170.6189
46565      183.7872      223.4540      238.9183
46566      271.9647      294.4512      327.3072
46567      344.6400      364.2629      374.6366
46568      400.4494      420.3040      435.7236
46569      482.6095      556.6386      584.4671
46570      657.6107      737.4061      826.6028
46571      861.0807      944.1200      974.8507
46572      990.8559      1007.4110      1056.6240
46573      1076.9270      1122.5322      1133.3653
46574      1158.8293      1178.3506      1203.3027
46575      1257.7722      1284.1964      1346.3769
46576      1382.7130      1402.8596      1416.6750
46577      1426.0756      1429.4385      1493.0088
46578      1495.1074      1508.3126      1565.6803
46579      1938.0536      3085.7690      3090.5665
46580      3103.6042      3149.8057      3168.7762
46581      3189.6831      3779.6365      3785.5323
46582      Zero-point correction (Hartree): 0.151280
46583
46584      TS.diHPCARP_Ic.16aldHshift.b.pmtmud
46585      -----
46586      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15111359
46587      Electronic state : 2-A
46588      Cartesian coordinates (Angs):
46589      O      2.511634      0.081587      -0.989197
46590      H      1.737361      1.028626      -0.650881
46591      C      0.661413      1.533239      -0.164606
46592      O      2.391501      -0.730006      0.113434
46593      C      -0.202774      0.429204      0.483530
46594      C      1.296670      -1.608501      -0.059946
46595      C      -0.045599      -0.899527      -0.289617
46596      O      0.353299      2.666099      -0.273659
46597      C      0.143651      0.312667      1.961306
46598      O      -1.557405      0.848769      0.474454
46599      H      -0.097212      1.246636      2.464563
46600      H      1.201257      0.096202      2.088650
46601      H      -0.449915      -0.492305      2.392294
46602      O      -1.951956      1.143802      -0.859842
46603      H      -1.859356      2.107568      -0.877047
46604      O      -0.998857      -1.831912      0.180417
46605      H      -0.219032      -0.724928      -1.350795
46606      O      -2.188470      -1.730331      -0.580206
46607      H      -2.641607      -0.983673      -0.161777
46608      H      1.487053      -2.294034      -0.884872
46609      H      1.243330      -2.170661      0.872651
46610      Rotational constants (GHz):      1.1063400      0.9327600      0.6483100
46611      Vibrational harmonic frequencies (cm-1):
46612      i2040.6513      71.0471      90.0330
46613      160.9176      170.6014      176.5005
46614      215.6917      220.8237      231.8938
46615      264.6683      286.1427      331.3315
46616      346.1891      370.1126      383.9938
46617      407.0512      434.9552      447.9957
46618      489.1640      511.5788      577.2628
46619      650.9950      717.5969      826.9172
46620      877.7416      940.5410      971.8431
46621      1000.9117      1033.7884      1046.1572
46622      1073.2026      1102.9007      1141.5970
46623      1162.1564      1188.9973      1196.8472
46624      1256.9682      1291.0484      1340.0538
46625      1381.9039      1399.9055      1411.7261
46626      1413.2685      1432.7514      1487.4409
46627      1497.0019      1502.7258      1562.8035
46628      1933.8226      3082.2437      3089.2330
46629      3113.9367      3146.3057      3161.8650
46630      3178.0891      3778.6989      3782.2066

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46631 Zero-point correction (Hartree): 0.151189
46632
46633 TS.diHPCARP_Ic.16aldHshift.b.pppud
46634 -----
46635 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14822747
46636 Electronic state : 2-A
46637 Cartesian coordinates (Angs):
46638 O 2.570115 -0.116194 -0.746428
46639 H 1.852315 0.919698 -0.437563
46640 C 0.805053 1.542845 -0.030541
46641 O 2.196674 -1.006460 0.234959
46642 C -0.250011 0.481686 0.389840
46643 C 1.024108 -1.696589 -0.161466
46644 C -0.083142 -0.725118 -0.565791
46645 O 0.685652 2.708591 0.017608
46646 C -0.039146 0.226852 1.879867
46647 O -1.555396 1.004438 0.290102
46648 H -0.273830 1.142996 2.418926
46649 H 0.995264 -0.044990 2.074294
46650 H -0.686415 -0.574693 2.225054
46651 O -1.807075 1.367066 -1.059516
46652 H -2.203035 0.555025 -1.410445
46653 O -1.307775 -1.396485 -0.785129
46654 H 0.141394 -0.340189 -1.561850
46655 O -1.798585 -1.910094 0.445796
46656 H -2.396105 -1.200712 0.724778
46657 H 1.236615 -2.366928 -0.994899
46658 H 0.723742 -2.275158 0.711113
46659 Rotational constants (GHz): 1.0760700 0.9875000 0.6678900
46660 Vibrational harmonic frequencies (cm-1):
46661 i1917.3977 74.9687 120.6616
46662 147.4621 157.7556 187.3277
46663 207.2669 226.6778 238.6124
46664 271.4127 295.6935 329.3807
46665 360.3136 369.4942 399.5810
46666 420.6668 438.7464 474.9052
46667 486.5405 554.2440 576.7102
46668 653.6034 736.3174 821.7172
46669 860.6879 945.3766 974.6135
46670 991.3186 1010.0993 1055.5854
46671 1081.5210 1122.8933 1130.7771
46672 1153.4642 1178.3113 1206.2265
46673 1258.5629 1286.9790 1354.5003
46674 1382.1896 1405.3722 1417.1707
46675 1429.4738 1440.2771 1493.4423
46676 1497.6343 1510.0599 1571.7777
46677 1965.4751 3085.6322 3089.7543
46678 3099.5501 3151.3801 3169.2657
46679 3182.3496 3768.2699 3771.5983
46680 Zero-point correction (Hartree): 0.151707
46681
46682 TS.diHPCARP_Ic.16aldHshift.e.mppmdu
46683 -----
46684 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14577406
46685 Electronic state : 2-A
46686 Cartesian coordinates (Angs):
46687 O 1.376976 -1.457655 1.092425
46688 H 0.458321 -0.624355 1.502937
46689 C -0.675977 -0.127300 1.231647
46690 O 0.734822 -1.926783 -0.033548
46691 C -0.676124 0.654987 -0.110951
46692 C 1.020809 -1.081238 -1.134231
46693 C 0.558353 0.380666 -1.002686
46694 O -1.637064 -0.355163 1.870759
46695 C -0.811862 2.135643 0.224018
46696 O -1.870041 0.351343 -0.800431
46697 H 0.008737 2.462137 0.854892
46698 H -1.761079 2.290706 0.732199
46699 H -0.795858 2.706737 -0.702538
46700 O -1.879574 -1.025630 -1.141497
46701 H -2.426674 -1.402756 -0.437713
46702 O 1.633842 1.261192 -0.721308

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46703      H      0.261736      0.711517      -2.001266
46704      O      1.986810      1.201329      0.652623
46705      H      2.400921      0.327436      0.743235
46706      H      2.096492      -1.081279     -1.328561
46707      H      0.500043      -1.555755     -1.962138
46708      Rotational constants (GHz):      1.1336400      0.9395200      0.8153100
46709      Vibrational harmonic frequencies (cm-1):
46710      i1898.1384      56.7240      98.8277
46711      150.5186      167.2809      196.3732
46712      216.8335      228.9371      239.3882
46713      265.9075      294.0761      322.0149
46714      355.0252      365.2182      397.5727
46715      416.6574      434.5934      470.9515
46716      507.8171      559.1182      617.6688
46717      666.7769      759.6159      807.6890
46718      850.0649      943.0481      963.0688
46719      992.0381      1039.1097     1052.1536
46720      1061.8370     1117.7263     1134.6305
46721      1173.3118     1180.7071     1227.6961
46722      1236.9862     1300.7191     1350.9072
46723      1369.4934     1403.4239     1411.1909
46724      1416.0456     1461.2704     1480.4504
46725      1489.9435     1497.2454     1599.2140
46726      1941.1544     3065.9291     3085.4865
46727      3087.1441     3157.9400     3166.1298
46728      3191.8651     3722.3645     3785.0142
46729      Zero-point correction (Hartree): 0.151614
46730
46731      TS.diHPCARP_Ic.16aldHshift.e.pmpmpdu
46732      -----
46733      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14484012
46734      Electronic state : 2-A
46735      Cartesian coordinates (Angs):
46736      O      1.746634      -1.183577      1.079446
46737      H      0.600835      -0.637443      1.423910
46738      C      -0.518630      -0.122538      1.206425
46739      O      1.340071      -1.783123      -0.088340
46740      C      -0.696381      0.326765      -0.276586
46741      C      1.449893      -0.868547      -1.163117
46742      C      0.632142      0.426887      -1.047016
46743      O      -1.361765      -0.062494      2.026687
46744      C      -1.464879      1.632260      -0.321355
46745      O      -1.359600      -0.738423      -0.950588
46746      H      -0.868971      2.419099      0.135277
46747      H      -2.404355      1.531711      0.212381
46748      H      -1.663063      1.887793      -1.361841
46749      O      -2.703972      -0.825392      -0.521434
46750      H      -2.667432      -1.529097      0.140905
46751      O      1.397094      1.546330      -0.636615
46752      H      0.362094      0.706081      -2.068867
46753      O      1.501123      1.594404      0.777470
46754      H      2.160146      0.907299      0.970602
46755      H      2.496884      -0.595052     -1.317309
46756      H      1.094311      -1.441158     -2.018174
46757      Rotational constants (GHz):      1.2087300      0.8441800      0.7776400
46758      Vibrational harmonic frequencies (cm-1):
46759      i1829.7674      30.9197      110.1076
46760      129.3786      146.1349      162.6753
46761      173.3541      223.5936      246.5074
46762      269.8449      283.2449      307.8929
46763      323.3951      352.8082      378.2195
46764      425.8548      458.9413      474.6652
46765      526.1793      546.3742      577.1653
46766      641.1437      765.0052      802.9255
46767      847.8614      925.7214      968.3997
46768      999.5350      1046.7454     1050.6576
46769      1062.9535     1118.0364     1144.0040
46770      1161.2259     1186.9464     1206.1373
46771      1256.7634     1302.0253     1364.1823
46772      1380.4233     1404.9502     1412.6658
46773      1428.1320     1449.1362     1473.6804
46774      1483.6593     1498.3337     1547.3270

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46775      1935.2114      3065.0354      3080.5549
46776      3085.6064      3143.0547      3165.3421
46777      3192.2652      3719.5297      3795.0041
46778 Zero-point correction (Hartree): 0.150946
46779
46780 TS.diHPCARP_Ic.16aldHshift.e.pptmud
46781 -----
46782 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14973277
46783 Electronic state : 2-A
46784 Cartesian coordinates (Angs):
46785 O      2.426351      -0.404054      -1.077155
46786 H      1.780610      0.706959      -0.830463
46787 C      0.931707      1.401984      -0.204812
46788 O      2.231066      -1.047935      0.123670
46789 C      -0.152031      0.490241      0.447344
46790 C      1.021492      -1.774465      0.068406
46791 C      -0.186426      -0.884738      -0.245724
46792 O      0.988436      2.569013      -0.094664
46793 C      0.104518      0.412458      1.943538
46794 O      -1.402234      1.137948      0.323788
46795 H      -0.005354      1.405812      2.372688
46796 H      1.110808      0.048184      2.137983
46797 H      -0.620328      -0.261931      2.397615
46798 O      -1.646925      1.398592      -1.050823
46799 H      -2.131317      0.600854      -1.318010
46800 O      -1.281938      -1.655990      0.216799
46801 H      -0.274569      -0.751330      -1.324333
46802 O      -2.468697      -1.254432      -0.457322
46803 H      -2.935536      -0.785443      0.248636
46804 H      1.086949      -2.571053      -0.672105
46805 H      0.904699      -2.210065      1.061128
46806 Rotational constants (GHz):      1.1198900      0.9269100      0.6562900
46807 Vibrational harmonic frequencies (cm-1):
46808 i1816.7582      64.4044      103.3896
46809      151.9976      177.8096      193.6046
46810      210.7607      227.5079      234.6597
46811      267.6461      272.0408      318.7367
46812      348.1842      376.4894      392.4690
46813      419.8414      462.8764      491.9427
46814      512.1584      558.5269      578.6092
46815      660.8343      701.4737      817.4159
46816      876.4941      945.6752      976.7141
46817      1006.0106      1026.5432      1050.4614
46818      1091.7938      1104.3725      1134.4973
46819      1157.7324      1186.2206      1201.9925
46820      1268.2518      1291.7180      1347.2304
46821      1387.5290      1403.2222      1416.1039
46822      1416.2705      1445.5945      1487.7527
46823      1495.9189      1503.4669      1573.9906
46824      1961.5786      3080.3481      3087.0329
46825      3103.7292      3143.3369      3161.6158
46826      3172.4639      3726.0075      3791.9120
46827 Zero-point correction (Hartree): 0.151651
46828
46829 TS.diHPCARP_Ic.16aldHshift.e.pptpud
46830 -----
46831 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14829469
46832 Electronic state : 2-A
46833 Cartesian coordinates (Angs):
46834 O      2.361108      -0.594030      -1.118924
46835 H      1.794998      0.576357      -0.886914
46836 C      1.013100      1.346772      -0.273358
46837 O      2.162538      -1.181738      0.109337
46838 C      -0.102839      0.536733      0.457372
46839 C      0.901039      -1.814277      0.121996
46840 C      -0.248412      -0.851539      -0.196849
46841 O      1.142521      2.512594      -0.231922
46842 C      0.219513      0.479046      1.942726
46843 O      -1.302338      1.265401      0.382075
46844 H      0.194777      1.488771      2.346292
46845 H      1.206310      0.052273      2.106509
46846 H      -0.534374      -0.127520      2.442617

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46847 O -1.630757 1.468254 -0.984676
46848 H -2.290396 0.770005 -1.114903
46849 O -1.389759 -1.526185 0.309316
46850 H -0.350201 -0.736955 -1.275712
46851 O -2.542274 -1.121229 -0.418332
46852 H -2.792352 -1.945100 -0.854774
46853 H 0.884346 -2.644072 -0.585079
46854 H 0.784173 -2.198719 1.135661
46855 Rotational constants (GHz): 1.1072200 0.9245900 0.6528700
46856 Vibrational harmonic frequencies (cm-1):
46857 i1762.3477 62.3132 99.7955
46858 147.3584 169.4960 201.8477
46859 211.7198 231.2916 233.7937
46860 253.2779 269.2173 286.9472
46861 326.0150 351.8314 383.6509
46862 416.4009 458.6208 479.9640
46863 493.4995 511.6231 563.7896
46864 656.9262 704.0300 817.3689
46865 871.0066 949.3443 977.7060
46866 1004.2920 1027.3707 1056.3519
46867 1090.2344 1099.1580 1133.3421
46868 1158.6188 1183.3881 1206.7260
46869 1268.6404 1291.1683 1345.9114
46870 1384.7402 1400.5036 1402.9297
46871 1420.5878 1449.6200 1486.2978
46872 1499.0215 1503.1480 1576.0682
46873 1960.9455 3081.2684 3082.4891
46874 3109.8720 3140.1048 3163.5545
46875 3174.2102 3757.0802 3821.0428
46876 Zero-point correction (Hartree): 0.151287
46877
46878
46879
46880 1,6-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-
46881 HPCARP-Ia), forming B' (di-HPCARP-Ib)
46882 =====
46883 =====
46884
46885 TS.diHPCARP_I.16OOHHshift.a.lmmpdu
46886 -----
46887 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14434491
46888 Electronic state : 2-A
46889 Cartesian coordinates (Angs):
46890 O -2.716305 0.447415 0.027728
46891 H -2.618942 -0.615690 -0.489138
46892 O -2.034622 -1.542799 -0.888764
46893 O -1.623520 1.096905 -0.446602
46894 O -1.023327 -1.670124 0.007633
46895 C -0.404771 0.686725 0.237801
46896 C 0.020480 -0.708606 -0.228284
46897 C -0.563426 0.827288 1.741080
46898 H -1.193622 0.031409 2.131033
46899 H -1.027601 1.785138 1.970339
46900 H 0.413714 0.781273 2.220975
46901 C 0.508772 1.797633 -0.283472
46902 O 1.427799 1.651566 -1.035994
46903 H 0.210115 2.800353 0.068105
46904 H 0.237573 -0.692382 -1.297684
46905 C 1.172798 -1.308211 0.580786
46906 O 2.293107 -0.470280 0.679346
46907 H 0.839756 -1.472480 1.606566
46908 H 1.450236 -2.267403 0.144221
46909 O 3.002092 -0.557251 -0.547707
46910 H 2.683854 0.237356 -1.007008
46911 Rotational constants (GHz): 1.3914700 0.7705300 0.6271800
46912 Vibrational harmonic frequencies (cm-1):
46913 i2900.2710 63.6798 74.5514
46914 109.2574 170.6995 200.3188
46915 216.4924 259.4547 271.6244
46916 284.6808 306.6560 321.0620
46917 357.5527 384.0491 418.7451
46918 469.1397 506.7588 517.4270

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46919	534.2904	588.3693	691.5843			
46920	702.5792	750.2962	893.4542			
46921	942.7683	953.6142	984.0406			
46922	1026.8572	1051.5114	1065.6648			
46923	1117.7405	1127.3551	1143.5065			
46924	1159.7511	1182.0620	1225.3039			
46925	1268.6950	1293.9434	1331.5224			
46926	1394.6947	1408.3468	1412.6068			
46927	1427.6957	1464.7999	1480.8461			
46928	1498.5681	1506.7922	1508.2370			
46929	1873.7097	2995.6367	3076.8281			
46930	3086.0078	3101.7863	3139.0855			
46931	3154.5228	3167.9279	3732.2629			
46932	Zero-point correction (Hartree): 0.151264					
46933						
46934	TS.diHPCARP_I.1600HHshift.a.tpppud					
46935	-----					
46936	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14493614					
46937	Electronic state : 2-A					
46938	Cartesian coordinates (Angs):					
46939	O	2.287396	0.904962	-0.690930		
46940	H	1.653419	1.765264	-0.172729		
46941	O	0.745521	2.233207	0.385918		
46942	O	1.347741	0.144040	-1.319845		
46943	O	0.340550	1.226626	1.211248		
46944	C	0.602904	-0.629768	-0.357025		
46945	C	-0.364729	0.228337	0.452364		
46946	C	-0.111266	-1.687888	-1.186097		
46947	H	0.624768	-2.349152	-1.642700		
46948	H	-0.698120	-1.218228	-1.972214		
46949	H	-0.776720	-2.267468	-0.549575		
46950	C	1.595090	-1.352112	0.553993		
46951	O	1.280299	-1.805731	1.613675		
46952	H	2.603036	-1.483878	0.123381		
46953	H	-0.801903	-0.409231	1.220493		
46954	C	-1.479117	0.891550	-0.355096		
46955	O	-2.519787	-0.014299	-0.655392		
46956	H	-1.859003	1.746518	0.206831		
46957	H	-1.126354	1.231800	-1.328317		
46958	O	-3.118737	-0.406428	0.574088		
46959	H	-3.980282	0.024643	0.515894		
46960	Rotational constants (GHz):			1.2117100	0.7732000	0.6582500
46961	Vibrational harmonic frequencies (cm-1):					
46962	i3042.5491		55.7411			71.1577
46963	100.0396		153.0256			177.5545
46964	199.7026		207.6340			240.5190
46965	264.1334		295.9211			304.4288
46966	311.3865		341.9520			352.3221
46967	415.0145		464.0325			534.2315
46968	559.5704		635.6343			677.6734
46969	697.0175		805.5530			914.4518
46970	946.0870		956.3284			970.5028
46971	1002.1026		1045.8024			1064.6635
46972	1111.4496		1115.7534			1132.5787
46973	1142.3733		1161.4783			1235.1781
46974	1259.2150		1291.1578			1336.1268
46975	1391.0240		1395.1477			1401.6162
46976	1412.3709		1425.0531			1478.4912
46977	1483.2930		1484.3724			1502.8183
46978	1874.2665		2991.1335			3075.6736
46979	3078.5656		3129.4750			3143.6605
46980	3154.5348		3171.3544			3825.5539
46981	Zero-point correction (Hartree): 0.150286					
46982						
46983	TS.diHPCARP_I.1600HHshift.a.ttmpud					
46984	-----					
46985	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14416966					
46986	Electronic state : 2-A					
46987	Cartesian coordinates (Angs):					
46988	O	1.602320	1.830632	-0.214718		
46989	H	0.488196	2.122941	0.098806		
46990	O	-0.620551	1.931987	0.375006		

46991	O	1.426610	0.794289	-1.082285	
46992	O	-0.573320	0.755562	1.060490	
46993	C	1.058561	-0.397242	-0.362023	
46994	C	-0.375270	-0.346286	0.156954	
46995	C	1.266872	-1.530127	-1.358777	
46996	H	2.325606	-1.620173	-1.598968	
46997	H	0.723474	-1.326268	-2.279629	
46998	H	0.919539	-2.467864	-0.928513	
46999	C	2.053523	-0.599637	0.781767	
47000	O	1.827902	-1.325662	1.703559	
47001	H	3.018702	-0.080893	0.651114	
47002	H	-0.509718	-1.210411	0.806981	
47003	C	-1.430253	-0.337707	-0.945935	
47004	O	-2.696103	0.038575	-0.467093	
47005	H	-1.199527	0.406298	-1.707972	
47006	H	-1.475877	-1.329138	-1.402435	
47007	O	-3.061146	-0.886604	0.548529	
47008	H	-2.976688	-0.338725	1.340804	
47009	Rotational constants (GHz):		1.3242900	0.7267800	0.6538500
47010	Vibrational harmonic frequencies (cm-1):				
47011	i2975.4805		59.1082		79.4399
47012	95.1037		136.0569		186.2043
47013	203.4302		219.9171		263.4117
47014	283.2168		300.7865		306.8149
47015	320.4928		336.2947		367.2148
47016	400.0281		460.1567		553.5999
47017	572.6181		623.0448		695.1268
47018	727.4341		813.2429		898.7853
47019	939.9861		956.9262		974.0674
47020	988.9245		1043.5685		1059.0203
47021	1103.0891		1123.1796		1135.4687
47022	1150.8918		1172.4725		1231.3044
47023	1260.1989		1305.0085		1337.1072
47024	1396.3341		1401.4386		1407.9087
47025	1412.4614		1420.3205		1482.2926
47026	1483.8891		1487.5563		1508.3644
47027	1873.9264		2998.2074		3067.6282
47028	3074.9898		3124.5409		3140.0778
47029	3151.8522		3164.1073		3799.4625
47030	Zero-point correction (Hartree):		0.150537		
47031	TS.diHPCARP_I.1600HHshift.b.hppmud				
47032	-----				
47033	IRC pathway available				
47034	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17424011				
47035	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05083632				
47036	T1 diagnostic: 0.025808				
47037	E(MP2/Aug-CC-pVTZ) (Hartree): -721.00671798				
47038	E(MP3/Aug-CC-pVTZ) (Hartree): -721.02328156				
47039	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01669881				
47040	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02896091				
47041	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47563139				
47042	E(UHF/Aug-CC-pVTZ) (Hartree): -718.46157635				
47043	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14834725				
47044	Electronic state : 2-A				
47045	Cartesian coordinates (Angs):				
47046	O	2.725577	0.403701	0.210175	
47047	H	2.456654	-0.753594	0.160297	
47048	O	1.811152	-1.724422	-0.029248	
47049	O	1.721258	0.955920	-0.508303	
47050	O	0.982955	-1.352371	-1.038247	
47051	C	0.423037	0.720480	0.097679	
47052	C	-0.117861	-0.584391	-0.532767	
47053	C	0.485584	0.767978	1.618614	
47054	H	0.961944	1.693968	1.938309	
47055	H	1.060416	-0.068097	2.006481	
47056	H	-0.527312	0.722943	2.014280	
47057	C	-0.384194	1.932349	-0.337600	
47058	O	-1.540335	1.889369	-0.653344	
47059	H	0.173826	2.883513	-0.303229	
47060	H	-0.666599	-0.332616	-1.440019	
47061	C	-0.999648	-1.444063	0.360393	
47062					

47063	O	-2.128020	-0.729769	0.807476			
47064	H	-1.302189	-2.338181	-0.186627			
47065	H	-0.467305	-1.740164	1.263881			
47066	O	-2.990193	-0.542436	-0.306874			
47067	H	-2.790098	0.378185	-0.544363			
47068	Rotational constants (GHz):				1.3755900	0.8153700	0.6333100
47069	Vibrational harmonic frequencies (cm-1):						
47070	i2676.1886		83.3658			106.6685	
47071	120.3894		178.5769			183.0831	
47072	234.9120		253.2197			273.9713	
47073	291.9858		332.9093			338.1520	
47074	359.2638		381.5088			450.8964	
47075	466.0848		509.3601			546.5559	
47076	558.7093		619.8472			676.2162	
47077	683.0533		776.6157			850.3227	
47078	911.7178		951.6124			969.0647	
47079	980.4807		1016.8024			1058.1151	
47080	1117.9840		1129.0212			1151.5976	
47081	1159.2608		1172.7698			1232.9429	
47082	1255.0153		1291.1161			1343.1677	
47083	1399.4054		1403.1287			1409.3041	
47084	1419.6748		1464.4725			1484.9526	
47085	1495.0830		1508.2320			1697.1141	
47086	1861.3295		3003.3154			3081.8990	
47087	3084.8889		3120.5555			3146.0366	
47088	3160.4392		3179.0963			3712.6952	
47089	Zero-point correction (Hartree):				0.151835		
47090							
47091	TS.diHPCARP_I.1600HHshift.b.lmmpdu						
47092	-----						
47093	IRC pathway available						
47094	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17821887						
47095	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05514167						
47096	T1 diagnostic: 0.026666						
47097	E(MP2/Aug-CC-pVTZ) (Hartree): -721.01074247						
47098	E(MP3/Aug-CC-pVTZ) (Hartree): -721.02724143						
47099	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.02028946						
47100	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03271031						
47101	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.48108139						
47102	E(UHF/Aug-CC-pVTZ) (Hartree): -718.46760514						
47103	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15172859						
47104	Electronic state : 2-A						
47105	Cartesian coordinates (Angs):						
47106	O	-2.360896	0.544569	-0.753197			
47107	H	-2.286010	-0.654526	-0.913879			
47108	O	-1.908597	-1.743106	-0.768614			
47109	O	-1.850817	0.717738	0.491853			
47110	O	-1.059080	-1.614281	0.280296			
47111	C	-0.408363	0.677566	0.446450			
47112	C	0.014657	-0.720465	-0.057444			
47113	C	0.006987	1.005617	1.871518			
47114	H	-0.395461	0.249900	2.545256			
47115	H	-0.403394	1.973514	2.156705			
47116	H	1.090994	1.033709	1.951617			
47117	C	0.047259	1.799095	-0.469646			
47118	O	1.025408	1.741641	-1.162400			
47119	H	-0.581618	2.704943	-0.429369			
47120	H	0.121891	-0.719482	-1.141150			
47121	C	1.268383	-1.298221	0.585828			
47122	O	2.372688	-0.439336	0.450838			
47123	H	1.125231	-1.420334	1.660077			
47124	H	1.480839	-2.271464	0.142157			
47125	O	2.769334	-0.462428	-0.913385			
47126	H	2.369674	0.363811	-1.234779			
47127	Rotational constants (GHz):				1.2743100	0.8126200	0.6743900
47128	Vibrational harmonic frequencies (cm-1):						
47129	i2662.3113		78.3717			103.0898	
47130	108.9915		166.6819			191.8717	
47131	239.3973		251.6507			274.2430	
47132	284.8295		323.5506			335.6778	
47133	350.6651		375.3111			421.0253	
47134	506.5024		533.8289			552.4292	

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47135      566.0777      605.3682      667.2356
47136      689.8052      754.7207      827.3945
47137      923.4620      948.5696      961.1911
47138      982.9138      1044.5715     1063.3959
47139      1121.5993     1134.0600     1158.9712
47140      1160.6258     1186.8282     1235.3132
47141      1265.5009     1295.7169     1343.7101
47142      1393.3001     1403.4930     1410.6745
47143      1416.8225     1473.6435     1484.2299
47144      1500.6762     1506.4569     1703.2302
47145      1861.3835     3001.0513     3074.8591
47146      3084.1789     3123.0653     3140.4417
47147      3149.4677     3174.9563     3699.7490
47148      Zero-point correction (Hartree): 0.151810
47149
47150      TS.diHPCARP_I.1600HHshift.b.lppmdu
47151      -----
47152      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14488929
47153      Electronic state : 2-A
47154      Cartesian coordinates (Angs):
47155      O      2.021212      1.530517      0.109810
47156      H      1.086076      2.139324      -0.334220
47157      O      -0.024628      2.375276      -0.630174
47158      O      1.451682      0.720601      1.036580
47159      O      -0.688359      1.336944      -0.064570
47160      C      0.843760      -0.423859      0.401058
47161      C      -0.207930      0.085499      -0.600923
47162      C      0.319858      -1.243865      1.569487
47163      H      -0.401449      -0.660624      2.136560
47164      H      1.153478      -1.511286      2.218630
47165      H      -0.162686      -2.151813      1.215635
47166      C      1.924909      -1.224313      -0.305649
47167      O      1.707093      -1.858718      -1.297944
47168      H      2.913933      -1.209170      0.186621
47169      H      0.269049      0.299139      -1.556633
47170      C      -1.397278      -0.828842      -0.846485
47171      O      -2.254403      -0.926572      0.272177
47172      H      -1.968698      -0.477241      -1.704635
47173      H      -1.029041      -1.835427      -1.050406
47174      O      -3.214519      0.115934      0.198545
47175      H      -2.745208      0.867533      0.588130
47176      Rotational constants (GHz):      1.2184600      0.8179300      0.6310600
47177      Vibrational harmonic frequencies (cm-1):
47178      i2745.0758      60.6123      80.1626
47179      99.3282      137.7034      165.8541
47180      195.0673      251.2977      255.9589
47181      277.1800      305.3928      322.5850
47182      353.9204      356.9555      360.3513
47183      435.0652      503.5558      523.7223
47184      543.7392      662.7144      679.5627
47185      684.4755      798.5689      845.9914
47186      900.9616      928.6703      961.0510
47187      981.4619      998.3223      1045.0653
47188      1109.3126      1136.6215      1152.0978
47189      1161.0902      1170.3849      1230.7932
47190      1268.2442      1313.6095      1359.9980
47191      1382.0469      1396.7861      1404.6035
47192      1415.1613      1440.2293      1472.2150
47193      1484.9754      1498.8265      1703.7372
47194      1866.2845      2985.2424      3078.5754
47195      3087.3106      3121.6287      3142.3984
47196      3156.8986      3176.8493      3781.6115
47197      Zero-point correction (Hartree): 0.150844
47198
47199      TS.diHPCARP_I.1600HHshift.b.lppmdu
47200      -----
47201      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14297900
47202      Electronic state : 2-A
47203      Cartesian coordinates (Angs):
47204      O      2.358376      0.951546      0.182657
47205      H      1.664435      1.824566      -0.301692
47206      O      0.701415      2.375604      -0.642631

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47207      O      1.526440      0.368971      1.080650
47208      O      -0.275425      1.599357      -0.107173
47209      C      0.620397      -0.544020      0.421657
47210      C      -0.159503      0.260067      -0.632441
47211      C      -0.178007      -1.134371      1.572630
47212      H      -0.795508      -0.361754      2.026154
47213      H      0.519707      -1.520866      2.315381
47214      H      -0.819634      -1.937049      1.221260
47215      C      1.437177      -1.648484      -0.226548
47216      O      1.115591      -2.173817      -1.254350
47217      H      2.333337      -1.956379      0.341768
47218      H      0.447319      0.334288      -1.535728
47219      C      -1.506311      -0.263749      -1.100325
47220      O      -2.427808      -0.654670      -0.110808
47221      H      -1.947970      0.494436      -1.753058
47222      H      -1.328162      -1.176904      -1.670192
47223      O      -2.717451      0.478857      0.695122
47224      H      -3.605138      0.716219      0.398534
47225      Rotational constants (GHz):      1.1662100      0.8654900      0.6678000
47226      Vibrational harmonic frequencies (cm-1):
47227      i2706.3129      52.3137      81.9946
47228      94.1182      133.2017      164.8433
47229      188.4814      226.6299      244.9557
47230      270.9678      281.8275      318.4801
47231      329.4691      357.1403      359.6338
47232      410.4105      473.6112      521.0028
47233      547.3202      661.5532      671.7511
47234      687.8201      837.1981      855.9414
47235      875.7719      928.3708      952.4398
47236      972.0197      1000.0055      1051.3089
47237      1115.5371      1144.2429      1154.4406
47238      1163.4635      1176.1752      1231.1544
47239      1273.3570      1327.4845      1373.4977
47240      1384.7393      1392.1584      1399.6449
47241      1413.6979      1428.6781      1463.0623
47242      1485.0154      1500.2418      1704.3003
47243      1864.7314      2982.6663      3055.5158
47244      3078.2445      3104.2418      3129.7930
47245      3157.0087      3182.1708      3818.0739
47246      Zero-point correction (Hartree): 0.150482
47247
47248      TS.diHPCARP_I.1600HHshift.b.tmpmdu
47249      -----
47250      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14667660
47251      Electronic state : 2-A
47252      Cartesian coordinates (Angs):
47253      O      2.405970      -0.699946      -0.564780
47254      H      2.445544      0.501244      -0.741451
47255      O      2.132835      1.613150      -0.636300
47256      O      1.753995      -0.803685      0.619178
47257      O      1.172255      1.544105      0.316964
47258      C      0.329196      -0.672707      0.416150
47259      C      0.064990      0.744664      -0.149765
47260      C      -0.252430      -0.937456      1.794948
47261      H      0.112705      -0.178215      2.486458
47262      H      0.078030      -1.913362      2.148452
47263      H      -1.338108      -0.908546      1.758708
47264      C      -0.080936      -1.787027      -0.532418
47265      O      -1.041070      -1.735211      -1.251072
47266      H      0.564701      -2.680442      -0.490382
47267      H      0.096094      0.733424      -1.239055
47268      C      -1.196469      1.495651      0.281505
47269      O      -2.331759      1.156330      -0.470896
47270      H      -1.400162      1.394922      1.348140
47271      H      -1.019940      2.547966      0.056430
47272      O      -2.866391      -0.056996      0.039344
47273      H      -2.531651      -0.697721      -0.609328
47274      Rotational constants (GHz):      1.3006900      0.8139400      0.6427500
47275      Vibrational harmonic frequencies (cm-1):
47276      i2612.8754      54.7849      97.0810
47277      109.2804      148.5639      202.7026
47278      221.0158      249.7167      277.2338

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47279	286.9146	303.9309	321.3221
47280	362.5353	381.8025	404.8721
47281	503.7972	525.3844	530.1566
47282	561.3599	585.7572	671.4369
47283	691.0893	761.6504	841.9954
47284	923.5641	946.9843	963.4054
47285	986.2274	1032.3445	1068.8027
47286	1106.1565	1138.7062	1159.6971
47287	1164.4232	1176.0433	1233.2216
47288	1259.8920	1304.2704	1328.6916
47289	1389.3398	1403.5088	1414.6653
47290	1417.0133	1466.0485	1479.3266
47291	1498.6601	1506.6928	1715.0190
47292	1858.4911	3005.8572	3073.2619
47293	3084.3222	3115.0759	3138.1638
47294	3147.2026	3179.1086	3711.9292

47295 Zero-point correction (Hartree): 0.151477

47296
47297 TS.diHPCARP_I.1600HHshift.b.ttmpdu

47298 -----
47299 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14498407

47300 Electronic state : 2-A

47301 Cartesian coordinates (Angs):

47302	O	1.827864	1.685214	-0.467908
47303	H	0.721427	2.130191	-0.622709
47304	O	-0.442201	2.213988	-0.539522
47305	O	1.708915	0.952522	0.667173
47306	O	-0.745172	1.207639	0.320298
47307	C	1.090246	-0.317319	0.380218
47308	C	-0.301086	-0.053702	-0.225727
47309	C	1.075635	-1.022266	1.727452
47310	H	0.460269	-0.460728	2.429007
47311	H	2.090326	-1.077056	2.119721
47312	H	0.684202	-2.032089	1.622729
47313	C	1.976451	-1.096135	-0.576967
47314	O	1.536829	-1.931111	-1.314004
47315	H	3.054377	-0.863134	-0.514108
47316	H	-0.237153	0.069309	-1.306104
47317	C	-1.343284	-1.112377	0.082572
47318	O	-2.560025	-0.829898	-0.569932
47319	H	-0.989836	-2.062709	-0.322022
47320	H	-1.523416	-1.211362	1.152925
47321	O	-3.349874	-0.018015	0.285928
47322	H	-3.058658	0.875662	0.059010

47323 Rotational constants (GHz): 1.2549300 0.7547400 0.5925200

47324 Vibrational harmonic frequencies (cm-1):

47325	i2770.9166	54.6627	70.0968
47326	96.9193	119.6419	161.6493
47327	183.0489	235.5667	272.4120
47328	283.6395	294.2517	307.7834
47329	342.4420	346.2932	369.8078
47330	406.8477	507.2637	523.9491
47331	567.8149	580.3258	672.0388
47332	685.6590	826.4238	839.3981
47333	872.7947	929.7119	962.7815
47334	971.1630	1009.2756	1102.8171
47335	1114.0621	1133.5114	1151.4452
47336	1158.8690	1183.6618	1231.7652
47337	1268.6257	1319.3073	1340.2982
47338	1378.8477	1398.2348	1409.8692
47339	1416.2590	1430.8327	1464.9574
47340	1493.2703	1502.8674	1697.7103
47341	1867.9905	2987.0729	3074.5628
47342	3081.4569	3121.0265	3141.5882
47343	3152.7790	3166.2016	3798.6970

47344 Zero-point correction (Hartree): 0.150546

47345
47346
47347
47348 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-di-
47349 HPCARP-Ia), forming C' (di-HPCARP-Ic)

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47350 =====
47351 =====
47352
47353 TS.diHPCARP_I.1700HHshift.BB.cmudu
47354 -----
47355 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15131991
47356 Electronic state : 2-A
47357 Cartesian coordinates (Angs):
47358 O -2.320313 -0.428460 0.976877
47359 H -1.235484 -0.586525 1.432448
47360 O -0.073345 -0.483328 1.673453
47361 O -2.185395 0.679951 0.213469
47362 O 0.193098 0.743212 1.161580
47363 C -1.725402 0.342028 -1.089210
47364 C 0.639995 0.673002 -0.184162
47365 C -0.280450 -0.150364 -1.105415
47366 C 2.088604 0.171340 -0.237482
47367 C 0.681732 2.130600 -0.641842
47368 O 2.766838 0.006340 0.729750
47369 H 2.484100 0.058380 -1.263518
47370 H 1.383392 2.681376 -0.018198
47371 H -0.301489 2.583604 -0.536073
47372 H 1.005647 2.197664 -1.679708
47373 H 0.118485 -0.038677 -2.122038
47374 O -0.379350 -1.531353 -0.806101
47375 O 0.915846 -2.065650 -0.628351
47376 H 0.974854 -2.088635 0.341408
47377 H -2.367775 -0.432687 -1.507767
47378 H -1.827628 1.260165 -1.663304
47379 Rotational constants (GHz): 1.3492300 0.8723800 0.7913600
47380 Vibrational harmonic frequencies (cm-1):
47381 i2320.7157 81.9865 119.9993
47382 140.0253 162.6427 179.2977
47383 220.3181 264.3513 282.7168
47384 292.1359 303.0506 365.5635
47385 368.4878 379.2914 411.9304
47386 448.8824 498.4904 550.4862
47387 595.2268 635.0113 661.4538
47388 774.1615 831.0680 849.6111
47389 883.2495 920.7528 937.2539
47390 972.2632 996.5508 1053.3642
47391 1075.4116 1144.6485 1166.8837
47392 1182.5014 1187.3744 1194.3245
47393 1253.3003 1311.9133 1352.4485
47394 1376.9033 1392.4453 1401.4552
47395 1420.5280 1430.0726 1472.0149
47396 1485.8673 1513.8474 1699.1774
47397 1875.9070 2966.3177 3021.9152
47398 3078.4118 3097.7321 3156.8605
47399 3160.1120 3168.2806 3725.9999
47400 Zero-point correction (Hartree): 0.151481
47401
47402 TS.diHPCARP_I.1700HHshift.BB.htdud
47403 -----
47404 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15107190
47405 Electronic state : 2-A
47406 Cartesian coordinates (Angs):
47407 O -2.694628 0.343757 -0.023142
47408 H -2.263939 -0.541030 -0.665904
47409 O -1.523175 -1.363708 -1.127418
47410 O -1.918760 0.310393 1.086386
47411 O -0.680652 -1.598053 -0.095910
47412 C -0.783693 1.145403 0.910814
47413 C 0.508467 -0.798765 -0.183627
47414 C 0.103049 0.691151 -0.251149
47415 C 1.207599 -1.103212 1.141887
47416 C 1.354155 -1.201735 -1.372921
47417 O 2.394776 -1.077852 1.270908
47418 H 0.527633 -1.346084 1.978369
47419 H 0.825268 -0.969221 -2.295046
47420 H 1.554253 -2.270524 -1.332422
47421 H 2.299148 -0.665966 -1.338250

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47422      H      -0.406651      0.854736      -1.201636
47423      O       1.306955      1.428157      -0.225163
47424      O       0.987320      2.761018      -0.608402
47425      H       1.499671      2.851633      -1.421471
47426      H      -1.107541      2.170717      0.734790
47427      H      -0.240006      1.088989      1.853466
47428      Rotational constants (GHz):      1.0673900      0.8959800      0.6703400
47429      Vibrational harmonic frequencies (cm-1):
47430      i2246.4061      55.0102      75.2989
47431      90.6959      119.6447      185.6984
47432      191.5261      205.6842      225.4751
47433      238.3730      285.0859      294.9454
47434      301.1115      338.3395      418.8810
47435      440.2935      470.1382      489.2029
47436      535.2106      615.3010      644.3541
47437      663.3028      776.6676      885.3934
47438      908.6654      934.4306      996.9262
47439      1011.5350      1021.6120      1061.4741
47440      1119.3103      1134.9369      1168.7530
47441      1177.8065      1180.4580      1211.5903
47442      1245.1358      1302.5741      1344.2482
47443      1373.9719      1396.8730      1402.5141
47444      1416.0754      1419.5438      1487.1288
47445      1492.1439      1494.7523      1697.2152
47446      1881.0557      2979.1030      3085.3607
47447      3092.4265      3100.4053      3152.2647
47448      3165.3632      3179.7400      3823.3367
47449      Zero-point correction (Hartree): 0.150369
47450
47451      TS.diHPCARP_I.1700HHshift.BB.lmddu
47452      -----
47453      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15109336
47454      Electronic state : 2-A
47455      Cartesian coordinates (Angs):
47456      O       2.543574      0.262595      0.605711
47457      H       1.609200      0.195611      1.345460
47458      O       0.574997      -0.089966      1.839298
47459      O       2.234226      -0.635684      -0.358711
47460      O       0.160554      -1.115455      1.056133
47461      C       1.450920      -0.023550      -1.369331
47462      C      -0.642822      -0.661874      -0.036497
47463      C       0.056965      0.405332      -0.907118
47464      C      -1.963140      -0.132068      0.547752
47465      C      -0.916189      -1.913628      -0.854408
47466      O      -2.998782      -0.223494      -0.042877
47467      H      -1.880331      0.285018      1.563399
47468      H      -1.436214      -2.642809      -0.237245
47469      H       0.016117      -2.354543      -1.200040
47470      H      -1.555890      -1.667742      -1.698458
47471      H      -0.573220      0.531810      -1.795388
47472      O       0.237361      1.671527      -0.300131
47473      O      -1.041338      2.209053      -0.010093
47474      H      -1.127308      2.904296      -0.674985
47475      H       1.977429      0.851718      -1.750435
47476      H       1.371077      -0.777232      -2.149341
47477      Rotational constants (GHz):      1.3508300      0.8399800      0.7386200
47478      Vibrational harmonic frequencies (cm-1):
47479      i2210.9492      36.4374      105.5111
47480      126.7402      143.5429      194.7245
47481      211.8527      219.9934      251.7359
47482      271.0713      279.4729      291.6644
47483      327.0781      363.2702      391.7952
47484      438.8386      485.3111      494.4833
47485      541.1665      644.7640      669.3559
47486      719.7557      816.1626      850.5367
47487      880.3678      924.5491      941.7663
47488      979.0453      1010.1058      1060.3816
47489      1067.9757      1150.2469      1160.2644
47490      1173.0792      1192.2282      1220.0597
47491      1242.8385      1301.5261      1345.3326
47492      1374.1840      1388.7014      1393.4586
47493      1407.8907      1414.6317      1471.4640

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47494      1485.1829          1508.1217          1700.7637
47495      1862.0847          3023.2038          3037.1071
47496      3088.4142          3093.9762          3159.1908
47497      3167.6178          3176.9520          3810.7517
47498      Zero-point correction (Hartree): 0.150561
47499
47500      TS.diHPCARP_I.1700HHshift.BB.lpuud
47501      -----
47502      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15071261
47503      Electronic state : 2-A
47504      Cartesian coordinates (Angs):
47505      O      2.523749      -0.942876      -0.237340
47506      H      2.187182      -0.075398      -0.966800
47507      O      1.569252      0.812759      -1.472533
47508      O      1.932239      -0.606104      0.933302
47509      O      0.964457      1.373363      -0.400243
47510      C      0.649332      -1.210461      1.026361
47511      C      -0.348494      0.826598      -0.178113
47512      C      -0.275691      -0.705318      -0.082116
47513      C      -0.745936      1.516432      1.123357
47514      C      -1.297775      1.274817      -1.280217
47515      O      -1.261568      0.969492      2.052744
47516      H      -0.531628      2.601216      1.127307
47517      H      -0.935901      0.902085      -2.236756
47518      H      -1.337841      2.363043      -1.314598
47519      H      -2.293572      0.877134      -1.096424
47520      H      0.080002      -1.080610      -1.040387
47521      O      -1.550171      -1.256302      0.176671
47522      O      -2.151650      -1.602659      -1.068707
47523      H      -2.292956      -2.549940      -0.949309
47524      H      0.751686      -2.292103      0.940571
47525      H      0.273938      -0.939218      2.009606
47526      Rotational constants (GHz): 1.1182300      0.8283100      0.7696800
47527      Vibrational harmonic frequencies (cm-1):
47528      i2245.0674          72.0983          86.4867
47529      92.2521          123.3787          185.4987
47530      191.8525          225.5499          233.7474
47531      247.1195          271.4535          309.2804
47532      336.6209          378.7949          393.6529
47533      428.4048          435.0874          482.0288
47534      537.7314          635.2318          646.0087
47535      672.4119          785.7261          896.1857
47536      908.4459          959.1023          977.3794
47537      983.3618          1030.0835          1050.3547
47538      1118.4319          1139.4998          1153.7259
47539      1170.1365          1178.0848          1195.7303
47540      1268.3769          1324.2488          1343.1776
47541      1381.6378          1399.2911          1402.4637
47542      1405.6280          1432.1021          1489.9782
47543      1493.4973          1497.9210          1695.8578
47544      1878.5459          2972.6762          3075.1629
47545      3095.0096          3122.5408          3154.5481
47546      3169.8345          3175.6321          3824.7760
47547      Zero-point correction (Hartree): 0.150664
47548
47549      TS.diHPCARP_I.1700HHshift.BB.ltdud
47550      -----
47551      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15023857
47552      Electronic state : 2-A
47553      Cartesian coordinates (Angs):
47554      O      -2.385071      1.162922      0.008767
47555      H      -2.277672      0.219162      -0.668232
47556      O      -1.853994      -0.794662      -1.180093
47557      O      -1.655767      0.838574      1.102708
47558      O      -1.143561      -1.337789      -0.165900
47559      C      -0.307653      1.263624      0.940138
47560      C      0.244288      -0.959667      -0.209276
47561      C      0.353944      0.571765      -0.251135
47562      C      0.778110      -1.604770      1.065423
47563      C      0.923086      -1.609305      -1.407189
47564      O      1.595933      -1.107711      1.780583
47565      H      0.357665      -2.608826      1.258674

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47566	H	0.450141	-1.251471	-2.320403	
47567	H	0.810773	-2.691602	-1.355417	
47568	H	1.980045	-1.353704	-1.416638	
47569	H	-0.123184	0.900604	-1.175372	
47570	O	1.724730	0.907103	-0.301295	
47571	O	1.802614	2.249678	-0.769297	
47572	H	2.260438	2.132810	-1.610855	
47573	H	-0.280678	2.342409	0.788926	
47574	H	0.192741	0.995815	1.867768	
47575	Rotational constants (GHz):		1.0459100	0.9030000	0.7234100
47576	Vibrational harmonic frequencies (cm-1):				
47577	i2189.9053		71.5265		78.3829
47578	89.1387		122.0506		173.0933
47579	189.8226		206.9362		225.8845
47580	230.9587		280.5422		290.7120
47581	332.9149		339.8603		413.6957
47582	433.2617		463.6883		470.8344
47583	534.2002		621.2587		645.5571
47584	671.9105		795.6194		898.8160
47585	905.9497		961.0733		972.9120
47586	993.3805		1019.1326		1063.9288
47587	1113.3854		1135.2513		1168.2018
47588	1174.6326		1185.4984		1187.8849
47589	1269.2465		1324.3347		1350.5935
47590	1370.7171		1394.7780		1400.2162
47591	1419.6258		1426.8934		1490.7585
47592	1494.2333		1498.5012		1697.9766
47593	1881.0537		2977.7132		3075.9697
47594	3098.5047		3100.3270		3153.5765
47595	3171.3647		3174.0768		3824.4902
47596	Zero-point correction (Hartree): 0.150489				
47597	TS.diHPCARP_I.1700HHshift.BB.ltud				
47598	-----				
47599	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15086985				
47600	Electronic state : 2-A				
47601	Cartesian coordinates (Angs):				
47602	O	-2.357733	1.222197	-0.000503	
47603	H	-2.277539	0.258270	-0.659078	
47604	O	-1.886375	-0.774342	-1.147529	
47605	O	-1.636255	0.898441	1.098758	
47606	O	-1.176618	-1.312950	-0.130298	
47607	C	-0.277643	1.280662	0.926383	
47608	C	0.218644	-0.968759	-0.202734	
47609	C	0.366878	0.558669	-0.256531	
47610	C	0.762415	-1.611699	1.067928	
47611	C	0.861636	-1.641190	-1.407538	
47612	O	1.571640	-1.103692	1.786361	
47613	H	0.359209	-2.623157	1.258176	
47614	H	0.368669	-1.290440	-2.312524	
47615	H	0.742096	-2.721732	-1.337498	
47616	H	1.918680	-1.390403	-1.449908	
47617	H	-0.096445	0.891334	-1.186101	
47618	O	1.745106	0.852566	-0.314181	
47619	O	1.858753	2.120576	-0.960086	
47620	H	2.454233	2.579815	-0.355471	
47621	H	-0.223410	2.356791	0.759265	
47622	H	0.214787	1.011052	1.857916	
47623	Rotational constants (GHz):		1.0500500	0.8980700	0.7251200
47624	Vibrational harmonic frequencies (cm-1):				
47625	i2208.4189		73.2533		81.2948
47626	86.2797		122.4750		190.3855
47627	197.6783		202.5413		225.4544
47628	229.1060		279.8639		291.5098
47629	335.1858		340.4377		412.5501
47630	433.0327		461.6064		469.6007
47631	533.4483		621.9922		645.2773
47632	673.4371		795.5302		890.9363
47633	907.0947		960.8648		974.7545
47634	995.1034		1021.2785		1066.7405
47635	1113.7143		1137.3749		1165.0104
47636	1173.8862		1182.2923		1187.8123

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47638      1271.0217      1325.7079      1349.3664
47639      1369.6458      1396.3389      1411.6390
47640      1412.8936      1430.9088      1489.6847
47641      1494.9918      1498.5238      1697.2950
47642      1878.2979      2979.7490      3077.5575
47643      3091.8350      3103.8951      3155.5518
47644      3170.2857      3174.7209      3833.3970
47645 Zero-point correction (Hartree): 0.150569
47646
47647 TS.diHPCARP_I.1700HHshift.BB.mmdud
47648 -----
47649 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15223118
47650 Electronic state : 2-A
47651 Cartesian coordinates (Angs):
47652   O      2.541939      -0.864809      -0.308230
47653   H      2.342221      0.276389      -0.540844
47654   O      1.794267      1.331712      -0.660260
47655   O      1.698635      -1.099367      0.724629
47656   O      0.899318      1.308603      0.355242
47657   C      0.448784      -1.568444      0.243165
47658   C     -0.384271      0.847309      -0.090969
47659   C     -0.200687      -0.561844      -0.706380
47660   C     -1.221263      0.802926      1.195417
47661   C     -0.993897      1.807439      -1.092739
47662   O     -0.783462      0.439966      2.246010
47663   H     -2.264036      1.142794      1.079950
47664   H     -0.365781      1.873626      -1.977971
47665   H     -1.085573      2.797408      -0.647365
47666   H     -1.982117      1.452660      -1.382315
47667   H      0.433067      -0.441364      -1.585947
47668   O     -1.393676      -1.065421      -1.256262
47669   O     -2.360564      -1.144680      -0.208758
47670   H     -2.589985      -2.082021      -0.221530
47671   H      0.595547      -2.507797      -0.293343
47672   H     -0.146996      -1.724042      1.139434
47673 Rotational constants (GHz):      1.1968000      0.8765800      0.7786100
47674 Vibrational harmonic frequencies (cm-1):
47675   i2248.1972      70.8289      96.6045
47676      124.2490      170.4964      189.1034
47677      204.8414      208.0929      220.4900
47678      270.7816      284.9797      313.4124
47679      316.5492      332.7742      393.9796
47680      437.5071      472.4325      535.6201
47681      576.1679      632.6665      651.1167
47682      670.6327      777.3335      900.4802
47683      916.4304      931.2127      972.3429
47684      999.0033      1015.9823      1054.0722
47685      1114.7047      1140.4507      1170.3725
47686      1172.7838      1181.5728      1201.6437
47687      1240.3820      1296.2936      1341.3562
47688      1361.4841      1389.0266      1404.0707
47689      1421.3155      1429.2270      1486.5725
47690      1487.1973      1499.1445      1697.6945
47691      1871.9733      2997.1234      3076.8336
47692      3078.0153      3113.7294      3154.0710
47693      3167.7082      3169.2359      3830.2900
47694 Zero-point correction (Hartree): 0.150893
47695
47696 TS.diHPCARP_I.1700HHshift.BB.tmudu
47697 -----
47698 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15365262
47699 Electronic state : 2-A
47700 Cartesian coordinates (Angs):
47701   O      2.548977      0.303720      0.450341
47702   H      1.641501      0.597940      1.134322
47703   O      0.567172      0.627274      1.682098
47704   O      2.133539      -0.826335      -0.164903
47705   O      0.081471      -0.600677      1.368129
47706   C      1.382920      -0.523972      -1.336541
47707   C     -0.679992      -0.603740      0.158800
47708   C      0.019932      0.091004      -1.025337
47709   C     -2.053862      0.024111      0.434333

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47710      C      -0.893022      -2.082345      -0.145018
47711      O      -2.978832      -0.132360      -0.304908
47712      H      -2.136299      0.558915      1.396824
47713      H      -1.451687      -2.544025      0.666686
47714      H      0.063156      -2.591472      -0.238014
47715      H      -1.473005      -2.183853      -1.059370
47716      H      -0.650217      -0.044150      -1.882159
47717      O      0.301585      1.470499      -0.866766
47718      O      -0.822303      2.136320      -0.328963
47719      H      -0.525456      2.260698      0.586605
47720      H      1.952340      0.166720      -1.957982
47721      H      1.270937      -1.478648      -1.844569
47722      Rotational constants (GHz):      1.3846100      0.8577500      0.7639800
47723      Vibrational harmonic frequencies (cm-1):
47724      i2294.8694      78.6778      114.6295
47725      147.0285      167.7693      211.6952
47726      227.9848      264.1768      271.8593
47727      289.8325      311.7185      328.8588
47728      366.3426      387.7054      438.6340
47729      466.1170      490.9859      501.0705
47730      558.5133      651.5800      667.0678
47731      709.7682      832.0237      852.1085
47732      891.6372      932.7830      952.4723
47733      974.6981      1002.1610      1048.6447
47734      1073.4096      1147.0077      1157.3506
47735      1178.4580      1187.2262      1214.2029
47736      1240.9433      1301.7300      1348.5771
47737      1376.0640      1386.9436      1393.5023
47738      1412.4691      1434.4101      1472.8934
47739      1488.1151      1515.1941      1696.7196
47740      1866.7641      2986.8774      3044.2536
47741      3087.0875      3100.4153      3162.5154
47742      3167.5709      3180.0001      3742.5355
47743      Zero-point correction (Hartree): 0.151502
47744
47745      TS.diHPCARP_I.1700HHshift.BB.tmuud
47746      -----
47747      IRC pathway available
47748      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18122416
47749      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05740314
47750      T1 diagnostic: 0.025077
47751      E(MP2/Aug-CC-pVTZ) (Hartree): -721.01490724
47752      E(MP3/Aug-CC-pVTZ) (Hartree): -721.02948376
47753      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.02445354
47754      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.03491421
47755      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47949160
47756      E(UHF/Aug-CC-pVTZ) (Hartree): -718.46593926
47757      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15617316
47758      Electronic state : 2-A
47759      Cartesian coordinates (Angs):
47760      O      2.619438      -0.906867      -0.069291
47761      H      2.467718      0.222298      -0.347683
47762      O      1.965697      1.303665      -0.517878
47763      O      1.702807      -1.099720      0.907170
47764      O      1.019087      1.330753      0.446518
47765      C      0.472388      -1.557959      0.360524
47766      C      -0.258229      0.881573      -0.037384
47767      C      -0.103501      -0.544583      -0.627365
47768      C      -1.121482      0.985711      1.207132
47769      C      -0.803509      1.841291      -1.087864
47770      O      -2.243446      0.561447      1.274649
47771      H      -0.661746      1.529994      2.048856
47772      H      -0.121385      1.863493      -1.935447
47773      H      -0.890250      2.845174      -0.674737
47774      H      -1.781208      1.496608      -1.416452
47775      H      0.594977      -0.434062      -1.458002
47776      O      -1.267651      -1.021665      -1.254838
47777      O      -2.120426      -1.670561      -0.321289
47778      H      -2.576586      -0.923909      0.102396
47779      H      0.622965      -2.508035      -0.152483
47780      H      -0.172539      -1.704185      1.222958
47781      Rotational constants (GHz):      1.2603100      0.8671000      0.6897500

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47782 Vibrational harmonic frequencies (cm-1):
47783 i2206.7030 55.5622 67.8997
47784 149.7917 158.5021 208.0271
47785 212.0075 227.5582 249.9695
47786 269.9579 298.5864 316.7789
47787 323.9106 391.7728 439.8607
47788 470.8027 508.4302 550.6660
47789 565.6359 628.7372 643.7946
47790 663.3514 777.3212 901.4018
47791 906.7912 953.2682 972.7759
47792 985.9454 1012.5705 1051.1433
47793 1117.2557 1145.4613 1163.3714
47794 1169.9156 1186.5794 1194.8388
47795 1248.9347 1299.3785 1336.9462
47796 1378.4599 1396.3112 1406.9197
47797 1429.9073 1479.1600 1485.1152
47798 1488.8864 1499.9724 1699.4224
47799 1856.0517 3004.9574 3078.7158
47800 3096.4301 3108.4210 3159.5040
47801 3171.2446 3174.2303 3694.5362
47802 Zero-point correction (Hartree): 0.151347
47803
47804 TS.diHPCARP_I.1700HHshift.BB.tpud
47805 -----
47806 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15240778
47807 Electronic state : 2-A
47808 Cartesian coordinates (Angs):
47809 O 2.745911 -0.555820 -0.412853
47810 H 2.373483 0.538819 -0.620329
47811 O 1.703513 1.528559 -0.616427
47812 O 2.122527 -0.830957 0.755770
47813 O 0.886653 1.333964 0.444426
47814 C 0.900008 -1.502442 0.515462
47815 C -0.348908 0.727723 0.035456
47816 C -0.084699 -0.753247 -0.391647
47817 C -1.201380 0.756278 1.292864
47818 C -0.985529 1.570243 -1.063920
47819 O -2.367453 0.473479 1.278108
47820 H -0.685610 1.049915 2.222875
47821 H -0.471611 1.405903 -2.006799
47822 H -0.898847 2.621709 -0.793157
47823 H -2.032814 1.314810 -1.178996
47824 H 0.266016 -0.745446 -1.425743
47825 O -1.217728 -1.580180 -0.264802
47826 O -2.246070 -1.142839 -1.133392
47827 H -2.812292 -0.667201 -0.503230
47828 H 1.101429 -2.474524 0.065195
47829 H 0.464471 -1.644972 1.504254
47830 Rotational constants (GHz): 1.3722300 0.8018700 0.6721000
47831 Vibrational harmonic frequencies (cm-1):
47832 i2187.2267 56.8052 107.1440
47833 128.1505 159.1784 192.8368
47834 203.6681 221.0840 261.3710
47835 268.9866 304.0785 338.2534
47836 353.2141 380.2145 443.0432
47837 480.3687 504.0226 515.6674
47838 532.0183 635.7229 654.0949
47839 668.4284 757.2860 860.9483
47840 909.4814 944.3971 987.2560
47841 1003.8750 1033.8075 1061.6329
47842 1104.7594 1153.0312 1158.7730
47843 1183.4251 1192.0944 1204.8696
47844 1234.5900 1297.8504 1325.2087
47845 1386.5579 1401.6153 1408.6657
47846 1424.7431 1460.4892 1485.1407
47847 1487.0620 1498.4260 1705.0479
47848 1856.9519 3003.1626 3086.8454
47849 3088.4062 3091.0301 3146.3315
47850 3169.4423 3204.6994 3728.3318
47851 Zero-point correction (Hartree): 0.151395
47852
47853 TS.diHPCARP_I.1700HHshift.BB.ttddu

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47854 -----
47855 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15439883
47856 Electronic state : 2-A
47857 Cartesian coordinates (Angs):
47858   O      -2.308658      -0.651475      -0.629372
47859   H      -1.352022      -0.805649      -1.309296
47860   O      -0.245311      -1.016912      -1.695310
47861   O      -1.875687      -1.081085       0.580864
47862   O       0.370813      -1.496670      -0.588160
47863   C      -1.301019      -0.005285       1.305565
47864   C       0.963419      -0.450395       0.185441
47865   C      -0.056663       0.597047       0.661980
47866   C       2.019892       0.262825      -0.671160
47867   C       1.622602      -1.156430       1.357327
47868   O       2.870243       0.941585      -0.177473
47869   H       1.939443       0.087036      -1.755896
47870   H       2.316903      -1.906990       0.985197
47871   H       0.877401      -1.653701       1.974744
47872   H       2.177024      -0.431279       1.947818
47873   H       0.445266       1.211492       1.417013
47874   O      -0.340230       1.423892      -0.454075
47875   O      -1.080865       2.537174       0.018315
47876   H      -1.918174       2.412067      -0.447882
47877   H      -2.045033       0.779797       1.439253
47878   H      -1.052635      -0.431418       2.275824
47879 Rotational constants (GHz):      1.2348000      0.8729600      0.7204600
47880 Vibrational harmonic frequencies (cm-1):
47881   i2291.7669      43.6870      78.9030
47882     94.7500      169.2994      186.8537
47883    215.3220      224.6135      245.4062
47884    269.0989      302.3237      316.5624
47885    328.0847      341.1228      388.0107
47886    426.6374      467.4444      521.3317
47887    540.3360      630.5444      667.5508
47888    735.7547      836.9407      851.1569
47889    876.8562      930.7619      942.5938
47890    994.4323     1010.1518     1040.8704
47891   1055.8421     1145.6039     1165.8967
47892   1170.2187     1181.7242     1226.7295
47893   1251.3462     1292.5761     1355.1556
47894   1378.8016     1387.5085     1390.1434
47895   1411.2645     1417.9987     1478.2289
47896   1487.3574     1508.1908     1701.7484
47897   1869.1951     3016.4455     3053.7622
47898   3085.9519     3099.7681     3154.0078
47899   3163.5575     3176.9273     3806.1218
47900 Zero-point correction (Hartree): 0.150608
47901
47902 TS.diHPCARP_I.1700HHshift.BB.ttudu
47903 -----
47904 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15366177
47905 Electronic state : 2-A
47906 Cartesian coordinates (Angs):
47907   O      -2.416722      -0.426094      -0.639407
47908   H      -1.490691      -0.691446      -1.296956
47909   O      -0.397513      -1.046128      -1.668831
47910   O      -2.031832      -0.801216       0.603753
47911   O       0.126326      -1.585151      -0.541667
47912   C      -1.341730       0.258744       1.248758
47913   C       0.847274      -0.608901       0.205401
47914   C       0.001599       0.608587       0.614162
47915   C       2.022855      -0.106792      -0.639521
47916   C       1.362861      -1.354150       1.426845
47917   O       2.853312       0.625952      -0.187800
47918   H       2.051573      -0.484800      -1.674976
47919   H       1.932832      -2.225307       1.109587
47920   H       0.531622      -1.694095       2.041564
47921   H       2.012212      -0.699160       2.002804
47922   H       0.593689       1.155215       1.353799
47923   O      -0.147278       1.444772      -0.522048
47924   O      -0.501265       2.732678      -0.037871
47925   H       0.299444       3.235900      -0.235570

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47926      H      -1.965111      1.153353      1.247119
47927      H      -1.202951      -0.093104      2.269727
47928      Rotational constants (GHz):      1.1868100      0.9006500      0.7188500
47929      Vibrational harmonic frequencies (cm-1):
47930      i2220.4894      60.8985      85.0616
47931      101.0792      148.1284      191.7936
47932      203.1597      226.0070      241.0161
47933      244.9921      267.9409      301.8295
47934      308.1055      354.3682      383.0960
47935      432.0717      461.7872      523.6689
47936      552.1829      625.8035      671.1586
47937      730.9560      802.5429      854.7380
47938      887.7813      940.0719      948.9387
47939      987.7818      1010.9126      1044.2046
47940      1054.7386      1139.8275      1169.9343
47941      1179.5614      1183.9105      1236.4582
47942      1246.9567      1300.0866      1348.5965
47943      1385.1114      1391.8893      1392.5300
47944      1409.7091      1411.4721      1473.0802
47945      1489.2826      1508.1591      1693.0333
47946      1865.3439      3009.6790      3067.7016
47947      3083.2177      3095.5312      3153.7080
47948      3161.0393      3174.1684      3809.8435
47949      Zero-point correction (Hartree): 0.150420
47950
47951      TS.diHPCARP_I.1700HHshift.BB.ttuud
47952      -----
47953      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15056613
47954      Electronic state : 2-A
47955      Cartesian coordinates (Angs):
47956      O      -2.670433      0.482477      -0.000018
47957      H      -2.289487      -0.420877      -0.655704
47958      O      -1.601196      -1.277900      -1.125879
47959      O      -1.885334      0.402653      1.100105
47960      O      -0.767507      -1.568638      -0.101497
47961      C      -0.709296      1.176285      0.914612
47962      C      0.464032      -0.835630      -0.185629
47963      C      0.141992      0.674089      -0.254164
47964      C      1.140928      -1.174429      1.141815
47965      C      1.291531      -1.284115      -1.372218
47966      O      2.322907      -1.105726      1.303997
47967      H      0.450638      -1.478208      1.949765
47968      H      0.781032      -1.019044      -2.295776
47969      H      1.429869      -2.362815      -1.332949
47970      H      2.262765      -0.798311      -1.334008
47971      H      -0.367553      0.859887      -1.200692
47972      O      1.380126      1.344859      -0.257146
47973      O      1.114906      2.647922      -0.782791
47974      H      1.754070      3.171056      -0.283987
47975      H      -0.981221      2.216653      0.738787
47976      H      -0.162983      1.089285      1.853908
47977      Rotational constants (GHz):      1.0713300      0.8930500      0.6772600
47978      Vibrational harmonic frequencies (cm-1):
47979      i2239.8421      55.1703      77.1179
47980      86.4227      115.8523      124.5051
47981      190.8566      206.8840      224.5181
47982      227.9632      282.6172      293.4673
47983      298.3828      337.9132      418.6519
47984      440.4319      466.6032      489.1832
47985      531.4139      615.8708      646.7259
47986      660.0494      776.4732      886.3312
47987      910.3776      935.7614      997.8401
47988      1010.6933      1022.8320      1065.1368
47989      1117.8012      1138.5379      1164.1071
47990      1177.8125      1181.2673      1212.2644
47991      1245.3475      1301.3998      1345.5453
47992      1370.0198      1397.2271      1409.7891
47993      1415.1446      1430.5365      1488.1433
47994      1491.9484      1495.6000      1697.8443
47995      1878.7312      2975.6964      3085.8245
47996      3088.7636      3102.5348      3148.8290
47997      3165.5107      3183.0605      3839.5042

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47998 Zero-point correction (Hartree): 0.150233
47999
48000 TS.diHPCARP_I.17OOHHshift.CR.hpddu
48001 -----
48002 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15355618
48003 Electronic state : 2-A
48004 Cartesian coordinates (Angs):
48005 O -2.725863 -0.703729 0.460164
48006 H -2.336142 0.359386 0.602908
48007 O -1.652642 1.376303 0.627972
48008 O -1.920876 -1.182637 -0.516708
48009 O -0.967873 1.383874 -0.544033
48010 C -0.628362 -1.503602 -0.006117
48011 C 0.360288 0.872460 -0.377459
48012 C 0.375027 -0.633708 -0.756710
48013 C 0.837628 1.249623 1.014270
48014 C 1.224363 1.648261 -1.368419
48015 O 1.586065 0.593718 1.686988
48016 H 0.500463 2.245271 1.341223
48017 H 1.295245 2.696591 -1.082570
48018 H 0.767625 1.588009 -2.355477
48019 H 2.217921 1.206557 -1.403780
48020 H 0.085434 -0.654055 -1.811205
48021 O 1.674896 -1.175377 -0.741012
48022 O 1.930400 -1.825069 0.495737
48023 H 2.105248 -1.070821 1.087128
48024 H -0.624044 -1.357842 1.070459
48025 H -0.418278 -2.547960 -0.234924
48026 Rotational constants (GHz): 1.1818000 0.8856100 0.6969700
48027 Vibrational harmonic frequencies (cm-1):
48028 i2257.3696 54.0607 103.5104
48029 138.3548 165.3119 190.9350
48030 222.5539 238.8964 258.1151
48031 288.6526 316.9109 335.6909
48032 354.1783 372.1289 428.4547
48033 454.0991 516.0819 573.2773
48034 599.5124 612.1849 651.4888
48035 672.1776 789.1688 861.0732
48036 925.9460 956.1019 965.8143
48037 985.7241 1000.2089 1050.1136
48038 1114.8755 1142.0362 1168.4861
48039 1172.0768 1191.2684 1202.3107
48040 1259.3954 1301.2584 1328.1266
48041 1379.2345 1397.0422 1402.1679
48042 1430.7225 1484.5485 1492.2586
48043 1494.6477 1500.5287 1663.7211
48044 1853.8875 3024.8773 3071.7750
48045 3074.4991 3102.5246 3152.2386
48046 3169.0775 3172.8308 3646.8494
48047 Zero-point correction (Hartree): 0.151439
48048
48049
48050
48051 1,7-hydroperoxide-H-shift in (2R,3S)-2-Me-2,4-diOOH-butanal-3-peroxyl (B', R,S-di-
48052 HPCARP-Ib), forming C' (di-HPCARP-Ic)
48053 =====
48054 =====
48055
48056 TS.diHPCARP_Ib.16OOHHshift.a.cmpdu
48057 -----
48058 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14542558
48059 Electronic state : 2-A
48060 Cartesian coordinates (Angs):
48061 O 2.987131 0.061070 0.047794
48062 H 2.357160 -0.898517 0.247883
48063 O 1.385649 -1.583566 0.303035
48064 O 2.107078 1.068984 0.296293
48065 O 0.707868 -1.268115 -0.836228
48066 C 1.152550 1.138362 -0.768032
48067 C 0.110602 0.035462 -0.733768
48068 H 1.698804 1.102430 -1.711313
48069 H 0.660682 2.103613 -0.659802

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48070	H	-0.441010	0.110974	-1.671629	
48071	C	-0.917714	0.094696	0.419043	
48072	C	-0.402332	0.520780	1.790326	
48073	H	0.057509	1.504996	1.737107	
48074	H	0.330540	-0.195001	2.150617	
48075	H	-1.241158	0.556480	2.485427	
48076	C	-2.030216	1.066956	0.037126	
48077	O	-1.501723	-1.173043	0.645083	
48078	O	-1.886754	1.981046	-0.724042	
48079	H	-2.985507	0.872061	0.557816	
48080	O	-2.108717	-1.597443	-0.568373	
48081	H	-1.438606	-2.206017	-0.912776	
48082	Rotational constants (GHz):		1.3777300	0.8075900	0.6535500
48083	Vibrational harmonic frequencies (cm-1):				
48084	i3044.8497		78.0766		94.3720
48085	122.7170		154.1210		162.2951
48086	215.0252		242.2959		255.9079
48087	258.0343		312.4811		318.9437
48088	332.7891		369.8060		398.7987
48089	434.8742		473.8478		536.8377
48090	541.0389		670.0597		684.1250
48091	694.5117		841.2492		903.8924
48092	932.6231		961.2302		971.0161
48093	994.5567		1051.2795		1059.7079
48094	1067.3734		1081.2168		1145.3235
48095	1154.1554		1190.4416		1233.1978
48096	1262.6120		1318.4737		1367.1294
48097	1386.6172		1393.3507		1405.2528
48098	1412.3768		1418.6010		1470.0251
48099	1475.9963		1480.4445		1505.5768
48100	1864.0905		2980.5367		3080.4916
48101	3087.5025		3114.4088		3156.6639
48102	3159.8113		3186.4151		3776.9546
48103	Zero-point correction (Hartree):		0.150909		
48104	TS.diHPCARP_Ib.1600HHshift.a.cmpmud				
48105	-----				
48107	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.14427722		
48108	Electronic state :		2-A		
48109	Cartesian coordinates (Angs):				
48110	O	-3.097487	-0.047192	0.361745	
48111	H	-2.562674	-1.001613	-0.031075	
48112	O	-1.661976	-1.658161	-0.453307	
48113	O	-2.566608	0.947106	-0.398997	
48114	O	-0.572991	-1.118617	0.152965	
48115	C	-1.227694	1.219002	0.026204	
48116	C	-0.250443	0.158226	-0.439474	
48117	H	-1.214431	1.317153	1.113409	
48118	H	-0.993239	2.174713	-0.438779	
48119	H	-0.288032	0.028252	-1.522951	
48120	C	1.188707	0.465964	-0.018620	
48121	C	1.632814	1.848300	-0.492292	
48122	H	1.155435	2.621057	0.107748	
48123	H	1.379172	1.986862	-1.542114	
48124	H	2.710356	1.946669	-0.370374	
48125	C	2.164616	-0.540137	-0.625405	
48126	O	1.342984	0.498454	1.392499	
48127	O	1.978741	-1.065195	-1.683071	
48128	H	3.089483	-0.677936	-0.040908	
48129	O	1.467926	-0.826867	1.891557	
48130	H	0.551215	-1.139516	1.915439	
48131	Rotational constants (GHz):		1.3958200	0.6745900	0.6405200
48132	Vibrational harmonic frequencies (cm-1):				
48133	i2954.7517		55.9873		83.6545
48134	99.2683		149.9679		204.9506
48135	218.0491		236.3275		251.0446
48136	273.7025		289.0399		328.3797
48137	348.2256		360.1010		398.9802
48138	401.6861		455.1114		533.9363
48139	560.3444		573.2662		639.7694
48140	690.7005		875.8742		904.9651
48141	940.7268		972.0210		976.6832

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48142      1001.8975      1052.9474      1059.1999
48143      1100.1338      1108.4384      1140.0192
48144      1150.1049      1183.3652      1227.9133
48145      1251.5778      1305.0166      1336.4739
48146      1374.6860      1399.3215      1409.4085
48147      1426.3572      1447.3799      1468.2424
48148      1487.6165      1487.8605      1510.6374
48149      1873.2771      3006.4206      3074.2713
48150      3082.8056      3103.0204      3150.6639
48151      3157.4232      3162.5812      3768.9870
48152      Zero-point correction (Hartree): 0.150657
48153
48154      TS.diHPCARP_Ib.16OOHHshift.a.cppmud
48155      -----
48156      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14556945
48157      Electronic state : 2-A
48158      Cartesian coordinates (Angs):
48159      O      3.148362      -0.202197      0.184432
48160      H      2.685827      0.823904      -0.092067
48161      O      1.833237      1.624186      -0.351931
48162      O      2.365870      -1.101183      -0.471700
48163      O      0.775869      1.213371      0.398736
48164      C      1.090712      -1.188041      0.175282
48165      C      0.225082      0.006120      -0.168762
48166      H      1.261981      -1.262484      1.250064
48167      H      0.634697      -2.097168      -0.211724
48168      H      0.202210      0.138093      -1.251847
48169      C      -1.209577      -0.088964      0.374329
48170      C      -1.303913      -0.569672      1.818049
48171      H      -0.693234      0.065854      2.457262
48172      H      -0.967324      -1.601563      1.899171
48173      H      -2.339205      -0.512038      2.150550
48174      C      -2.054657      -1.005867      -0.504141
48175      O      -1.829073      1.184301      0.399014
48176      O      -1.618785      -1.939050      -1.114570
48177      H      -3.128774      -0.745690      -0.503773
48178      O      -1.808689      1.711492      -0.919355
48179      H      -1.076387      2.342276      -0.863211
48180      Rotational constants (GHz):      1.3585400      0.7242700      0.5916100
48181      Vibrational harmonic frequencies (cm-1):
48182      i3009.8343      56.8110      71.8885
48183      101.9618      129.4307      156.5089
48184      217.5827      233.6533      248.3376
48185      277.3319      290.7122      305.5061
48186      340.3685      364.2453      379.9975
48187      432.1804      445.3734      527.8549
48188      557.6288      567.2353      657.1833
48189      688.4576      870.6475      897.6353
48190      933.5447      962.6793      985.1382
48191      1021.6181      1046.5039      1054.8827
48192      1103.7765      1118.6352      1139.8283
48193      1151.4388      1184.1999      1241.3741
48194      1269.4420      1312.4461      1328.8198
48195      1381.0259      1397.2229      1407.9550
48196      1411.3232      1426.0191      1465.1799
48197      1487.7321      1494.2459      1504.9200
48198      1869.4132      2983.1671      3075.3074
48199      3086.2538      3104.3518      3155.9739
48200      3161.2092      3163.7660      3782.5751
48201      Zero-point correction (Hartree): 0.150429
48202
48203      TS.diHPCARP_Ib.16OOHHshift.a.httpdu
48204      -----
48205      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14655169
48206      Electronic state : 2-A
48207      Cartesian coordinates (Angs):
48208      O      2.833099      -0.723465      -0.230206
48209      H      2.456326      0.266599      -0.704633
48210      O      1.707772      1.178296      -0.889317
48211      O      1.683813      -1.379870      0.086730
48212      O      1.307586      1.523514      0.365604
48213      C      1.075634      -0.756545      1.225223

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48214	C	0.391102	0.552653	0.882912	
48215	H	1.843872	-0.606667	1.983884	
48216	H	0.328747	-1.470110	1.571941	
48217	H	0.053019	1.006663	1.816786	
48218	C	-0.878944	0.404936	0.008967	
48219	C	-1.315478	1.739115	-0.576445	
48220	H	-0.627402	2.060099	-1.355983	
48221	H	-1.331906	2.494543	0.207635	
48222	H	-2.314404	1.637978	-0.993576	
48223	C	-0.711280	-0.626493	-1.108033	
48224	O	-1.797288	-0.084629	0.977658	
48225	O	-1.264280	-1.692364	-1.087771	
48226	H	-0.080815	-0.316929	-1.955389	
48227	O	-3.064334	-0.293657	0.381754	
48228	H	-2.944584	-1.176775	-0.002029	
48229	Rotational constants (GHz):		1.5198000	0.7563900	0.6559100
48230	Vibrational harmonic frequencies (cm-1):				
48231	i3026.8812		68.8410		101.7455
48232	118.2738		158.9235		202.6571
48233	230.4086		238.5225		267.9683
48234	283.6200		306.6487		336.5399
48235	349.2396		371.6549		390.7609
48236	472.6125		510.0572		528.4077
48237	550.2650		630.0789		693.1144
48238	818.9053		834.0171		860.1294
48239	927.1338		945.0516		965.2709
48240	1018.3384		1050.4794		1057.8439
48241	1064.1631		1085.5660		1144.1408
48242	1148.7773		1187.4486		1198.4089
48243	1260.4199		1312.8432		1358.2968
48244	1377.4802		1398.7124		1403.4581
48245	1415.4903		1447.0191		1464.1013
48246	1481.8151		1489.1240		1501.8659
48247	1845.6379		3027.7962		3082.1240
48248	3087.4774		3098.8158		3153.6002
48249	3160.1014		3173.0358		3743.6202
48250	Zero-point correction (Hartree): 0.151268				
48251	TS.diHPCARP_Ib.16OOHHshift.a.lmppud				
48252	-----				
48253	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14593946				
48254	Electronic state : 2-A				
48255	Cartesian coordinates (Angs):				
48256	O	3.096799	0.148354	0.492747	
48257	H	2.602081	1.044583	-0.058372	
48258	O	1.764547	1.663850	-0.647736	
48259	O	2.594997	-0.947219	-0.139137	
48260	O	0.606271	1.222138	-0.088813	
48261	C	1.215688	-1.111289	0.214892	
48262	C	0.349849	-0.125030	-0.539233	
48263	H	1.103673	-0.982931	1.290382	
48264	H	0.970766	-2.133443	-0.070088	
48265	H	0.602901	-0.144001	-1.602819	
48266	C	-1.148828	-0.406681	-0.364033	
48267	C	-1.629467	-1.436480	-1.383312	
48268	H	-1.028564	-2.341794	-1.316465	
48269	H	-1.550806	-1.036901	-2.393182	
48270	H	-2.667316	-1.689852	-1.177150	
48271	C	-1.936892	0.881197	-0.589068	
48272	O	-1.462579	-0.973610	0.888065	
48273	O	-2.749026	1.292138	0.188869	
48274	H	-1.734311	1.397204	-1.544642	
48275	O	-1.050066	-0.085783	1.915441	
48276	H	-1.808077	0.517887	1.961377	
48277	Rotational constants (GHz):		1.5360200	0.6630100	0.6144100
48278	Vibrational harmonic frequencies (cm-1):				
48279	i3051.4645		75.7222		95.7165
48280	108.1074		167.8821		190.1370
48281	211.5682		231.3090		240.9073
48282	267.2682		311.2441		329.9848
48283	349.8598		372.8613		411.4540
48284	434.4376		467.8246		487.7677

48286	543.6377	588.6200	686.9436			
48287	752.2152	863.6620	905.8338			
48288	931.7054	967.5275	970.8149			
48289	998.9663	1047.7588	1058.3522			
48290	1099.0520	1107.9782	1135.9883			
48291	1146.2426	1185.6571	1217.7379			
48292	1283.9425	1304.2970	1324.4781			
48293	1377.8991	1404.1104	1417.3175			
48294	1425.6709	1433.1345	1461.4061			
48295	1489.2017	1489.7996	1504.6656			
48296	1867.5671	2978.6421	3073.1214			
48297	3079.1372	3102.7323	3157.6025			
48298	3163.5859	3166.4282	3752.5999			
48299	Zero-point correction (Hartree): 0.150860					
48300						
48301	TS.diHPCARP_Ib.16OOHshift.a.lmtmud					
48302	-----					
48303	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14398305					
48304	Electronic state : 2-A					
48305	Cartesian coordinates (Angs):					
48306	O	-3.214420	-0.117317	-0.643838		
48307	H	-2.785075	0.902670	-0.285999		
48308	O	-1.997914	1.672823	0.178438		
48309	O	-2.674802	-1.020574	0.218758		
48310	O	-0.800695	1.191708	-0.249586		
48311	C	-1.280553	-1.180509	-0.068722		
48312	C	-0.484259	-0.012649	0.477565		
48313	H	-1.147540	-1.273194	-1.145427		
48314	H	-0.996426	-2.107758	0.425505		
48315	H	-0.749076	0.168760	1.522724		
48316	C	1.029490	-0.208778	0.366247		
48317	C	1.544049	-1.142487	1.460572		
48318	H	1.027980	-2.099515	1.414172		
48319	H	1.381489	-0.702812	2.444223		
48320	H	2.606874	-1.317791	1.319439		
48321	C	1.692795	1.156529	0.533254		
48322	O	1.250564	-0.718725	-0.933864		
48323	O	2.462319	1.618178	-0.259440		
48324	H	1.437232	1.689535	1.467886		
48325	O	2.632132	-0.980484	-1.113765		
48326	H	2.957947	-0.097399	-1.349637		
48327	Rotational constants (GHz):			1.6309400	0.6232800	0.5424800
48328	Vibrational harmonic frequencies (cm-1):					
48329	i3018.6811		54.4375			93.4215
48330	104.5159		165.3476			171.2042
48331	204.9976		226.3214			245.7585
48332	285.0240		295.3117			330.6882
48333	358.4318		372.0786			393.6246
48334	425.7551		480.1861			505.3758
48335	543.7376		572.9289			688.0637
48336	776.7179		836.1878			899.6988
48337	925.8827		962.5125			975.9311
48338	1008.5071		1049.0245			1062.1941
48339	1096.6694		1108.7243			1138.8590
48340	1145.5971		1193.7913			1216.9414
48341	1260.4581		1306.0184			1335.4104
48342	1372.6136		1403.0470			1417.0576
48343	1426.0436		1451.1239			1462.8362
48344	1487.4607		1490.0745			1508.5794
48345	1868.4017		2970.4491			3076.4261
48346	3081.7280		3105.0166			3153.9535
48347	3167.4089		3176.7977			3746.3567
48348	Zero-point correction (Hartree): 0.150773					
48349						
48350	TS.diHPCARP_Ib.16OOHshift.a.ltp pdu					
48351	-----					
48352	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14064360					
48353	Electronic state : 2-A					
48354	Cartesian coordinates (Angs):					
48355	O	2.863091	-0.219193	-0.370561		
48356	H	2.355276	0.680653	0.175943		
48357	O	1.490653	1.290713	0.714895		

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48358      O      1.825679      -0.834823      -0.999754
48359      O      0.912184      0.380025      1.547562
48360      C      1.005146      -1.492609      -0.027959
48361      C      0.133622      -0.552239      0.784585
48362      H      1.660841      -2.053195      0.639487
48363      H      0.375437      -2.173062      -0.597566
48364      H      -0.336853      -1.164988      1.554605
48365      C      -1.006437      0.168713      0.028061
48366      C      -1.954196      0.851782      0.988406
48367      H      -1.423386      1.627843      1.536118
48368      H      -2.356587      0.131353      1.698723
48369      H      -2.763426      1.322550      0.435138
48370      C      -0.514562      1.154711      -1.054068
48371      O      -1.663593      -0.795413      -0.799133
48372      O      -0.885756      2.289057      -1.095421
48373      H      0.150084      0.721090      -1.816097
48374      O      -2.113745      -1.875137      0.012459
48375      H      -3.070926      -1.756224      -0.020879
48376      Rotational constants (GHz):      1.2518900      0.8326800      0.6886200
48377      Vibrational harmonic frequencies (cm-1):
48378      i3072.7679      39.7729      102.6659
48379      109.0763      126.4706      176.5180
48380      204.6235      228.6587      247.4049
48381      256.4932      275.9099      303.7944
48382      319.7411      342.8418      369.7886
48383      419.8275      477.9194      499.8989
48384      561.4625      622.3940      692.0596
48385      745.2587      822.8841      879.1988
48386      904.2809      955.0473      978.0189
48387      1012.4296      1041.7438      1060.2849
48388      1075.2074      1079.8525      1144.2298
48389      1151.3818      1178.2633      1209.9693
48390      1249.2808      1320.3666      1369.8435
48391      1381.9017      1396.6725      1402.9434
48392      1406.6345      1427.6303      1463.0646
48393      1470.8628      1490.6443      1493.5008
48394      1870.5580      3027.9884      3082.7957
48395      3087.2046      3110.0734      3161.6039
48396      3162.1412      3169.3086      3826.4863
48397      Zero-point correction (Hartree): 0.150329
48398
48399      TS.diHPCARP_Ib.1600HHshift.a.ltpud
48400      -----
48401      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14517921
48402      Electronic state : 2-A
48403      Cartesian coordinates (Angs):
48404      O      3.035099      -0.598949      0.608795
48405      H      2.881840      0.510113      0.326287
48406      O      2.287483      1.473589      -0.073846
48407      O      2.334577      -1.271238      -0.343087
48408      O      1.017126      1.233579      0.341706
48409      C      0.927572      -1.162424      -0.091839
48410      C      0.408408      0.209795      -0.474635
48411      H      0.740733      -1.392130      0.959521
48412      H      0.476454      -1.922780      -0.721600
48413      H      0.664448      0.423752      -1.515180
48414      C      -1.109717      0.416815      -0.289969
48415      C      -1.519167      1.770572      -0.870098
48416      H      -1.309832      1.772363      -1.938800
48417      H      -0.958607      2.573086      -0.396396
48418      H      -2.585178      1.925157      -0.716800
48419      C      -1.522236      0.426648      1.176410
48420      O      -1.853943      -0.521910      -1.035644
48421      O      -2.488684      -0.155811      1.586828
48422      H      -0.901481      1.052449      1.838170
48423      O      -1.785837      -1.806288      -0.431334
48424      H      -2.484114      -1.734225      0.238244
48425      Rotational constants (GHz):      1.4805300      0.6651900      0.5752100
48426      Vibrational harmonic frequencies (cm-1):
48427      i2951.2169      42.2898      86.5993
48428      131.7570      177.0698      197.7776
48429      206.8025      240.4710      244.2854

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48430      277.6309      300.2623      318.1282
48431      335.7488      371.1859      403.4286
48432      433.3653      484.3057      507.5921
48433      534.9336      570.0422      689.3499
48434      738.5778      843.1862      892.9777
48435      929.7811      974.7675      989.3779
48436      1014.6704      1053.7316      1059.5895
48437      1095.1411      1114.2893      1141.7140
48438      1153.1335      1178.9136      1232.4093
48439      1251.6959      1305.0921      1339.8949
48440      1364.9755      1399.4872      1422.7149
48441      1427.9991      1441.6088      1459.0528
48442      1491.7149      1493.7509      1500.0272
48443      1852.3432      3017.2485      3077.1566
48444      3078.7750      3088.5927      3158.8724
48445      3172.1681      3184.4146      3746.6002
48446      Zero-point correction (Hartree): 0.150905
48447
48448      TS.diHPCARP_Ib.16OOHHshift.a.lttmud
48449      -----
48450      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14569205
48451      Electronic state : 2-A
48452      Cartesian coordinates (Angs):
48453      O      3.129093      -0.697397      0.343283
48454      H      2.956130      0.441269      0.233327
48455      O      2.351131      1.454392      0.016078
48456      O      2.361341      -1.239693      -0.640097
48457      O      1.100831      1.168316      0.463744
48458      C      0.979782      -1.151147      -0.277597
48459      C      0.454334      0.260968      -0.446621
48460      H      0.865446      -1.503193      0.750060
48461      H      0.462882      -1.820736      -0.960931
48462      H      0.637300      0.616113      -1.463497
48463      C      -1.049298      0.377064      -0.133118
48464      C      -1.560945      1.780892      -0.427610
48465      H      -1.389138      2.007929      -1.478536
48466      H      -1.034784      2.511218      0.183991
48467      H      -2.627348      1.840834      -0.225179
48468      C      -1.297717      0.038188      1.334146
48469      O      -1.627523      -0.604232      -0.970951
48470      O      -1.902766      -0.938020      1.683528
48471      H      -0.897662      0.761551      2.064513
48472      O      -3.035308      -0.583119      -0.813985
48473      H      -3.144152      -1.172751      -0.051752
48474      Rotational constants (GHz):      1.619990      0.6095500      0.5611700
48475      Vibrational harmonic frequencies (cm-1):
48476      i2966.9554      47.3583      71.8864
48477      114.5147      146.8227      162.8714
48478      213.3506      225.8492      242.7014
48479      268.1524      294.4623      329.4227
48480      361.8017      373.7912      396.9434
48481      431.7128      465.5360      503.2792
48482      539.3400      578.7516      688.6566
48483      742.3065      837.1314      896.6469
48484      927.5430      972.8298      990.8930
48485      1020.7498      1050.9290      1056.5385
48486      1096.6695      1121.3629      1146.1681
48487      1153.2038      1176.9863      1223.7240
48488      1278.9665      1305.9727      1322.0755
48489      1363.3106      1402.1064      1417.4467
48490      1429.6383      1441.9993      1465.5441
48491      1487.5113      1489.6519      1501.0964
48492      1853.4625      2999.7982      3078.0589
48493      3082.7691      3090.3514      3161.9168
48494      3166.0539      3172.8522      3757.3031
48495      Zero-point correction (Hartree): 0.150675
48496
48497      TS.diHPCARP_Ib.16OOHHshift.b.cmpmud
48498      -----
48499      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14513672
48500      Electronic state : 2-A
48501      Cartesian coordinates (Angs):

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48502	O	3.073860	0.046626	-0.436136		
48503	H	2.479947	1.046390	-0.217486		
48504	O	1.587771	1.760316	0.108362		
48505	O	2.426658	-0.871392	0.322056		
48506	O	0.683708	0.879857	0.602691		
48507	C	1.205650	-1.257361	-0.312834		
48508	C	0.280409	-0.043539	-0.430514		
48509	H	0.787202	-1.997126	0.368899		
48510	H	1.420826	-1.711911	-1.280423		
48511	H	0.380021	0.479692	-1.380020		
48512	C	-1.186674	-0.405984	-0.215689		
48513	C	-1.618844	-1.479616	-1.211573		
48514	H	-1.109394	-2.418845	-1.000413		
48515	H	-1.388729	-1.159371	-2.226430		
48516	H	-2.690690	-1.649454	-1.124625		
48517	C	-2.096979	0.801364	-0.420347		
48518	O	-1.418380	-0.972621	1.063749		
48519	O	-1.839157	1.680261	-1.188890		
48520	H	-3.042053	0.758046	0.146299		
48521	O	-1.487199	0.066111	2.032104		
48522	H	-0.556593	0.250135	2.228448		
48523	Rotational constants (GHz):			1.3839800	0.7026800	0.6539600
48524	Vibrational harmonic frequencies (cm-1):					
48525	i2705.6063		40.4263			80.3010
48526	97.4148		141.5424			189.9644
48527	212.7236		237.6404			244.8821
48528	275.7286		312.1667			322.4068
48529	337.4319		383.3430			416.1125
48530	422.8703		452.3171			556.0653
48531	561.1690		615.8137			672.9998
48532	683.8769		814.2944			857.2263
48533	918.5642		941.1540			970.5522
48534	988.5448		999.7269			1052.1923
48535	1077.7196		1125.2631			1141.6941
48536	1168.9287		1189.0068			1242.7159
48537	1258.8131		1295.7607			1345.8160
48538	1379.5929		1400.8231			1410.2884
48539	1417.2218		1446.0242			1486.9743
48540	1489.9593		1507.5264			1700.9283
48541	1873.1936		3006.1825			3074.6047
48542	3082.9470		3130.5968			3148.6937
48543	3153.0146		3161.3184			3772.7227
48544	Zero-point correction (Hartree):			0.151015		
48545	TS.diHPCARP_Ib.16OOHHshift.b.cppmud					
48546	-----					
48547	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14560090					
48548	Electronic state : 2-A					
48549	Cartesian coordinates (Angs):					
48551	O	2.998427	-0.206386	-0.623978		
48552	H	2.548635	0.869363	-0.460965		
48553	O	1.781079	1.716160	-0.103898		
48554	O	2.399468	-0.946383	0.339746		
48555	O	0.931128	0.997260	0.669591		
48556	C	1.061957	-1.276818	-0.058420		
48557	C	0.250381	0.022082	-0.144867		
48558	H	0.713691	-1.938828	0.730092		
48559	H	1.078000	-1.814476	-1.002751		
48560	H	0.245455	0.402579	-1.164163		
48561	C	-1.189596	-0.045411	0.363083		
48562	C	-1.308555	-0.384261	1.845203		
48563	H	-0.754530	0.347944	2.428935		
48564	H	-0.919672	-1.379137	2.048023		
48565	H	-2.356342	-0.351729	2.139278		
48566	C	-2.003496	-1.048524	-0.442141		
48567	O	-1.819412	1.222187	0.259953		
48568	O	-1.529547	-2.006355	-0.983206		
48569	H	-3.086867	-0.832380	-0.458433		
48570	O	-1.893284	1.571175	-1.117204		
48571	H	-1.275392	2.312993	-1.165186		
48572	Rotational constants (GHz):			1.3552200	0.7314900	0.6077100
48573	Vibrational harmonic frequencies (cm-1):					

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48574      i2653.7676          44.6193          48.9006
48575      85.2088             141.5715         150.6475
48576      191.3664             229.5140         243.7017
48577      261.0407             307.8512         318.9886
48578      334.1580             360.7063         369.8047
48579      430.0156             464.5582         529.6280
48580      559.5860             644.5873         658.1003
48581      681.0941             831.9326         835.8943
48582      930.6125             940.4654         959.2670
48583      978.4293             1032.0515        1049.1606
48584      1072.2602            1122.9495        1150.8558
48585      1168.3663            1193.6301        1246.5530
48586      1270.2234            1290.8558        1354.3980
48587      1375.9352            1393.5073        1405.2603
48588      1411.3112            1412.7396        1481.0568
48589      1495.9807            1505.1666        1711.8742
48590      1867.1837            2987.6205        3083.4026
48591      3121.1722            3132.5951        3160.8825
48592      3171.7025            3182.9356        3803.6326
48593      Zero-point correction (Hartree): 0.150786
48594
48595      TS.diHPCARP_Ib.1600HHshift.b.lmppud
48596      -----
48597      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14526001
48598      Electronic state : 2-A
48599      Cartesian coordinates (Angs):
48600      O      -3.127268          -0.016618          0.295761
48601      H      -2.564458          1.018741          0.350149
48602      O      -1.664145          1.804895          0.286006
48603      O      -2.417511          -0.712298         -0.625490
48604      O      -0.709332          1.070842         -0.341167
48605      C      -1.222440          -1.237378         -0.039408
48606      C      -0.384949          -0.072827          0.482076
48607      H      -0.723698          -1.740569         -0.863189
48608      H      -1.478898          -1.947927          0.747590
48609      H      -0.672880          0.201851          1.496855
48610      C      1.127386          -0.327075          0.461653
48611      C      1.554281          -1.114856          1.697447
48612      H      0.984580          -2.040634          1.764144
48613      H      1.384532          -0.530047          2.600149
48614      H      2.611620          -1.360033          1.622473
48615      C      1.839024          1.022930          0.464095
48616      O      1.555749          -1.111216         -0.625833
48617      O      2.678679          1.318445         -0.336181
48618      H      1.539836          1.712596          1.274816
48619      O      1.132780          -0.489967         -1.829428
48620      H      1.847925          0.148593         -1.977506
48621      Rotational constants (GHz):      1.5276500      0.6807600      0.6309700
48622      Vibrational harmonic frequencies (cm-1):
48623      i2758.6151          57.7026          80.5713
48624      99.2194             164.6216         173.7754
48625      214.5895            224.2844         263.7618
48626      284.2020            317.3724         324.8155
48627      369.8485            381.8637         400.2743
48628      457.0557            458.5650         479.6428
48629      578.0933            642.0969         673.5097
48630      749.8075            851.9313         865.3872
48631      893.1128            933.1833         971.2148
48632      996.1363            1001.8281        1051.8337
48633      1069.7266           1128.8835        1135.1691
48634      1163.8581           1195.6631        1216.5232
48635      1287.6223           1293.2608        1343.7554
48636      1387.3919           1402.2608        1413.0864
48637      1420.4713           1428.5916        1488.0949
48638      1490.9997           1505.4927        1702.5722
48639      1869.2272           2969.2482        3076.1075
48640      3085.1543           3105.9482        3154.7308
48641      3163.9684           3177.1125        3754.0131
48642      Zero-point correction (Hartree): 0.151246
48643
48644      TS.diHPCARP_Ib.1600HHshift.b.lmtud
48645      -----

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48646 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14356109
48647 Electronic state : 2-A
48648 Cartesian coordinates (Angs):
48649 O -3.269317 -0.141891 0.165465
48650 H -2.758850 0.923156 0.130494
48651 O -1.899085 1.741479 0.013031
48652 O -2.483054 -0.890630 -0.645262
48653 O -0.885767 1.008505 -0.515156
48654 C -1.294787 -1.278281 0.047721
48655 C -0.510399 -0.017824 0.423550
48656 H -0.747918 -1.876438 -0.677253
48657 H -1.558187 -1.876242 0.920605
48658 H -0.785655 0.346463 1.413748
48659 C 1.005005 -0.196698 0.376140
48660 C 1.455645 -1.136203 1.494247
48661 H 0.953892 -2.097669 1.392417
48662 H 1.216652 -0.714524 2.470326
48663 H 2.527587 -1.298910 1.427969
48664 C 1.641868 1.175435 0.569642
48665 O 1.295056 -0.703704 -0.909383
48666 O 2.433351 1.651647 -0.191867
48667 H 1.335166 1.708611 1.489566
48668 O 2.686137 -0.955261 -1.014640
48669 H 3.014758 -0.074180 -1.253175
48670 Rotational constants (GHz): 1.6471800 0.6364400 0.5524900
48671 Vibrational harmonic frequencies (cm-1):
48672 i2719.2749 52.8743 63.0295
48673 88.8812 156.3335 180.8792
48674 191.3603 226.8857 271.6815
48675 280.1204 299.8833 326.7457
48676 365.9816 380.4794 409.6615
48677 435.5460 472.8358 503.0685
48678 570.0428 638.1560 672.5704
48679 769.9305 833.2946 838.2587
48680 893.6675 925.7694 970.0379
48681 991.0194 1010.7537 1054.1935
48682 1078.8278 1124.1163 1140.9105
48683 1166.9563 1194.5282 1227.6065
48684 1271.3405 1294.4976 1355.3099
48685 1376.1325 1401.9957 1413.7974
48686 1422.7709 1449.1512 1486.4339
48687 1490.5280 1507.5249 1701.8928
48688 1869.8289 2963.1841 3076.7894
48689 3087.0060 3102.4364 3148.9261
48690 3166.7249 3177.4969 3753.9891
48691 Zero-point correction (Hartree): 0.151099
48692
48693 TS.diHPCARP_Ib.1600HHshift.b.ltpud
48694 -----
48695 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14612492
48696 Electronic state : 2-A
48697 Cartesian coordinates (Angs):
48698 O 3.034081 -0.702638 -0.295149
48699 H 2.846569 0.455374 -0.255946
48700 O 2.260173 1.488948 -0.075963
48701 O 2.144169 -1.194654 0.599906
48702 O 1.131479 1.049380 0.533464
48703 C 0.834834 -1.249479 0.017328
48704 C 0.407943 0.173945 -0.357185
48705 H 0.220639 -1.668216 0.812453
48706 H 0.830379 -1.922162 -0.837345
48707 H 0.700339 0.426538 -1.375482
48708 C -1.088666 0.503121 -0.206328
48709 C -1.344763 1.977308 -0.500581
48710 H -0.982942 2.211770 -1.500470
48711 H -0.824999 2.605841 0.218521
48712 H -2.414026 2.174100 -0.453693
48713 C -1.572546 0.209634 1.205634
48714 O -1.851373 -0.189966 -1.167824
48715 O -2.526094 -0.478120 1.446288
48716 H -0.990879 0.694149 2.010396
48717 O -1.737513 -1.589308 -0.949402

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48718      H      -2.445265      -1.733692      -0.302216
48719 Rotational constants (GHz):      1.4915700      0.6810500      0.5924900
48720 Vibrational harmonic frequencies (cm-1):
48721      i2685.1501      43.2563      84.3329
48722      112.3541      162.6487      190.9969
48723      202.2171      210.8199      260.5523
48724      294.7147      315.8474      334.0361
48725      337.2832      370.0236      424.6072
48726      440.0570      477.0695      492.0012
48727      565.3894      624.1450      677.8238
48728      733.2925      838.7448      840.9566
48729      901.7955      932.2694      973.9185
48730      985.8482      1020.5366      1053.5247
48731      1081.2825      1107.1874      1149.8380
48732      1167.0722      1198.1577      1240.6227
48733      1257.0813      1292.2946      1350.8473
48734      1360.1023      1401.5974      1407.5383
48735      1420.4651      1432.2005      1485.4492
48736      1491.6534      1499.5038      1708.2347
48737      1857.0459      2983.2165      3080.4182
48738      3106.5003      3117.7596      3160.0621
48739      3167.0896      3172.2422      3755.6110
48740 Zero-point correction (Hartree): 0.151161
48741
48742 TS.diHPCARP_Ib.16OOHHshift.b.lttmud
48743 -----
48744 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14590825
48745 Electronic state : 2-A
48746 Cartesian coordinates (Angs):
48747      O      3.137622      -0.587408      -0.492419
48748      H      2.920665      0.524191      -0.203041
48749      O      2.311460      1.488939      0.182833
48750      O      2.222298      -1.287271      0.221378
48751      O      1.180650      0.923212      0.671803
48752      C      0.940948      -1.200687      -0.410868
48753      C      0.475683      0.259801      -0.391417
48754      H      0.300126      -1.834281      0.200449
48755      H      0.995692      -1.601218      -1.421725
48756      H      0.711021      0.778116      -1.320209
48757      C      -1.026266      0.410861      -0.106086
48758      C      -1.478632      1.854526      -0.263083
48759      H      -1.297502      2.174181      -1.287885
48760      H      -0.917827      2.497063      0.414280
48761      H      -2.540869      1.946456      -0.049639
48762      C      -1.326572      -0.074119      1.309223
48763      O      -1.598621      -0.459015      -1.061434
48764      O      -1.941460      -1.080328      1.534830
48765      H      -0.952042      0.568615      2.123381
48766      O      -3.009669      -0.429805      -0.935912
48767      H      -3.148466      -1.102011      -0.250856
48768 Rotational constants (GHz):      1.6381900      0.6226900      0.5714000
48769 Vibrational harmonic frequencies (cm-1):
48770      i2685.0963      49.3911      69.9180
48771      106.5996      133.5369      170.0889
48772      209.5016      235.3238      246.3677
48773      282.5227      322.5064      340.4602
48774      351.4904      369.6605      420.1148
48775      441.6457      466.3871      496.4952
48776      580.0972      628.5423      677.4012
48777      739.1853      811.4069      836.7913
48778      897.2618      930.8634      972.4724
48779      996.7434      1016.2978      1053.5349
48780      1092.8797      1118.1806      1152.7621
48781      1168.4597      1198.3527      1227.0629
48782      1278.8342      1293.9050      1349.7487
48783      1356.9031      1402.7078      1411.0904
48784      1422.0608      1439.9355      1488.4126
48785      1494.1321      1502.4274      1700.1711
48786      1853.2864      3006.5529      3079.9880
48787      3101.1364      3113.6855      3158.5099
48788      3161.1933      3169.4205      3756.1045
48789 Zero-point correction (Hartree): 0.151158

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48790
48791 TS.diHPCARP_Ib.1600HHshift.b.pmpud
48792 -----
48793 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14377047
48794 Electronic state : 2-A
48795 Cartesian coordinates (Angs):
48796 O -3.071075 0.047667 0.015896
48797 H -2.524368 1.081614 -0.181439
48798 O -1.642235 1.863410 -0.311768
48799 O -2.028332 -0.817143 0.078030
48800 O -0.581711 1.089192 -0.641478
48801 C -1.135057 -0.428580 1.137954
48802 C -0.041421 0.453500 0.531588
48803 H -0.738857 -1.343838 1.568929
48804 H -1.723161 0.106706 1.878964
48805 H 0.274044 1.225624 1.237265
48806 C 1.230182 -0.242543 0.035281
48807 C 1.937548 -1.007016 1.146989
48808 H 1.349563 -1.867049 1.456759
48809 H 2.111298 -0.348089 1.996419
48810 H 2.898184 -1.368234 0.782689
48811 C 2.184191 0.843072 -0.474649
48812 O 1.022199 -1.043366 -1.114771
48813 O 2.486707 1.784970 0.197186
48814 H 2.594064 0.673446 -1.484201
48815 O 0.232064 -2.169554 -0.772643
48816 H -0.634366 -1.912186 -1.121972
48817 Rotational constants (GHz): 1.3947400 0.7859600 0.6172500
48818 Vibrational harmonic frequencies (cm-1):
48819 i2745.6926 47.4838 80.3308
48820 106.7511 160.6129 166.6455
48821 216.2772 231.3786 238.9154
48822 266.2098 307.4071 319.1819
48823 331.9440 391.0198 437.1054
48824 450.1079 463.6032 510.3515
48825 559.4851 641.2339 683.2874
48826 743.5258 782.1706 828.3235
48827 915.4059 920.1778 957.3283
48828 991.2199 1029.8035 1046.3799
48829 1062.7659 1110.9621 1147.6496
48830 1165.6491 1188.3374 1226.3768
48831 1267.3668 1293.7636 1352.5933
48832 1385.3825 1395.7356 1396.9694
48833 1409.9134 1440.0019 1482.6025
48834 1490.7376 1513.8103 1700.7700
48835 1871.8847 3007.9490 3078.8805
48836 3088.6802 3119.6332 3153.2283
48837 3171.6159 3180.5659 3765.6891
48838 Zero-point correction (Hartree): 0.151027
48839
48840 TS.diHPCARP_Ib.1600HHshift.b.pmpud
48841 -----
48842 IRC pathway available
48843 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.17358521
48844 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.05049003
48845 T1 diagnostic: 0.025657
48846 E(MP2/Aug-CC-pVTZ) (Hartree): -721.00668290
48847 E(MP3/Aug-CC-pVTZ) (Hartree): -721.02254436
48848 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.01674488
48849 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.02827625
48850 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.47633207
48851 E(UHF/Aug-CC-pVTZ) (Hartree): -718.46218137
48852 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.14691999
48853 Electronic state : 2-A
48854 Cartesian coordinates (Angs):
48855 O 3.026758 -0.139288 0.078099
48856 H 2.545102 0.952317 0.079296
48857 O 1.709318 1.784573 0.026257
48858 O 1.925784 -0.932299 0.048535
48859 O 0.588586 1.121417 0.396809
48860 C 1.151927 -0.640594 -1.129657
48861 C 0.073233 0.361788 -0.715592

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48862      H      0.726499      -1.585520      -1.458888
48863      H      1.827820      -0.247987      -1.884247
48864      H      -0.180813      1.059643      -1.514721
48865      C      -1.202894      -0.331539      -0.223184
48866      C      -1.993957      -0.883247      -1.405909
48867      H      -1.403652      -1.608010      -1.964548
48868      H      -2.285704      -0.065398      -2.061133
48869      H      -2.888150      -1.384850      -1.040502
48870      C      -2.112557      0.647855      0.515785
48871      O      -0.926523      -1.460186      0.585521
48872      O      -2.359610      1.733203      0.077250
48873      H      -2.567113      0.254063      1.439401
48874      O      -0.437631      -1.024284      1.846185
48875      H      0.518041      -0.964911      1.687449
48876      Rotational constants (GHz):      1.4434000      0.7598300      0.6752800
48877      Vibrational harmonic frequencies (cm-1):
48878      i2707.7150      82.2351      85.7563
48879      97.3784      144.1289      202.2102
48880      208.7549      224.5766      254.8342
48881      284.4192      300.7294      328.9950
48882      338.5796      383.1293      393.3290
48883      458.9815      499.9293      541.9911
48884      553.8255      627.0558      682.1145
48885      745.7591      792.9715      836.5654
48886      921.0129      939.7643      959.9423
48887      969.3558      1026.0771      1031.7668
48888      1058.8412      1104.7807      1138.2889
48889      1160.8260      1185.8790      1247.8771
48890      1251.9002      1290.3948      1342.0481
48891      1372.7057      1389.4128      1398.6993
48892      1409.9919      1456.7298      1483.2541
48893      1491.0384      1507.0472      1704.8664
48894      1868.7665      3011.0423      3078.4531
48895      3101.2260      3117.0520      3154.6848
48896      3168.2527      3177.0868      3740.9798
48897      Zero-point correction (Hartree): 0.151107
48898
48899
48900
48901      1,4-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,S-
48902      di-HPCARP-Ia), forming OH + dihydroperoxide-keto-aldehyde
48903      =====
48904      =====
48905
48906      TS.diHPCARP_I.14HPHshift.mppmtd
48907      -----
48908      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12617375
48909      Electronic state : 2-A
48910      Cartesian coordinates (Angs):
48911      C      0.263306      -0.546122      -0.474426
48912      C      0.370192      0.659827      0.519817
48913      O      -0.342429      0.158053      1.650128
48914      O      0.121131      -1.142342      1.826958
48915      H      0.210719      -1.350464      0.567843
48916      C      1.790023      1.072111      0.866570
48917      C      -0.405075      1.872839      0.028394
48918      H      2.334486      1.318991      -0.042470
48919      H      2.295075      0.265028      1.387348
48920      H      1.754294      1.951911      1.508373
48921      O      -0.156298      2.393266      -1.021112
48922      H      -1.182964      2.251567      0.713133
48923      O      1.299995      -0.837022      -1.310154
48924      O      2.457046      -1.221452      -0.573050
48925      H      2.621236      -2.095200      -0.951749
48926      C      -0.993903      -0.584137      -1.325701
48927      O      -2.116973      -0.106575      -0.631530
48928      H      -0.870014      0.096375      -2.172038
48929      H      -1.168467      -1.595397      -1.694062
48930      O      -2.517258      -1.105869      0.293910
48931      H      -2.103331      -0.794397      1.114498
48932      Rotational constants (GHz):      1.0947700      0.8615100      0.7889100
48933      Vibrational harmonic frequencies (cm-1):

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48934      i2126.5827          80.1138          89.6309
48935      117.3742           165.3003         178.6385
48936      185.0123           194.7920         216.1413
48937      227.1573           234.8638         276.8962
48938      314.6492           322.2969         381.2620
48939      412.7624           453.2019         470.9003
48940      498.4314           520.0230         586.9852
48941      643.4078           709.9296         733.4324
48942      909.4256           940.2986         960.2852
48943      992.8546           1010.2106        1037.3150
48944      1058.0132          1113.8797        1143.5313
48945      1146.6296          1174.7132        1218.0262
48946      1245.5181          1282.9008        1295.5652
48947      1393.9485          1396.3859        1408.6094
48948      1430.0005          1439.2792        1462.1390
48949      1488.2260          1501.4538        1764.4583
48950      1860.7270          2993.8775        3068.5851
48951      3080.7335          3124.8226        3156.8262
48952      3193.0898          3751.9054        3812.5463
48953      Zero-point correction (Hartree): 0.150063
48954
48955      TS.diHPCARP_I.14HPHshift.mptmmtd
48956      -----
48957      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12584309
48958      Electronic state : 2-A
48959      Cartesian coordinates (Angs):
48960      C      0.255727      -0.547295      -0.486520
48961      C      0.376442      0.635441      0.535075
48962      O     -0.354902      0.125054      1.646896
48963      O      0.084308     -1.186009      1.802920
48964      H      0.184240     -1.372647      0.537323
48965      C      1.798988      1.015284      0.907738
48966      C     -0.368463      1.872275      0.056129
48967      H      2.346429      1.306062      0.012667
48968      H      2.292764      0.182143      1.397025
48969      H      1.768912      1.867804      1.585735
48970      O     -0.072398      2.421053     -0.966815
48971      H     -1.169448      2.237915      0.720315
48972      O      1.286359     -0.841996     -1.323912
48973      O      2.380960     -1.369772     -0.576250
48974      H      3.125247     -0.959420     -1.035883
48975      C     -1.000475     -0.551001     -1.340220
48976      O     -2.114638     -0.050287     -0.647769
48977      H     -0.858327      0.130362     -2.183359
48978      H     -1.195339     -1.556078     -1.714338
48979      O     -2.552467     -1.049709      0.260104
48980      H     -2.125562     -0.771034      1.085924
48981      Rotational constants (GHz):      1.0925100      0.8626700      0.7883500
48982      Vibrational harmonic frequencies (cm-1):
48983      i2133.1475          78.9468          87.4746
48984      103.5365           124.2497         178.3616
48985      183.1893           195.7493         217.5262
48986      227.7611           235.2064         278.6286
48987      311.7763           323.3539         379.3104
48988      412.7017           455.3026         471.5195
48989      503.8062           520.4930         587.2090
48990      640.5965           710.8428         735.1629
48991      909.3170           940.2268         958.9913
48992      992.4704           1014.6033        1037.5046
48993      1058.3786          1117.2375        1144.8500
48994      1146.6918          1174.7125        1220.0506
48995      1244.8413          1285.0928        1296.0794
48996      1392.1057          1395.8109        1407.5342
48997      1432.0439          1440.1937        1461.8698
48998      1489.8192          1499.4290        1759.5616
48999      1858.6340          3000.2947        3067.5723
49000      3078.1606          3126.7365        3149.1656
49001      3192.1618          3750.9138        3822.3844
49002      Zero-point correction (Hartree): 0.149968
49003
49004      TS.diHPCARP_I.14HPHshift.mtppptd
49005      -----

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49006 IRC pathway available
49007 E(CCS(D(T)/Aug-CC-pVTZ) (Hartree): -721.16066851
49008 E(CCS(D/Aug-CC-pVTZ) (Hartree): -721.03881510
49009 T1 diagnostic: 0.022879
49010 E(MP2/Aug-CC-pVTZ) (Hartree): -720.99744736
49011 E(MP3/Aug-CC-pVTZ) (Hartree): -721.01390962
49012 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.00572614
49013 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.01891557
49014 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.46663936
49015 E(UHF/Aug-CC-pVTZ) (Hartree): -718.45522397
49016 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13353156
49017 Electronic state : 2-A
49018 Cartesian coordinates (Angs):
49019 C -0.029189 -0.770541 -0.048801
49020 C -1.121338 0.312213 0.147614
49021 O -1.959838 0.032599 -0.965343
49022 O -2.164146 -1.342779 -0.911828
49023 H -0.965759 -1.586904 -0.444155
49024 C -1.831013 0.190843 1.484782
49025 C -0.575104 1.716919 -0.051804
49026 H -1.147159 0.455946 2.287099
49027 H -2.186476 -0.826083 1.628148
49028 H -2.680197 0.872264 1.497023
49029 O 0.146251 2.240273 0.755631
49030 H -0.887716 2.225666 -0.978734
49031 O 0.563867 -1.048357 1.150202
49032 O 1.751120 -1.800256 1.005646
49033 H 2.395237 -1.092261 0.826271
49034 C 0.851159 -0.603836 -1.266374
49035 O 1.528010 0.643643 -1.288482
49036 H 1.555602 -1.428284 -1.351956
49037 H 0.214061 -0.570749 -2.149387
49038 O 2.385863 0.713033 -0.158405
49039 H 1.926285 1.371563 0.393836
49040 Rotational constants (GHz): 1.1963900 0.8703200 0.7530100
49041 Vibrational harmonic frequencies (cm-1):
49042 i2050.2337 84.7480 133.2844
49043 144.4517 172.3144 187.9931
49044 195.1285 217.8516 233.7847
49045 240.1071 272.4346 287.5796
49046 323.9816 366.1608 402.0284
49047 457.7281 468.1649 483.1043
49048 534.4884 552.2656 579.6335
49049 707.3480 736.5605 817.4230
49050 897.0546 913.9506 955.0696
49051 981.4234 1006.8394 1035.9823
49052 1046.1993 1093.6995 1129.5146
49053 1170.5638 1193.3500 1233.2538
49054 1263.3554 1307.8519 1343.3597
49055 1388.0299 1395.4097 1409.9528
49056 1462.3611 1470.1493 1479.0655
49057 1488.7160 1498.7119 1781.1856
49058 1838.9531 3009.9684 3085.9199
49059 3108.9679 3163.1863 3165.8050
49060 3183.7077 3667.6002 3686.3221
49061 Zero-point correction (Hartree): 0.151393
49062
49063 TS.diHPCARP_I.14HPHshift.mttmtd
49064 -----
49065 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.12730593
49066 Electronic state : 2-A
49067 Cartesian coordinates (Angs):
49068 C -0.481698 -0.463349 -0.250996
49069 C -0.094440 1.033755 -0.128580
49070 O 1.054147 1.112026 -0.971117
49071 O 0.701546 0.407148 -2.125020
49072 H 0.010339 -0.489857 -1.441239
49073 C -1.198545 1.972746 -0.586563
49074 C 0.363470 1.400473 1.274702
49075 H -2.047384 1.903361 0.089518
49076 H -1.510386 1.717804 -1.596300
49077 H -0.816498 2.992534 -0.577702

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49078 O -0.352912 1.253520 2.223323
49079 H 1.377758 1.826328 1.351825
49080 O -1.840994 -0.597391 -0.265140
49081 O -2.160676 -1.983652 -0.218032
49082 H -3.048387 -1.938837 0.159198
49083 C 0.253652 -1.435866 0.663352
49084 O 1.561148 -0.993913 0.930356
49085 H -0.254224 -1.440369 1.631586
49086 H 0.268643 -2.442776 0.253402
49087 O 2.364709 -1.288968 -0.201907
49088 H 2.349766 -0.444904 -0.681477
49089 Rotational constants (GHz): 0.9665700 0.9120300 0.7995400
49090 Vibrational harmonic frequencies (cm-1):
49091 i1898.2964 73.5012 85.8629
49092 101.2000 105.8105 135.4010
49093 176.9402 194.2359 208.3664
49094 217.7786 249.8362 262.6238
49095 288.7094 328.2302 355.2508
49096 410.0712 452.5274 472.5414
49097 481.0388 516.7729 601.3996
49098 625.4799 702.3394 766.5144
49099 914.8541 945.2405 962.4463
49100 989.7354 1020.5668 1034.3953
49101 1068.6315 1127.1771 1141.3670
49102 1159.5081 1199.1884 1238.5954
49103 1244.3356 1292.7361 1301.8956
49104 1391.6726 1394.3983 1407.6538
49105 1439.5998 1454.7552 1460.9126
49106 1490.3998 1499.1003 1765.1215
49107 1861.5175 3001.2706 3074.3940
49108 3082.6050 3151.2632 3161.6375
49109 3178.5347 3719.6736 3834.0426
49110 Zero-point correction (Hartree): 0.149953
49111
49112
49113
49114 1,5-alpha-hydroperoxide-H-shift in (2R,3S)-2-Me-3,4-diOOH-butanal-2-peroxyl (A', R,R-
49115 di-HPCARP-Ia), forming OH + dihydroperoxide-dialdehyde
49116 =====
49117 =====
49118
49119 TS.diHPCARP_I.15HPHshift.dcmumudu
49120 -----
49121 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13701735
49122 Electronic state : 2-A
49123 Cartesian coordinates (Angs):
49124 O -0.959759 -0.218098 1.498876
49125 O 0.321778 -0.573897 1.897613
49126 H 0.978120 0.173530 1.178932
49127 C 1.202913 0.675854 -0.010539
49128 C -0.131952 0.478117 -0.695444
49129 C -1.060771 -0.466987 0.108843
49130 C -2.522903 -0.288294 -0.264328
49131 H -2.638701 -0.390470 -1.341554
49132 H -2.854662 0.701134 0.040547
49133 H -3.127612 -1.042999 0.236635
49134 C -0.673488 -1.921889 -0.146617
49135 O -0.282373 -2.326522 -1.202878
49136 H -0.846290 -2.584671 0.719408
49137 H 0.028081 0.002584 -1.667007
49138 O -0.747471 1.703682 -1.019632
49139 O -0.980040 2.396953 0.209437
49140 H -0.703955 3.288590 -0.034304
49141 H 1.515046 1.707051 0.145752
49142 O 2.155582 -0.107298 -0.622043
49143 O 3.394347 0.126605 0.028192
49144 H 3.550667 -0.726947 0.453577
49145 Rotational constants (GHz): 1.0883400 0.8288000 0.6596100
49146 Vibrational harmonic frequencies (cm-1):
49147 i1907.3004 30.1507 74.0731
49148 96.0430 133.4798 146.5446
49149 159.5737 190.9000 193.9459

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49150      219.3526      234.9587      268.7859
49151      295.6006      318.2087      331.5292
49152      352.4404      374.4099      463.1004
49153      525.1356      585.3100      604.0308
49154      683.6339      698.8429      853.5464
49155      934.7521      957.8443      964.3574
49156      980.4427      1010.2780     1027.1509
49157      1076.1453     1091.2212     1131.0865
49158      1157.0558     1207.5662     1226.0123
49159      1238.1163     1268.1449     1290.0724
49160      1323.8911     1383.4393     1396.6166
49161      1408.1829     1420.5547     1433.5544
49162      1483.9347     1502.5399     1582.6369
49163      1867.2608     2993.8341     3079.7128
49164      3088.1853     3127.8545     3158.4644
49165      3176.0683     3812.0905     3836.6573
49166      Zero-point correction (Hartree): 0.149150
49167
49168      TS.diHPCARP_I.15HPHshift.dcmupddu
49169      -----
49170      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13644197
49171      Electronic state : 2-A
49172      Cartesian coordinates (Angs):
49173      O      -0.951176     -0.499988      1.472660
49174      O      0.320858     -0.597896      2.022471
49175      H      0.857628      0.336992      1.438581
49176      C      0.966151      1.125897      0.400169
49177      C     -0.053590      0.523000     -0.555384
49178      C     -0.820585     -0.667537      0.067504
49179      C     -2.225785     -0.822935     -0.492346
49180      H     -2.175437     -0.882177     -1.577564
49181      H     -2.831984      0.032010     -0.206256
49182      H     -2.676838     -1.734473     -0.102047
49183      C     -0.089401     -1.983974     -0.187223
49184      O      0.459109     -2.247020     -1.217152
49185      H     -0.179131     -2.706852      0.642701
49186      H      0.462293      0.146905     -1.440852
49187      O     -0.915223      1.517848     -1.078071
49188      O     -1.631430      2.090618      0.019361
49189      H     -1.601770      3.024922     -0.218457
49190      H      0.697898      2.111135      0.771699
49191      O      2.272603      1.190654     -0.023410
49192      O      2.642412     -0.073222     -0.552400
49193      H      3.209365     -0.423109      0.148199
49194      Rotational constants (GHz): 1.0350200 0.9234700 0.7141800
49195      Vibrational harmonic frequencies (cm-1):
49196      i1907.9227      41.8434      77.6734
49197      122.7739      147.9373      160.7574
49198      185.8792      205.6468      211.6171
49199      240.1571      256.4850      271.5226
49200      295.0377      306.9820      331.2295
49201      365.1895      425.5768      464.7018
49202      555.1580      564.6517      594.4110
49203      670.8302      682.5813      866.6833
49204      917.0684      933.7318      955.3843
49205      977.4142      980.0389      996.3951
49206      1068.9583      1084.2246     1120.3615
49207      1149.4108      1191.0860     1222.3253
49208      1233.2455      1242.5323     1284.9686
49209      1335.6081      1388.6601     1394.7462
49210      1407.8032      1408.9533     1433.2283
49211      1484.0772      1504.4081     1623.0752
49212      1870.1496      2987.6659     3081.3823
49213      3108.4014      3159.1566     3164.1954
49214      3183.2336      3802.8220     3838.1436
49215      Zero-point correction (Hartree): 0.149398
49216
49217      TS.diHPCARP_I.15HPHshift.dcmutduu
49218      -----
49219      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13715849
49220      Electronic state : 2-A
49221      Cartesian coordinates (Angs):

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49222	O	2.052552	-0.325903	-0.840269		
49223	O	1.579282	-1.624875	-0.888276		
49224	H	0.415798	-1.452392	-1.239340		
49225	C	-0.731573	-0.814382	-1.074189		
49226	C	-0.147989	0.543990	-0.744622		
49227	C	1.197195	0.414214	0.014216		
49228	C	1.856610	1.764092	0.237701		
49229	H	1.201764	2.396004	0.832548		
49230	H	2.035414	2.239744	-0.725540		
49231	H	2.809644	1.636692	0.749359		
49232	C	1.120568	-0.317822	1.350809		
49233	O	0.167088	-0.343887	2.076501		
49234	H	2.077533	-0.790155	1.633842		
49235	H	0.086954	1.017112	-1.703875		
49236	O	-0.957285	1.411796	0.018374		
49237	O	-2.184937	1.571842	-0.669490		
49238	H	-2.704595	0.851748	-0.271542		
49239	H	-1.248666	-0.887066	-2.030801		
49240	O	-1.288143	-1.592829	-0.082177		
49241	O	-2.220085	-0.850168	0.714397		
49242	H	-1.630502	-0.520059	1.419378		
49243	Rotational constants (GHz):			1.2432400	0.8695000	0.7718400
49244	Vibrational harmonic frequencies (cm-1):					
49245	i2059.8533		85.9034			116.3783
49246	156.9504		184.1787			196.8980
49247	201.8305		214.0711			236.1898
49248	254.5673		283.0455			304.1705
49249	317.6204		386.4348			399.8848
49250	429.8233		520.2411			536.5077
49251	559.3683		627.4003			641.9312
49252	686.2532		763.3014			838.3560
49253	882.4733		928.6655			947.7187
49254	972.2108		996.8974			1029.7990
49255	1050.3588		1080.1966			1143.7646
49256	1174.4479		1205.4055			1213.5214
49257	1235.7674		1272.8874			1332.6345
49258	1364.3325		1394.3251			1405.0515
49259	1416.6747		1454.9384			1468.2996
49260	1488.5860		1498.8287			1549.9999
49261	1863.8816		2994.1137			3051.1163
49262	3076.5423		3112.4202			3153.0517
49263	3173.7066		3634.5460			3711.3818
49264	Zero-point correction (Hartree):			0.150860		
49265	TS.diHPCARP_I.15HPHshift.dcpdpddu					
49266	-----					
49267	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13528292					
49268	Electronic state : 2-A					
49269	Cartesian coordinates (Angs):					
49270	O	-1.558995	0.375210	1.220528		
49271	O	-1.194375	-0.853689	1.762179		
49272	H	0.055573	-0.853838	1.455060		
49273	C	1.053260	-0.310439	0.863883		
49274	C	0.368968	0.506259	-0.222352		
49275	C	-1.161685	0.355138	-0.143991		
49276	C	-1.914960	1.462431	-0.857894		
49277	H	-1.531678	1.583457	-1.869539		
49278	H	-1.779785	2.397961	-0.321523		
49279	H	-2.976761	1.222984	-0.895313		
49280	C	-1.614860	-1.000195	-0.682847		
49281	O	-0.923184	-1.773355	-1.285305		
49282	H	-2.678125	-1.210048	-0.476514		
49283	H	0.712544	0.179614	-1.204749		
49284	O	0.632725	1.887585	-0.061702		
49285	O	2.008342	2.071598	-0.367783		
49286	H	2.351783	2.418718	0.464590		
49287	H	1.445976	0.303228	1.674195		
49288	O	2.030313	-1.215305	0.531212		
49289	O	1.884584	-1.744021	-0.770355		
49290	H	0.980844	-2.105439	-0.797199		
49291	Rotational constants (GHz):			1.0532500	0.9047100	0.6879700
49292	Vibrational harmonic frequencies (cm-1):					
49293						

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49294      i1723.5889          59.6860          98.1345
49295      105.3003           124.6891         181.5084
49296      194.3040           202.7535         219.0762
49297      219.7647           253.5082         285.5309
49298      323.6429           341.4024         345.5299
49299      367.7885             409.3809         476.2953
49300      543.1046             560.7649         600.0070
49301      626.9002             638.0954         867.6623
49302      924.1817             950.7690         954.7966
49303      980.4005             998.8492        1041.1001
49304      1063.0383            1086.2032        1133.1179
49305      1163.2504            1223.9820        1237.9270
49306      1247.6451            1299.5095        1303.5638
49307      1341.4790            1404.1843        1410.2088
49308      1413.8101            1419.6198        1483.5543
49309      1485.3049            1499.3498        1647.2405
49310      1858.5769            3004.0270        3080.0477
49311      3110.8460            3124.6632        3158.0092
49312      3173.4893            3690.1924        3826.8222
49313      Zero-point correction (Hartree): 0.149868
49314
49315      TS.diHPCARP_I.15HPHshift.dcpdpudu
49316      -----
49317      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13605166
49318      Electronic state : 2-A
49319      Cartesian coordinates (Angs):
49320      O      1.510460      -0.877625      -1.130193
49321      O      1.062724      -2.042393      -0.517842
49322      H      -0.160883      -1.773210      -0.469892
49323      C      -0.997717      -0.792968      -0.665716
49324      C      -0.253471      0.333150      0.023917
49325      C      1.266110      0.189464      -0.221073
49326      C      1.926831      1.419963      -0.822612
49327      H      1.761107      2.281143      -0.180412
49328      H      1.508742      1.624984      -1.805588
49329      H      2.996006      1.236939      -0.922160
49330      C      1.998976      -0.143784      1.078945
49331      O      1.646827      0.232192      2.157081
49332      H      2.926297      -0.722301      0.920308
49333      H      -0.431656      0.320743      1.097558
49334      O      -0.684329      1.594246      -0.483707
49335      O      -1.998580      1.806648      0.021245
49336      H      -2.534433      1.728942      -0.778944
49337      H      -0.960575      -0.736367      -1.754303
49338      O      -2.307872      -1.007961      -0.328929
49339      O      -2.488959      -0.953487      1.073242
49340      H      -2.671150      -0.008788      1.205496
49341      Rotational constants (GHz):      1.2131700      0.7448800      0.6562000
49342      Vibrational harmonic frequencies (cm-1):
49343      i1924.5398          35.9367          95.8847
49344      103.9233           137.7752         169.6119
49345      201.7957           233.9869         251.0562
49346      254.7167           286.5923         299.3248
49347      322.3969           340.7699         374.2030
49348      386.4243           463.0560         491.0701
49349      534.9321           561.9273         603.9504
49350      636.0542           662.2551         896.6951
49351      911.4487           934.8124         964.6591
49352      978.4138           1001.7803        1025.3881
49353      1062.9140          1091.1252        1102.4995
49354      1180.1097          1215.6085        1225.0862
49355      1240.7567          1253.0237        1314.4053
49356      1386.7690          1393.6926        1408.4928
49357      1411.0644          1422.9952        1444.1990
49358      1488.0608          1500.3026        1703.7513
49359      1877.0876          2989.4927        3080.5133
49360      3118.5896          3132.0057        3158.8645
49361      3175.6439          3735.1291        3811.9740
49362      Zero-point correction (Hartree): 0.150553
49363
49364      TS.diHPCARP_I.15HPHshift.dctdmudu
49365      -----

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49366 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13629878
49367 Electronic state : 2-A
49368 Cartesian coordinates (Angs):
49369 O 0.745559 -1.203547 -1.331854
49370 O -0.268474 -2.052160 -0.903255
49371 H -1.105444 -1.208355 -0.583452
49372 C -1.368757 0.050182 -0.347726
49373 C -0.033908 0.588302 0.114746
49374 C 1.113301 -0.397579 -0.218286
49375 C 2.418654 0.281940 -0.593989
49376 H 2.773886 0.888372 0.234868
49377 H 2.261127 0.924978 -1.456876
49378 H 3.159031 -0.478366 -0.838557
49379 C 1.384592 -1.332337 0.957439
49380 O 1.221759 -1.027738 2.103318
49381 H 1.802696 -2.308713 0.655529
49382 H -0.053559 0.744465 1.194483
49383 O 0.098000 1.841163 -0.544681
49384 O 1.016441 2.641679 0.189334
49385 H 0.424940 3.297874 0.579291
49386 H -1.676109 0.390792 -1.337261
49387 O -2.321088 0.249633 0.619852
49388 O -3.590810 -0.026404 0.053321
49389 H -3.880955 -0.775114 0.590581
49390 Rotational constants (GHz): 1.0702400 0.7566000 0.5996400
49391 Vibrational harmonic frequencies (cm-1):
49392 i1910.2460 20.0138 82.0619
49393 102.4555 121.5341 140.6969
49394 168.8585 199.4362 232.0934
49395 243.0149 258.7504 273.2945
49396 294.3209 317.7511 338.4892
49397 360.6220 384.1542 414.2750
49398 523.8050 567.8704 640.1931
49399 645.8289 672.4653 839.1322
49400 920.0185 931.2186 967.5321
49401 983.8958 1022.1373 1037.4266
49402 1069.0403 1089.4532 1141.7775
49403 1153.1111 1215.4956 1229.5801
49404 1239.6132 1261.7474 1289.5679
49405 1361.3666 1396.6677 1402.1798
49406 1408.0558 1414.4047 1426.5283
49407 1487.9544 1499.3560 1658.0329
49408 1868.7633 2988.6432 3082.1941
49409 3102.9539 3113.9165 3161.9819
49410 3179.5263 3815.4910 3816.9794
49411 Zero-point correction (Hartree): 0.149397
49412
49413 TS.diHPCARP_I.15HPHshift.dctumudu
49414 -----
49415 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13461423
49416 Electronic state : 2-A
49417 Cartesian coordinates (Angs):
49418 O 0.544882 -1.015564 -1.497072
49419 O -0.829726 -1.173224 -1.618450
49420 H -1.205111 -0.067445 -1.232527
49421 C -1.131833 0.873507 -0.327198
49422 C 0.280330 0.704578 0.188596
49423 C 0.833959 -0.702713 -0.146200
49424 C 2.345341 -0.799491 -0.012853
49425 H 2.651734 -0.483850 0.981567
49426 H 2.812562 -0.168575 -0.767517
49427 H 2.664101 -1.827154 -0.182155
49428 C 0.212087 -1.759124 0.761685
49429 O 0.020015 -1.583821 1.929675
49430 H 0.015364 -2.723441 0.261088
49431 H 0.290909 0.827421 1.274221
49432 O 1.042733 1.732189 -0.419138
49433 O 2.047377 2.130630 0.506622
49434 H 2.850786 1.994939 -0.010424
49435 H -1.343325 1.818366 -0.825893
49436 O -2.029876 0.546917 0.661968
49437 O -3.334509 0.726764 0.134921

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49438      H      -3.663488      -0.181932      0.129254
49439 Rotational constants (GHz):      1.0905300      0.7795000      0.6480600
49440 Vibrational harmonic frequencies (cm-1):
49441      i1864.0107      24.8901      64.9356
49442      89.8875      112.0275      136.0018
49443      143.4185      173.6218      200.9093
49444      229.3601      251.8878      282.8014
49445      305.4389      313.9733      333.3809
49446      366.3462      374.8180      419.9863
49447      520.4149      569.2281      643.2048
49448      662.4011      686.6990      826.2052
49449      931.7864      956.1358      971.0617
49450      996.1848      1015.6583      1055.1224
49451      1078.4300      1102.6347      1127.4960
49452      1163.0251      1207.4281      1225.9951
49453      1239.8696      1267.4798      1294.3906
49454      1330.8664      1392.6407      1394.2553
49455      1403.6962      1411.1862      1422.5865
49456      1490.8530      1508.7000      1582.0941
49457      1867.8038      2988.7946      3075.8778
49458      3090.6870      3123.6198      3148.8555
49459      3174.0309      3812.5290      3828.8280
49460 Zero-point correction (Hartree): 0.149021
49461
49462 TS.diHPCARP_I.15HPHshift.dmmmdmudu
49463 -----
49464 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13934951
49465 Electronic state : 2-A
49466 Cartesian coordinates (Angs):
49467      O      1.032703      -0.012387      1.414658
49468      O      -0.259969      -0.014316      1.926938
49469      H      -0.874800      -0.642430      1.038134
49470      C      -1.134741      -0.772019      -0.231270
49471      C      0.209548      -0.417894      -0.821623
49472      C      0.999066      0.540471      0.105727
49473      C      2.445427      0.694900      -0.335767
49474      H      2.468486      1.079478      -1.353585
49475      H      2.952813      -0.266950      -0.311084
49476      H      2.963082      1.391946      0.321214
49477      C      0.361849      1.924509      0.145595
49478      O      0.020654      2.501315      -0.845763
49479      H      0.302044      2.373688      1.152004
49480      H      0.084930      0.086108      -1.783814
49481      O      0.958032      -1.582324      -1.103073
49482      O      0.886824      -2.464437      0.010770
49483      H      1.465351      -2.045875      0.666487
49484      H      -1.477633      -1.792252      -0.390197
49485      O      -2.053899      0.196113      -0.553741
49486      O      -3.300288      -0.188765      0.004425
49487      H      -3.443623      0.514885      0.651148
49488 Rotational constants (GHz):      1.0878700      0.8775800      0.6758300
49489 Vibrational harmonic frequencies (cm-1):
49490      i1820.0196      49.6197      76.7627
49491      96.0819      133.7358      145.3122
49492      154.3487      179.8555      210.3174
49493      218.5861      277.2533      295.3348
49494      304.8461      330.7000      348.2095
49495      371.7190      407.3631      477.1684
49496      517.6854      574.8610      621.0245
49497      679.8676      702.9927      850.5373
49498      928.4791      958.3627      961.8290
49499      973.1698      1014.5268      1033.2702
49500      1074.0890      1102.5458      1130.0923
49501      1161.1048      1208.9774      1222.0762
49502      1241.9049      1268.1740      1286.6221
49503      1318.7884      1394.0591      1395.9940
49504      1410.8628      1422.7061      1445.1404
49505      1489.0835      1496.2451      1575.2021
49506      1866.7263      2995.5530      3080.0046
49507      3088.6751      3141.9060      3160.0295
49508      3168.8285      3758.2728      3812.7058
49509 Zero-point correction (Hartree): 0.149471

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49510
49511 TS.diHPCARP_I.15HPHshift.dmmddpddu
49512 -----
49513 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13715708
49514 Electronic state : 2-A
49515 Cartesian coordinates (Angs):
49516 O 0.814278 0.511584 1.444500
49517 O -0.242420 -0.169637 2.034596
49518 H -0.383020 -1.105205 1.232008
49519 C -0.458076 -1.535875 0.005327
49520 C 0.277357 -0.422661 -0.729938
49521 C 0.450797 0.869185 0.113296
49522 C 1.580925 1.740916 -0.414938
49523 H 1.363384 2.010469 -1.446075
49524 H 2.532825 1.216140 -0.384798
49525 H 1.653415 2.648396 0.181814
49526 C -0.812274 1.727248 0.126301
49527 O -1.262882 2.204610 -0.873735
49528 H -1.227545 1.928879 1.127842
49529 H -0.259788 -0.154438 -1.643462
49530 O 1.535961 -0.900808 -1.174516
49531 O 2.204668 -1.522688 -0.084792
49532 H 2.469695 -0.780674 0.479574
49533 H 0.044047 -2.497198 -0.041449
49534 O -1.777119 -1.747937 -0.311565
49535 O -2.439915 -0.492771 -0.343656
49536 H -3.085961 -0.598070 0.367613
49537 Rotational constants (GHz): 1.0643800 0.9603400 0.7298500
49538 Vibrational harmonic frequencies (cm-1):
49539 i1844.7949 63.9377 78.9097
49540 113.6686 144.4970 172.8210
49541 177.1425 201.6612 220.2202
49542 231.7420 276.3830 304.2283
49543 308.5105 312.3102 328.6241
49544 386.5969 436.0977 467.3049
49545 539.1297 550.6829 598.7322
49546 682.8468 700.4375 854.6908
49547 918.8952 937.9850 960.6864
49548 965.9712 989.9975 1013.6334
49549 1070.8699 1081.1320 1113.1768
49550 1149.3267 1196.9629 1213.9310
49551 1239.0797 1251.3140 1276.8256
49552 1322.5917 1390.4584 1397.2970
49553 1410.9206 1426.4523 1440.2569
49554 1484.8486 1501.6397 1592.8007
49555 1866.5919 3007.1078 3084.4517
49556 3092.9684 3163.7844 3172.5798
49557 3177.7609 3762.3874 3810.4337
49558 Zero-point correction (Hartree): 0.149530
49559
49560 TS.diHPCARP_I.15HPHshift.dmmddpddu
49561 -----
49562 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13808710
49563 Electronic state : 2-A
49564 Cartesian coordinates (Angs):
49565 O 0.840038 0.561895 1.412382
49566 O -0.169248 -0.164019 2.031149
49567 H -0.318754 -1.096781 1.229648
49568 C -0.391303 -1.537594 -0.000975
49569 C 0.307335 -0.401929 -0.737987
49570 C 0.419821 0.898515 0.095505
49571 C 1.476026 1.843071 -0.461295
49572 H 1.229967 2.083363 -1.493462
49573 H 2.460143 1.380905 -0.435658
49574 H 1.496617 2.760666 0.124340
49575 C -0.894922 1.667982 0.135284
49576 O -1.479238 1.972606 -0.866869
49577 H -1.225418 1.977974 1.139757
49578 H -0.230112 -0.159526 -1.659134
49579 O 1.587842 -0.824763 -1.174854
49580 O 2.275268 -1.427784 -0.085988
49581 H 2.486709 -0.682425 0.496792

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49582      H      0.143894      -2.480827      -0.046131
49583      O      -1.703851      -1.791893      -0.311237
49584      O      -2.460695      -0.613251      -0.075677
49585      H      -2.665723      -0.305938      -0.970590
49586      Rotational constants (GHz):      1.0978200      0.9500600      0.7350800
49587      Vibrational harmonic frequencies (cm-1):
49588      i1899.7500      76.6230      90.5413
49589      103.8071      159.2446      169.3007
49590      186.0278      217.0591      229.2827
49591      276.9310      284.3279      299.5477
49592      306.4146      315.1486      327.0257
49593      384.3427      433.9246      467.7619
49594      542.7519      549.8780      599.0737
49595      677.7606      693.3684      857.1310
49596      924.5881      939.4799      959.4595
49597      965.8081      982.5689      1015.0597
49598      1071.8069      1080.9184      1115.2029
49599      1150.5992      1191.9041      1218.7158
49600      1236.9250      1238.4885      1280.3083
49601      1318.9130      1392.0571      1394.9292
49602      1410.6089      1420.2565      1442.9388
49603      1485.6766      1499.0208      1592.7210
49604      1852.4527      3016.4821      3081.3957
49605      3082.7730      3161.6545      3170.5023
49606      3178.6372      3755.0410      3787.6572
49607      Zero-point correction (Hartree): 0.149591
49608
49609      TS.diHPCARP_I.15HPHshift.dmmtdtddu
49610      -----
49611      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13952485
49612      Electronic state : 2-A
49613      Cartesian coordinates (Angs):
49614      O      1.243262      0.734636      1.100114
49615      O      0.497867      0.028824      2.030750
49616      H      0.128107      -0.944902      1.387481
49617      C      -0.435672      -1.395988      0.272976
49618      C      0.205823      -0.455574      -0.710880
49619      C      0.446801      0.932830      -0.059360
49620      C      1.224528      1.867816      -0.970602
49621      H      0.658479      2.027974      -1.886189
49622      H      2.185103      1.423543      -1.221552
49623      H      1.386842      2.825279      -0.478316
49624      C      -0.863434      1.604759      0.322733
49625      O      -1.805849      1.651437      -0.421470
49626      H      -0.861754      2.103330      1.305649
49627      H      -0.441037      -0.308119      -1.578906
49628      O      1.404720      -0.980808      -1.237783
49629      O      2.167981      -1.570685      -0.191961
49630      H      2.580508      -0.805838      0.235979
49631      H      -0.169358      -2.446740      0.175132
49632      O      -1.759274      -1.140983      0.568276
49633      O      -2.531193      -1.103729      -0.639547
49634      H      -2.675278      -0.147122      -0.735527
49635      Rotational constants (GHz):      1.1507900      0.9182800      0.7466600
49636      Vibrational harmonic frequencies (cm-1):
49637      i1977.5623      85.0599      93.5388
49638      145.1467      163.4224      178.5270
49639      193.8582      205.5014      220.2138
49640      264.1986      290.0965      296.3904
49641      315.6796      332.6559      391.0882
49642      425.3439      471.6557      494.3991
49643      528.7005      585.1775      619.6915
49644      668.0180      684.1364      818.5466
49645      918.2503      930.7419      956.5511
49646      967.8848      974.4600      1005.8536
49647      1077.5716      1105.6556      1131.7486
49648      1153.8799      1164.1887      1215.4754
49649      1240.0672      1258.0215      1273.8957
49650      1309.8415      1391.5526      1398.4404
49651      1410.4894      1433.3758      1438.5134
49652      1489.5522      1496.3717      1559.4095
49653      1844.2809      3017.3462      3080.3196

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49654          3093.5009          3134.9985          3160.9501
49655          3169.5362          3714.7506          3765.3632
49656 Zero-point correction (Hartree): 0.149798
49657
49658 TS.diHPCARP_I.15HPHshift.dmmdtudu
49659 -----
49660 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13438733
49661 Electronic state : 2-A
49662 Cartesian coordinates (Angs):
49663 O          1.389289          0.306935          1.151973
49664 O          0.428601         -0.096407          2.063102
49665 H         -0.210231         -0.884257          1.423690
49666 C         -0.875092         -1.134843          0.282333
49667 C          0.044377         -0.453177         -0.693098
49668 C          0.750317          0.764569         -0.037632
49669 C          1.847087          1.329378         -0.922198
49670 H          1.401494          1.682385         -1.849846
49671 H          2.583598          0.562498         -1.150487
49672 H          2.334978          2.164598         -0.422904
49673 C         -0.257204          1.868531          0.273968
49674 O         -0.909070          2.378096         -0.590525
49675 H         -0.299542          2.189940          1.327432
49676 H         -0.533533         -0.073244         -1.542142
49677 O          0.978908         -1.355644         -1.244808
49678 O          1.520690         -2.160480         -0.203410
49679 H          2.165492         -1.572201          0.217019
49680 H         -0.994657         -2.209365          0.162441
49681 O         -2.034098         -0.430996          0.543580
49682 O         -2.859075         -0.530341         -0.633374
49683 H         -3.626477         -0.996402         -0.277755
49684 Rotational constants (GHz):      1.0693500      0.9195700      0.7206000
49685 Vibrational harmonic frequencies (cm-1):
49686 i1959.1184          52.9881          83.1329
49687          94.1469          107.0531          140.1422
49688          159.7374          193.2219          212.8817
49689          215.4578          275.9761          291.1360
49690          304.8594          311.3378          334.6356
49691          397.4531          420.6120          486.3006
49692          516.9997          559.8416          622.5958
49693          665.6016          695.7980          809.7615
49694          906.3590          924.9048          949.8520
49695          960.7289          977.5041          1000.1178
49696          1078.0636          1094.6853          1126.5217
49697          1139.4928          1165.7591          1205.6512
49698          1233.8579          1253.2770          1272.4481
49699          1307.5052          1376.5983          1394.0978
49700          1396.7756          1410.7521          1434.9704
49701          1489.9738          1495.0810          1558.3104
49702          1863.8361          3010.8003          3071.1056
49703          3082.5669          3142.4347          3162.8417
49704          3171.2344          3767.9549          3824.7751
49705 Zero-point correction (Hartree): 0.148542
49706
49707 TS.diHPCARP_I.15HPHshift.dmmupddu
49708 -----
49709 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13644129
49710 Electronic state : 2-A
49711 Cartesian coordinates (Angs):
49712 O          0.949661          0.500610          1.473211
49713 O         -0.322805          0.596177          2.022411
49714 H         -0.857419         -0.339762          1.438303
49715 C         -0.965009         -1.127679          0.399057
49716 C          0.054445         -0.522985         -0.555677
49717 C          0.819584          0.668358          0.068036
49718 C          2.224925          0.825664         -0.490940
49719 H          2.175116          0.885300         -1.576156
49720 H          2.831983         -0.028668         -0.204843
49721 H          2.674643          1.737593         -0.100018
49722 C          0.086852          1.983892         -0.186884
49723 O         -0.460406          2.246735         -1.217534
49724 H          0.174198          2.706386          0.643622
49725 H         -0.461470         -0.147209         -1.441273

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49726	O	0.917644	-1.516495	-1.078313	
49727	O	1.633936	-2.088815	0.019295	
49728	H	1.604998	-3.023132	-0.218560	
49729	H	-0.696190	-2.113205	0.769402	
49730	O	-2.271383	-1.192649	-0.024745	
49731	O	-2.641832	0.071797	-0.551959	
49732	H	-3.209162	0.420307	0.149028	
49733	Rotational constants (GHz):		1.0350700	0.9235400	0.7142600
49734	Vibrational harmonic frequencies (cm-1):				
49735	i1908.0072		41.6052		77.7009
49736	122.6207		147.8581		160.7368
49737	185.6003		205.4477		211.3918
49738	240.0860		256.4065		271.5690
49739	295.0459		306.9616		331.0534
49740	365.1748		425.5924		464.6666
49741	555.0466		564.5619		594.4854
49742	670.9766		682.5852		866.5486
49743	917.0909		933.6849		955.3813
49744	977.3353		979.9753		996.4301
49745	1068.9674		1084.1700		1120.3311
49746	1149.1665		1191.0127		1222.3173
49747	1233.2298		1242.5388		1284.5804
49748	1335.4182		1388.6116		1394.7304
49749	1407.8151		1408.8802		1433.1973
49750	1484.0699		1504.4240		1622.8289
49751	1870.1192		2987.6428		3081.4298
49752	3108.3139		3159.2094		3164.2649
49753	3183.2771		3802.7451		3838.1760
49754	Zero-point correction (Hartree): 0.149391				
49755	TS.diHPCARP_I.15HPHshift.dmmupudu				
49756	-----				
49757	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13672114				
49758	Electronic state : 2-A				
49759	Cartesian coordinates (Angs):				
49760	O	0.794617	0.638495	1.467361	
49761	O	-0.426305	0.277245	2.019189	
49762	H	-0.661210	-0.732006	1.376627	
49763	C	-0.623780	-1.404611	0.242048	
49764	C	0.244856	-0.494157	-0.616332	
49765	C	0.595344	0.840157	0.078572	
49766	C	1.872060	1.464028	-0.463850	
49767	H	1.798074	1.561464	-1.545106	
49768	H	2.718338	0.828606	-0.216552	
49769	H	2.017977	2.448864	-0.022049	
49770	C	-0.527228	1.855204	-0.115237	
49771	O	-1.151205	1.958606	-1.134186	
49772	H	-0.669027	2.537230	0.739852	
49773	H	-0.288643	-0.241383	-1.536230	
49774	O	1.387784	-1.175581	-1.095559	
49775	O	2.163360	-1.553510	0.044880	
49776	H	2.434723	-2.442976	-0.211730	
49777	H	-0.172921	-2.368791	0.458315	
49778	O	-1.909525	-1.631610	-0.188668	
49779	O	-2.609627	-0.395452	-0.197638	
49780	H	-2.537611	-0.100284	-1.117366	
49781	Rotational constants (GHz): 1.0932100 0.9223100 0.7268500				
49782	Vibrational harmonic frequencies (cm-1):				
49783	i1975.0781		67.9501		93.7240
49784	110.3031		145.6390		157.7768
49785	185.6546		192.4196		229.2830
49786	241.7690		278.0484		288.4989
49787	306.4121		315.0277		331.2561
49788	366.8174		431.7439		460.0196
49789	537.4217		563.4324		596.6649
49790	674.8711		680.8873		866.0671
49791	921.4291		935.0755		956.3382
49792	972.9496		978.7842		1006.1498
49793	1071.9583		1084.9951		1123.1321
49794	1149.7202		1183.8407		1219.0824
49795	1230.5563		1242.8474		1290.8679
49796	1329.5255		1392.4331		1393.7485


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49798      1406.4046      1412.1524      1435.5160
49799      1483.0239      1503.5138      1598.2480
49800      1855.4269      3005.4979      3080.1583
49801      3089.8337      3158.7248      3170.3090
49802      3178.5994      3778.2990      3837.8575
49803 Zero-point correction (Hartree): 0.149445
49804
49805 TS.diHPCARP_I.15HPHshift.dmmupuuu
49806 -----
49807 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13762485
49808 Electronic state : 2-A
49809 Cartesian coordinates (Angs):
49810 O      1.777991      -0.656849      -1.024945
49811 O      1.214460      -1.881693      -0.693076
49812 H      0.028238      -1.651959      -0.930319
49813 C     -0.976300      -0.811626      -1.006148
49814 C     -0.255472      0.509434      -0.732316
49815 C      1.187471      0.330670      -0.195242
49816 C      1.994761      1.606018      -0.373647
49817 H      1.490021      2.419918      0.143388
49818 H      2.073199      1.839125      -1.434583
49819 H      2.997476      1.485385      0.033871
49820 C      1.345346      -0.109483      1.258406
49821 O      0.690411      0.302002      2.171289
49822 H      2.199140      -0.794371      1.403098
49823 H     -0.153599      1.044484      -1.679310
49824 O     -0.991279      1.309440      0.171012
49825 O     -2.174044      1.712530      -0.506638
49826 H     -2.804542      1.029527      -0.233497
49827 H     -1.394391      -0.917268      -2.003975
49828 O     -1.965687      -1.144274      -0.114767
49829 O     -1.416110      -1.294639      1.185272
49830 H     -1.296306      -0.377043      1.489838
49831 Rotational constants (GHz):      1.1783000      0.8728400      0.7820200
49832 Vibrational harmonic frequencies (cm-1):
49833 i1959.3752      49.7343      109.7124
49834      123.5620      145.4033      184.1951
49835      200.9140      228.3134      234.8472
49836      264.4677      293.0587      308.8795
49837      336.2245      384.0535      388.3303
49838      398.5123      441.7051      519.7800
49839      533.3276      577.3071      611.5528
49840      682.4897      747.5206      806.6978
49841      915.9014      928.6058      958.3594
49842      979.1155      1002.3524      1020.7812
49843      1057.7127      1071.1684      1141.1556
49844      1180.3709      1193.9429      1206.2966
49845      1213.6267      1270.3648      1340.7028
49846      1366.7771      1381.2463      1400.3590
49847      1411.9124      1426.1194      1444.1044
49848      1487.0176      1501.4597      1596.2348
49849      1868.7867      2992.6013      3073.7654
49850      3076.4312      3153.0458      3153.3553
49851      3165.7869      3691.6573      3770.3931
49852 Zero-point correction (Hartree): 0.150387
49853
49854 TS.diHPCARP_I.15HPHshift.dmmutddu
49855 -----
49856 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13656359
49857 Electronic state : 2-A
49858 Cartesian coordinates (Angs):
49859 O      1.195846      0.759606      1.182713
49860 O      0.269472      0.263107      2.079316
49861 H     -0.072880      -0.756271      1.534292
49862 C     -0.566487      -1.312019      0.418133
49863 C      0.176945      -0.514130      -0.619900
49864 C      0.563911      0.885966      -0.075886
49865 C      1.547604      1.602174      -0.985754
49866 H      1.141772      1.655723      -1.994147
49867 H      2.481662      1.045508      -1.003701
49868 H      1.734995      2.609920      -0.618128
49869 C     -0.683463      1.746731      0.084054

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49870	O	-1.616002	1.710820	-0.672401	
49871	H	-0.636439	2.458081	0.925498	
49872	H	-0.464181	-0.347719	-1.488595	
49873	O	1.275766	-1.210956	-1.153961	
49874	O	2.143453	-1.555471	-0.070353	
49875	H	2.303336	-2.487879	-0.260176	
49876	H	-0.349111	-2.379441	0.442505	
49877	O	-1.895369	-0.983804	0.594746	
49878	O	-2.587626	-1.007540	-0.661663	
49879	H	-2.654523	-0.056349	-0.848615	
49880	Rotational constants (GHz):			1.1379400	0.9041200 0.7460900
49881	Vibrational harmonic frequencies (cm-1):				
49882	i2007.0084		64.8670		87.1648
49883	118.6639		155.4613		161.5144
49884	176.6230		215.8638		220.3116
49885	222.2774		254.0707		287.2818
49886	295.7115		314.7458		359.5599
49887	419.4752		467.8780		486.7318
49888	533.3803		578.0885		613.3932
49889	669.1377		674.1705		822.2486
49890	916.3575		931.1857		955.0924
49891	969.5498		976.9623		1004.0117
49892	1083.8962		1106.4277		1134.1558
49893	1154.4075		1166.2737		1222.8946
49894	1237.6620		1262.3901		1278.4975
49895	1318.5643		1383.9754		1395.4552
49896	1406.6937		1430.1372		1434.6443
49897	1484.9278		1498.4725		1556.7625
49898	1847.1028		3007.4848		3079.4815
49899	3099.2995		3115.0715		3159.5251
49900	3172.1579		3720.7072		3833.3970
49901	Zero-point correction (Hartree): 0.149316				
49902					
49903	TS.diHPCARP_I.15HPHshift.dmpdmudu				
49904	-----				
49905	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13714992				
49906	Electronic state : 2-A				
49907	Cartesian coordinates (Angs):				
49908	O	-1.147801	-0.586152	1.472544	
49909	O	0.006250	-1.328745	1.690633	
49910	H	0.853081	-0.540457	1.247994	
49911	C	1.234479	0.295780	0.323175	
49912	C	-0.090294	0.695051	-0.289427	
49913	C	-1.216211	-0.291066	0.089944	
49914	C	-2.606331	0.267440	-0.173708	
49915	H	-2.662935	0.632052	-1.197509	
49916	H	-2.808998	1.087657	0.509537	
49917	H	-3.350811	-0.514166	-0.027598	
49918	C	-1.073392	-1.590986	-0.697919	
49919	O	-0.689064	-1.641103	-1.829223	
49920	H	-1.424659	-2.479669	-0.144600	
49921	H	-0.012315	0.705733	-1.380764	
49922	O	-0.497154	1.960782	0.184802	
49923	O	0.367054	2.916141	-0.423543	
49924	H	0.640253	3.436009	0.341854	
49925	H	1.775883	1.090782	0.834475	
49926	O	1.999449	-0.391370	-0.587394	
49927	O	3.245078	-0.682846	0.026311	
49928	H	3.230495	-1.648890	0.031188	
49929	Rotational constants (GHz):			1.0000000	0.8432200 0.6397600
49930	Vibrational harmonic frequencies (cm-1):				
49931	i1850.9810		41.0289		65.8703
49932	88.9539		114.8241		144.1276
49933	156.3957		175.8529		184.0388
49934	221.6449		226.9177		249.0212
49935	275.0388		297.6701		321.8726
49936	366.0272		370.4527		502.3408
49937	526.1802		564.3626		592.6919
49938	640.2674		690.8436		851.2656
49939	932.3903		962.4650		977.9535
49940	1011.3939		1017.4805		1044.6527
49941	1076.0976		1096.7652		1137.6301

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49942      1163.5893      1202.4059      1230.9629
49943      1240.4627      1269.9969      1307.7563
49944      1321.1745      1394.1430      1400.1834
49945      1408.9657      1416.0825      1424.7420
49946      1484.7848      1500.1217      1581.0613
49947      1870.9383      2988.2411      3072.2712
49948      3079.9049      3120.1686      3157.8544
49949      3177.2786      3816.6674      3835.9951
49950 Zero-point correction (Hartree): 0.148970
49951
49952 TS.diHPCARP_I.15HPHshift.dmpdpudu
49953 -----
49954 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13743092
49955 Electronic state : 2-A
49956 Cartesian coordinates (Angs):
49957 O      1.099115      -0.698533      1.455566
49958 O      1.034793      0.626753      1.863042
49959 H      -0.106506      0.902811      1.501066
49960 C      -1.104924      0.773359      0.659848
49961 C      -0.592850      -0.349368      -0.234253
49962 C      0.870612      -0.734415      0.058171
49963 C      1.226177      -2.141049      -0.405328
49964 H      0.947925      -2.261678      -1.450169
49965 H      0.690997      -2.871906      0.194520
49966 H      2.297806      -2.302313      -0.294883
49967 C      1.836815      0.220476      -0.636403
49968 O      1.656723      0.650650      -1.740181
49969 H      2.758549      0.416057      -0.063258
49970 H      -0.657679      -0.049590      -1.285429
49971 O      -1.357242      -1.522393      -0.036326
49972 O      -2.651460      -1.245321      -0.565350
49973 H      -3.217607      -1.584554      0.138239
49974 H      -1.976949      0.496035      1.246254
49975 O      -1.368523      1.987145      0.076621
49976 O      -0.159081      2.503788      -0.459802
49977 H      -0.186107      2.224412      -1.387119
49978 Rotational constants (GHz): 0.9864900      0.9392700      0.7090400
49979 Vibrational harmonic frequencies (cm-1):
49980 i1929.9468      60.4726      83.8991
49981 98.0891      133.2346      163.9115
49982 182.1222      185.6746      225.8772
49983 243.8988      267.8957      280.2268
49984 296.0785      318.4205      342.4856
49985 352.0748      414.5904      479.3588
49986 541.0715      568.6011      568.9655
49987 642.9262      681.2589      850.5958
49988 925.0885      949.0960      966.9772
49989 976.1140      996.6333      1037.9608
49990 1067.6679      1081.8223      1128.4590
49991 1156.1631      1186.1561      1219.2270
49992 1236.9385      1239.5978      1308.8310
49993 1331.1325      1395.0448      1405.7553
49994 1408.2720      1415.1427      1421.7665
49995 1483.9201      1501.5849      1598.2911
49996 1859.6173      3006.0437      3059.9523
49997 3080.4529      3159.0334      3159.8346
49998 3178.6627      3776.3630      3834.7971
49999 Zero-point correction (Hartree): 0.149298
50000
50001 TS.diHPCARP_I.15HPHshift.dmpdtddu
50002 -----
50003 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13679817
50004 Electronic state : 2-A
50005 Cartesian coordinates (Angs):
50006 O      -1.494035      0.710812      1.140276
50007 O      -1.074309      -0.308278      1.977586
50008 H      0.124386      -0.319378      1.760137
50009 C      1.105615      -0.351511      0.865318
50010 C      0.476602      0.481629      -0.221998
50011 C      -1.064852      0.397454      -0.170514
50012 C      -1.744320      1.383521      -1.108376
50013 H      -1.351598      1.256557      -2.115432

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50014	H	-1.546368	2.397491	-0.771833	
50015	H	-2.819659	1.210599	-1.116970	
50016	C	-1.541263	-1.005341	-0.526227	
50017	O	-1.004147	-1.706620	-1.338912	
50018	H	-2.475612	-1.300397	-0.020127	
50019	H	0.800265	0.148165	-1.210500	
50020	O	0.796969	1.845621	-0.047531	
50021	O	2.136385	2.009002	-0.502828	
50022	H	2.544702	2.437261	0.259301	
50023	H	1.981966	0.092168	1.338668	
50024	O	1.192266	-1.711093	0.655941	
50025	O	1.748041	-1.986360	-0.635731	
50026	H	0.941870	-2.181646	-1.142863	
50027	Rotational constants (GHz):			0.9742900	0.9657800 0.7221100
50028	Vibrational harmonic frequencies (cm-1):				
50029	i1976.4903		72.6658		82.2023
50030	118.4724		148.6411		160.7946
50031	189.6372		198.8654		207.4912
50032	223.1259		258.3670		270.2481
50033	304.5649		320.0288		347.0905
50034	427.8964		475.0651		502.6786
50035	531.0677		568.6592		614.9288
50036	634.8184		683.1032		817.9993
50037	924.2949		937.0445		956.5580
50038	980.9592		1007.7901		1040.0799
50039	1078.4288		1102.4953		1139.4979
50040	1161.8920		1166.6191		1228.6582
50041	1240.9556		1260.8490		1296.6978
50042	1315.5418		1394.7755		1398.0762
50043	1408.0723		1414.1825		1444.2268
50044	1486.1314		1498.8732		1557.2679
50045	1853.0672		3012.4066		3080.5176
50046	3089.5420		3107.3837		3158.2012
50047	3178.8489		3720.2905		3830.6169
50048	Zero-point correction (Hartree):			0.149514	
50049	-----				
50050	TS.diHPCARP_I.15HPHshift.dmpumudu				
50051	-----				
50052	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13752963				
50053	Electronic state : 2-A				
50054	Cartesian coordinates (Angs):				
50055	O	-1.135717	-0.606501	1.474342	
50056	O	0.016487	-1.358946	1.666161	
50057	H	0.862644	-0.557372	1.243960	
50058	C	1.242592	0.286392	0.327287	
50059	C	-0.082054	0.696529	-0.278770	
50060	C	-1.215686	-0.282507	0.100495	
50061	C	-2.602740	0.298593	-0.131682	
50062	H	-2.677327	0.665262	-1.153772	
50063	H	-2.778635	1.117817	0.560353	
50064	H	-3.355407	-0.472493	0.027317	
50065	C	-1.100783	-1.566335	-0.718424	
50066	O	-0.763745	-1.589612	-1.865881	
50067	H	-1.425862	-2.468268	-0.171100	
50068	H	-0.005395	0.705649	-1.370929	
50069	O	-0.472511	1.965194	0.207361	
50070	O	0.490715	2.906072	-0.245930	
50071	H	-0.006628	3.386615	-0.919677	
50072	H	1.789489	1.077270	0.838298	
50073	O	1.991809	-0.403005	-0.596379	
50074	O	3.241687	-0.710195	-0.000886	
50075	H	3.199350	-1.674577	0.041812	
50076	Rotational constants (GHz):			1.0037500	0.8403400 0.6398100
50077	Vibrational harmonic frequencies (cm-1):				
50078	i1836.9637		40.9131		65.6036
50079	90.7100		116.9653		151.4188
50080	157.0539		186.9240		205.4279
50081	227.1678		232.8134		256.7355
50082	277.5596		297.3331		320.0610
50083	366.0260		371.9345		503.1117
50084	528.0191		563.9428		592.5742
50085	642.3734		692.8168		853.4970

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50086          932.6307          963.0486          977.1666
50087          1014.5295         1022.5229         1042.5599
50088          1077.8441         1095.4408         1142.5011
50089          1163.5125         1202.3028         1229.8840
50090          1243.2563         1273.8680         1306.5513
50091          1326.4401         1392.7967         1395.8264
50092          1407.5167         1413.3357         1425.6391
50093          1485.5335         1501.4225         1580.1418
50094          1869.3646         2993.3503         3061.4409
50095          3079.1703         3129.1788         3156.3975
50096          3175.9844         3813.9321         3815.1812
50097 Zero-point correction (Hartree): 0.149109
50098
50099 TS.diHPCARP_I.15HPHshift.dmpupudu
50100 -----
50101 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13778507
50102 Electronic state : 2-A
50103 Cartesian coordinates (Angs):
50104 O          1.083539         -0.681137          1.470641
50105 O          1.017472          0.647879          1.864439
50106 H         -0.125903          0.916040          1.503759
50107 C         -1.111328          0.795156          0.646784
50108 C         -0.600537         -0.339916         -0.232627
50109 C          0.858803         -0.734944          0.074538
50110 C          1.200549         -2.154083         -0.362116
50111 H          0.947052         -2.283123         -1.412391
50112 H          0.641265         -2.867694          0.236566
50113 H          2.266784         -2.330539         -0.226473
50114 C          1.834533          0.197375         -0.637956
50115 O          1.684255          0.557501         -1.771126
50116 H          2.731850          0.444691         -0.046790
50117 H         -0.654482         -0.047418         -1.286829
50118 O         -1.378773         -1.502629         -0.015870
50119 O         -2.711671         -1.187952         -0.399111
50120 H         -2.830834         -1.761448         -1.166291
50121 H         -2.002905          0.537469          1.212128
50122 O         -1.332407          2.009893          0.046908
50123 O         -0.099274          2.475285         -0.485696
50124 H         -0.170079          2.259782         -1.426900
50125 Rotational constants (GHz):    0.9916300    0.9358000    0.7116300
50126 Vibrational harmonic frequencies (cm-1):
50127 i1922.5192          62.3756          74.1035
50128          97.8230          137.3344          166.5980
50129          183.4715          184.5233          226.2427
50130          247.2369          266.5521          270.6945
50131          288.5987          312.6795          341.3390
50132          351.2728          414.8460          483.1945
50133          540.1502          566.8344          568.1994
50134          646.2820          688.5307          851.8975
50135          926.4338          951.6615          965.5878
50136          974.9747          998.6150         1035.1203
50137          1072.4875         1082.1619         1130.4289
50138          1153.8726         1184.4068         1221.9085
50139          1239.9136         1240.4248         1305.8709
50140          1335.3287         1391.9171         1398.1330
50141          1406.7037         1407.6129         1423.6750
50142          1485.0948         1502.8748         1596.7055
50143          1857.7684         3009.6268         3053.1924
50144          3080.3443         3157.9974         3164.4521
50145          3178.6713         3786.7419         3824.3185
50146 Zero-point correction (Hartree): 0.149256
50147
50148 TS.diHPCARP_I.15HPHshift.dmpupuuu
50149 -----
50150 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13806530
50151 Electronic state : 2-A
50152 Cartesian coordinates (Angs):
50153 O         -1.565772          1.424613         -0.196326
50154 O         -0.606129          2.232246          0.396972
50155 H          0.399834          1.947782         -0.290948
50156 C          1.148263          1.051021         -0.858029
50157 C          0.086566         -0.014676         -1.100595

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50158 C -1.134360 0.070574 -0.136707
50159 C -2.285257 -0.764573 -0.675595
50160 H -1.984298 -1.808924 -0.720230
50161 H -2.548149 -0.421130 -1.674582
50162 H -3.156087 -0.672498 -0.029139
50163 C -0.910161 -0.316824 1.320836
50164 O -0.669522 -1.444816 1.665721
50165 H -1.069338 0.494218 2.045410
50166 H -0.348826 0.241276 -2.069661
50167 O 0.561719 -1.323645 -1.351669
50168 O 1.232819 -1.882350 -0.231377
50169 H 0.497170 -2.239987 0.296624
50170 H 1.558819 1.480391 -1.768698
50171 O 2.213585 0.805613 -0.037797
50172 O 1.758448 0.366163 1.229965
50173 H 1.819386 -0.596849 1.107839
50174 Rotational constants (GHz): 1.1297900 0.9903600 0.8132900
50175 Vibrational harmonic frequencies (cm-1):
50176 i1941.9455 100.4323 118.9786
50177 138.7897 186.3656 195.2484
50178 212.7454 227.7950 248.0120
50179 268.6393 277.8143 301.0431
50180 306.3301 396.5633 410.1982
50181 435.6809 458.3696 514.2507
50182 543.4345 612.9689 634.5976
50183 693.6062 738.4600 855.6170
50184 901.4124 925.7578 940.1480
50185 985.4143 988.5601 999.5620
50186 1065.3882 1073.1073 1134.5401
50187 1189.7206 1200.6748 1223.6409
50188 1234.4651 1252.2482 1354.6308
50189 1369.8749 1399.3086 1402.0609
50190 1416.2507 1447.2798 1482.0447
50191 1490.4039 1504.2467 1583.9276
50192 1835.5238 3047.4574 3079.4837
50193 3082.9706 3151.8676 3158.9626
50194 3170.6788 3672.3849 3699.2077
50195 Zero-point correction (Hartree): 0.151132
50196
50197 TS.diHPCARP_I.15HPHshift.dmpoutddu
50198 -----
50199 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13670431
50200 Electronic state : 2-A
50201 Cartesian coordinates (Angs):
50202 O -1.510777 0.666231 1.145785
50203 O -1.056958 -0.341834 1.978748
50204 H 0.143296 -0.309330 1.760559
50205 C 1.118631 -0.314685 0.861920
50206 C 0.461918 0.494141 -0.227723
50207 C -1.077161 0.370116 -0.165823
50208 C -1.789673 1.340745 -1.095846
50209 H -1.406489 1.223715 -2.107942
50210 H -1.615628 2.358809 -0.757511
50211 H -2.860501 1.141857 -1.093955
50212 C -1.513386 -1.045252 -0.525872
50213 O -0.968371 -1.719741 -1.356004
50214 H -2.426723 -1.376688 -0.004397
50215 H 0.787624 0.154709 -1.214253
50216 O 0.749344 1.867636 -0.059171
50217 O 2.138269 2.040195 -0.305254
50218 H 2.130398 2.517808 -1.144151
50219 H 1.983687 0.156079 1.327956
50220 O 1.235867 -1.673217 0.650470
50221 O 1.795934 -1.935531 -0.642453
50222 H 0.995899 -2.167256 -1.143217
50223 Rotational constants (GHz): 0.9802600 0.9631900 0.7223400
50224 Vibrational harmonic frequencies (cm-1):
50225 i1973.0191 70.7682 83.1843
50226 126.2189 148.0448 156.2714
50227 181.4417 197.4322 215.0727
50228 220.4556 259.0699 269.9277
50229 304.9609 317.7199 347.5771

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50230	429.9481	470.4426	492.7538			
50231	531.6033	567.1973	613.8497			
50232	635.0241	684.4635	820.4628			
50233	925.2093	936.0956	956.0112			
50234	979.5597	1009.4407	1038.0475			
50235	1078.9545	1100.9279	1142.0315			
50236	1160.8617	1165.0597	1227.5022			
50237	1243.4324	1264.5767	1295.9606			
50238	1317.8574	1394.0473	1397.5654			
50239	1408.3096	1412.0695	1441.5277			
50240	1486.9271	1500.0371	1556.1848			
50241	1852.0493	3011.9528	3078.4757			
50242	3080.7661	3122.0193	3156.6044			
50243	3176.3031	3716.7165	3821.4300			
50244	Zero-point correction (Hartree): 0.149444					
50245						
50246	TS.diHPCARP_I.15HPHshift.dmpduu					
50247	-----					
50248	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13684140					
50249	Electronic state : 2-A					
50250	Cartesian coordinates (Angs):					
50251	O	-1.868422	1.202494	-0.299819		
50252	O	-1.031260	2.163248	0.245535		
50253	H	0.013258	1.953948	-0.371373		
50254	C	0.924182	1.059151	-0.692621		
50255	C	-0.014058	-0.075988	-1.031249		
50256	C	-1.268686	-0.073808	-0.114443		
50257	C	-2.288041	-1.101834	-0.577972		
50258	H	-1.839835	-2.092117	-0.541968		
50259	H	-2.586021	-0.877298	-1.601005		
50260	H	-3.170866	-1.079404	0.059130		
50261	C	-1.021900	-0.296143	1.369704		
50262	O	-0.386254	-1.220059	1.804220		
50263	H	-1.546213	0.408509	2.033409		
50264	H	-0.409673	0.118590	-2.031351		
50265	O	0.579230	-1.356019	-1.190476		
50266	O	1.460202	-1.689218	-0.129083		
50267	H	0.857992	-1.813973	0.632423		
50268	H	1.548392	1.430659	-1.501522		
50269	O	1.594909	0.968637	0.506939		
50270	O	2.941396	0.588001	0.246180		
50271	H	2.825576	-0.373857	0.133781		
50272	Rotational constants (GHz):			1.2518100	0.8793100	0.7270000
50273	Vibrational harmonic frequencies (cm-1):					
50274	i2055.8886		64.3566			94.6891
50275	109.2416		171.0359			205.9384
50276	217.4418		241.5987			257.6440
50277	269.8460		276.2345			288.4727
50278	314.4473		375.9266			397.0948
50279	448.5448		496.2516			527.1830
50280	583.0461		637.2075			674.4081
50281	689.4614		716.0880			866.3594
50282	896.7088		920.3507			962.2001
50283	966.0968		986.6233			1014.0448
50284	1047.1062		1072.1433			1126.6758
50285	1167.3501		1193.2985			1208.2801
50286	1248.7789		1277.1856			1346.7470
50287	1361.2204		1378.6070			1401.4302
50288	1414.8799		1457.0005			1485.5979
50289	1498.9529		1514.5742			1551.3164
50290	1844.4770		3030.0969			3076.6268
50291	3084.6247		3147.6764			3154.2815
50292	3171.8757		3545.0514			3648.5341
50293	Zero-point correction (Hartree): 0.150639					
50294						
50295	TS.diHPCARP_I.15HPHshift.dmtppdu					
50296	-----					
50297	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13601312					
50298	Electronic state : 2-A					
50299	Cartesian coordinates (Angs):					
50300	O	0.741465	-1.217897	-1.370854		
50301	O	-0.521698	-1.796550	-1.360820		

50302	H	-1.191898	-0.792352	-1.197095			
50303	C	-1.273165	0.471043	-0.850363			
50304	C	-0.011378	0.657348	-0.021953			
50305	C	0.923682	-0.570605	-0.115199			
50306	C	2.401521	-0.227427	-0.029993			
50307	H	2.616893	0.244918	0.924622			
50308	H	2.664562	0.459693	-0.830891			
50309	H	2.986185	-1.140977	-0.129412			
50310	C	0.615975	-1.581001	0.985744			
50311	O	0.269268	-1.274345	2.089069			
50312	H	0.805379	-2.628242	0.690790			
50313	H	-0.277128	0.811690	1.023512			
50314	O	0.579836	1.839819	-0.550956			
50315	O	1.434163	2.400009	0.438624			
50316	H	0.923284	3.171343	0.715328			
50317	H	-1.242684	0.991833	-1.806176			
50318	O	-2.472546	0.777740	-0.258341			
50319	O	-2.534847	0.138653	1.007684			
50320	H	-3.189527	-0.553503	0.844657			
50321	Rotational constants (GHz):				0.9997100	0.8733000	0.7062100
50322	Vibrational harmonic frequencies (cm-1):						
50323	i1907.1830			28.2970		60.9274	
50324	110.4116			125.0592		153.2251	
50325	161.6592			206.6613		231.9959	
50326	266.5880			269.5116		284.0467	
50327	311.8007			327.0384		335.3499	
50328	350.1793			395.8313		478.6162	
50329	553.6880			567.1553		617.6572	
50330	638.5989			666.1976		848.0493	
50331	908.6859			931.4124		967.4042	
50332	973.1924			983.6045		1021.3118	
50333	1063.9388			1076.5437		1136.3029	
50334	1150.9228			1191.2549		1218.5005	
50335	1236.5470			1240.4944		1288.5250	
50336	1356.8915			1397.3148		1399.1812	
50337	1406.9224			1409.0038		1425.8076	
50338	1493.4133			1505.2349		1647.4229	
50339	1869.9068			2986.0141		3083.2453	
50340	3121.4199			3140.9503		3162.6417	
50341	3183.3119			3809.3229		3816.3388	
50342	Zero-point correction (Hartree):				0.149429		
50343							
50344	TS.diHPCARP_I.15HPHshift.dmtduuu						
50345	-----						
50346	E(CCSD(T)/Aug-CC-pVTZ) (Hartree):				-721.16683979		
50347	E(CCSD/Aug-CC-pVTZ) (Hartree):				-721.04541648		
50348	T1 diagnostic:				0.020002		
50349	E(MP2/Aug-CC-pVTZ) (Hartree):				-721.00647164		
50350	E(MP3/Aug-CC-pVTZ) (Hartree):				-721.02304042		
50351	E(PMP2/Aug-CC-pVTZ) (Hartree):				-721.01398645		
50352	E(PMP3/Aug-CC-pVTZ) (Hartree):				-721.02736423		
50353	E(PUHF/Aug-CC-pVTZ) (Hartree):				-718.47134936		
50354	E(UHF/Aug-CC-pVTZ) (Hartree):				-718.46060932		
50355	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.14125335		
50356	Electronic state : 2-A						
50357	Cartesian coordinates (Angs):						
50358	O	-0.426497	2.018945	-0.325281			
50359	O	0.830183	2.202764	0.222478			
50360	H	1.456818	1.382964	-0.450478			
50361	C	1.544109	0.196172	-0.965922			
50362	C	0.079135	-0.244069	-0.988492			
50363	C	-0.851103	0.679907	-0.121428			
50364	C	-2.296575	0.683537	-0.604096			
50365	H	-2.750537	-0.293301	-0.482091			
50366	H	-2.318938	0.957313	-1.657739			
50367	H	-2.863255	1.422841	-0.040066			
50368	C	-0.805790	0.323965	1.355380			
50369	O	-1.179066	-0.744878	1.767554			
50370	H	-0.451596	1.118551	2.027836			
50371	H	-0.293876	-0.165749	-2.012764			
50372	O	0.103411	-1.599071	-0.590226			
50373	O	-1.198459	-2.149699	-0.651388			

50374	H	-1.485757	-2.019191	0.270451		
50375	H	2.014541	0.288717	-1.940893		
50376	O	2.400552	-0.526749	-0.175973		
50377	O	1.882530	-0.590434	1.143475		
50378	H	1.372716	-1.416248	1.107984		
50379	Rotational constants (GHz):			1.1114900	1.0092500	0.7762500
50380	Vibrational harmonic frequencies (cm-1):					
50381	i1894.1350		85.6247			120.8925
50382	138.8282		172.8195			182.1285
50383	212.4704		224.0268			255.6514
50384	273.2632		282.5595			310.4962
50385	340.9308		359.6163			418.6002
50386	447.6934		464.2974			489.5957
50387	539.8136		610.4689			627.9672
50388	695.9895		737.1806			761.4606
50389	906.1852		940.6244			966.8332
50390	982.4255		999.1701			1045.6772
50391	1055.8927		1094.1414			1132.0723
50392	1179.9077		1193.3619			1203.0833
50393	1224.9959		1252.6017			1326.9514
50394	1361.6015		1381.1613			1401.0039
50395	1417.3442		1439.5369			1476.9953
50396	1485.5292		1501.1909			1593.3949
50397	1830.4098		3043.0286			3070.7068
50398	3084.1583		3153.8816			3160.6650
50399	3205.5933		3651.4724			3739.5221
50400	Zero-point correction (Hartree): 0.150937					
50401	TS.diHPCARP_I.15HPHshift.dmtdddu					
50402	-----					
50403	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.13671017					
50404	Electronic state : 2-A					
50405	Cartesian coordinates (Angs):					
50406	O	-0.757685	-1.385799	1.156447		
50408	O	0.453671	-1.328784	1.820453		
50409	H	0.701281	-0.152040	1.766864		
50410	C	0.827484	0.927317	0.982143		
50411	C	-0.309011	0.685702	0.022544		
50412	C	-0.582369	-0.831955	-0.133699		
50413	C	-1.858248	-1.131766	-0.904122		
50414	H	-1.813160	-0.668671	-1.887186		
50415	H	-2.707819	-0.727890	-0.358486		
50416	H	-1.979438	-2.208759	-1.012849		
50417	C	0.578810	-1.523924	-0.832125		
50418	O	1.189543	-1.030639	-1.741980		
50419	H	0.775498	-2.550741	-0.481291		
50420	H	-0.066758	1.096902	-0.959204		
50421	O	-1.435857	1.349232	0.559318		
50422	O	-2.291571	1.715993	-0.516319		
50423	H	-2.239158	2.679348	-0.477321		
50424	H	0.733440	1.815324	1.606568		
50425	O	2.094203	0.683067	0.494514		
50426	O	2.305270	1.405874	-0.725919		
50427	H	2.195527	0.692727	-1.377655		
50428	Rotational constants (GHz):			1.0719900	0.8709400	0.7474700
50429	Vibrational harmonic frequencies (cm-1):					
50430	i1980.8606		70.0882			89.5166
50431	112.3270		160.9950			165.6403
50432	188.3150		225.5146			230.4933
50433	251.2511		276.5899			281.2064
50434	305.9585		333.9978			358.5595
50435	382.9024		492.4772			502.0335
50436	522.5537		571.2364			622.5134
50437	653.7694		675.6199			792.1907
50438	923.6072		934.3166			956.7113
50439	976.2277		1002.7863			1021.2948
50440	1084.4655		1110.8912			1129.6098
50441	1156.6116		1165.6348			1223.7613
50442	1240.0635		1262.2198			1278.2216
50443	1321.0913		1388.9894			1399.4583
50444	1409.4505		1411.5971			1442.3292
50445	1484.3585		1504.8793			1561.1253

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50446      1846.1325          3008.9019          3080.3816
50447      3094.3048          3115.4282          3160.3798
50448      3176.7952          3711.2528          3818.8613
50449 Zero-point correction (Hartree): 0.149602
50450
50451
50452

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50453 #####
50454 Raw quantum chemical M06-2X/aug-cc-pVTZ data for tri-HPACYL-I
50455 #####
50456

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50457 (2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)
50458 =====
50459

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50460 triHPacyl.mmpmptmmpd
50461 -----

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50462 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17413953
50463 Electronic state : 2-A
50464 Cartesian coordinates (Angs):

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50465	O	0.356195	1.967623	1.359047
50466	O	0.399742	0.557214	1.290376
50467	C	0.982018	0.107730	0.068857
50468	C	-0.047337	-0.140040	-1.058972
50469	C	-1.099829	-1.226907	-0.842833
50470	O	-2.040470	-0.947469	0.177962
50471	O	-1.519319	-1.390584	1.419732
50472	H	-0.419852	2.164320	0.799971
50473	C	2.121540	1.003666	-0.395477
50474	H	2.785795	1.217562	0.438557
50475	H	1.723894	1.938244	-0.780135
50476	H	2.675081	0.494461	-1.182327
50477	C	1.599321	-1.260837	0.426899
50478	O	2.043090	-2.028914	-0.337358
50479	H	-1.000487	-0.622567	1.719282
50480	H	0.541854	-0.462954	-1.922583
50481	O	-0.644862	1.055874	-1.540639
50482	O	-1.490411	1.648280	-0.557069
50483	H	-2.139171	0.954355	-0.347724
50484	H	-1.694786	-1.284805	-1.756122
50485	H	-0.638318	-2.196477	-0.656168

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50486 Rotational constants (GHz): 1.0563000 0.9539500 0.7627600
50487 Vibrational harmonic frequencies (cm-1):

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50488	43.9242	79.5076	112.9979
50489	141.7707	196.2849	202.2560
50490	217.3571	244.8839	263.4347
50491	276.1148	289.3387	310.9194
50492	332.5692	344.3689	432.2396
50493	440.5730	465.8092	504.9517
50494	517.5765	612.2424	621.2137
50495	691.4783	706.6044	818.3034
50496	887.9365	904.0014	921.0832
50497	977.4381	995.0162	1061.1348
50498	1076.4520	1107.4028	1130.2175
50499	1149.0642	1182.1467	1224.7631
50500	1315.0244	1346.9596	1363.9347
50501	1405.3107	1411.7558	1470.3895
50502	1477.5086	1481.4807	1488.2629
50503	1494.2752	1496.0781	1981.7803
50504	3074.5878	3083.8348	3087.4611
50505	3139.1145	3167.2852	3182.2456
50506	3592.4439	3664.0687	3694.5928

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50507 Zero-point correction (Hartree): 0.156970
50508

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50509 triHPacyl.mmpmptttmpd
50510 -----

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50511 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17356137
50512 Electronic state : 2-A
50513 Cartesian coordinates (Angs):

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50514	O	0.275501	0.451755	2.130871
50515	O	-0.589750	0.987414	1.148559
50516	C	-0.998659	-0.048107	0.262121
50517	C	0.151318	-0.686466	-0.539825

50518	C	1.141954	0.284503	-1.169593	
50519	O	1.762710	1.136882	-0.219003	
50520	O	1.193987	2.434131	-0.309632	
50521	H	1.137024	0.494898	1.677856	
50522	C	-1.862743	-1.073312	0.979541	
50523	H	-2.744306	-0.584211	1.389727	
50524	H	-1.286487	-1.512530	1.789035	
50525	H	-2.171907	-1.852276	0.284593	
50526	C	-1.886282	0.702854	-0.749480	
50527	O	-2.358820	0.253474	-1.720078	
50528	H	0.438771	2.361636	0.298853	
50529	H	-0.316639	-1.265041	-1.342806	
50530	O	0.820755	-1.584969	0.335190	
50531	O	1.623032	-2.430178	-0.484346	
50532	H	1.246183	-3.295443	-0.283042	
50533	H	1.938022	-0.304828	-1.624478	
50534	H	0.666495	0.892881	-1.938801	
50535	Rotational constants (GHz):		0.9631400	0.9023800	0.7464600
50536	Vibrational harmonic frequencies (cm-1):				
50537		47.2276	84.4727		98.7121
50538		150.3593	169.4999		178.8788
50539		191.4403	208.1385		221.6683
50540		228.2546	250.0938		280.0501
50541		288.2511	323.1339		393.2397
50542		407.5169	449.8471		495.1341
50543		502.9013	537.7298		595.4034
50544		617.9824	696.2067		819.3224
50545		851.2487	908.8938		955.2576
50546		978.7168	1033.0095		1052.3946
50547		1063.7737	1116.3128		1129.7307
50548		1140.8345	1187.2635		1231.4529
50549		1302.7858	1357.7265		1377.5208
50550		1397.9669	1402.3137		1409.9919
50551		1462.6319	1472.5700		1481.7045
50552		1483.7794	1498.8045		1993.4191
50553		3056.9457	3081.9299		3089.1302
50554		3141.8822	3160.0773		3180.3186
50555		3671.3034	3690.4569		3827.7606
50556	Zero-point correction (Hartree):		0.155884		
50557	-----				
50558	triHPacyl.mmpmptppd				
50559	-----				
50560	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17392274		
50561	Electronic state : 2-A				
50562	Cartesian coordinates (Angs):				
50563	O	0.300401	0.521428	2.104170	
50564	O	-0.531855	1.064896	1.097240	
50565	C	-1.015876	0.014697	0.265168	
50566	C	0.086116	-0.710904	-0.528129	
50567	C	1.112112	0.193123	-1.196024	
50568	O	1.838869	0.973682	-0.256330	
50569	O	1.424824	2.327998	-0.341082	
50570	H	1.159870	0.484998	1.647908	
50571	C	-1.917969	-0.934223	1.037382	
50572	H	-2.767164	-0.384484	1.438998	
50573	H	-1.351446	-1.371754	1.854191	
50574	H	-2.273748	-1.725056	0.379539	
50575	C	-1.882627	0.772648	-0.759118	
50576	O	-2.387796	0.316185	-1.709667	
50577	H	0.644212	2.332953	0.239540	
50578	H	-0.421792	-1.290404	-1.305369	
50579	O	0.712496	-1.618802	0.367203	
50580	O	1.386230	-2.581340	-0.439067	
50581	H	2.291181	-2.504043	-0.112861	
50582	H	1.836482	-0.439532	-1.709545	
50583	H	0.646522	0.852900	-1.927804	
50584	Rotational constants (GHz):		0.9710000	0.8933600	0.7419600
50585	Vibrational harmonic frequencies (cm-1):				
50586		47.9769	77.6098		97.5819
50587		153.0863	174.5483		182.7237
50588		196.5908	211.3788		221.3106
50589		227.7634	255.7228		278.5700

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50590      290.3237      323.1038      392.3103
50591      410.3599      450.1608      484.3545
50592      502.2789      537.4390      601.4298
50593      618.6371      697.0189      812.7950
50594      849.8034      910.2579      958.0084
50595      978.8007      1035.7219     1052.8273
50596      1063.6667     1116.2921     1129.5417
50597      1140.5833     1186.4490     1231.3464
50598      1297.6112     1363.3289     1374.2657
50599      1395.7695     1403.1811     1411.4658
50600      1465.2883     1476.3819     1481.4880
50601      1483.8672     1498.5380     1993.8031
50602      3063.9492     3083.8490     3088.7599
50603      3139.7739     3162.4116     3183.7856
50604      3684.4896     3704.1467     3830.2620
50605 Zero-point correction (Hartree): 0.156020
50606
50607 triHPacyl.mmpptmmd
50608 -----
50609 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17438675
50610 Electronic state : 2-A
50611 Cartesian coordinates (Angs):
50612 O      0.207461      2.090821      -1.177110
50613 O     -0.177206      0.729983      -1.243613
50614 C     -0.924524      0.348610      -0.092360
50615 C     -0.054297     -0.225054      1.050915
50616 C      0.622369     -1.571620      0.739428
50617 O      0.867283     -1.842092     -0.619989
50618 O      1.942233     -1.025752     -1.062856
50619 H      0.973994      2.047193     -0.575173
50620 C     -1.841220      1.459680      0.402308
50621 H     -2.368686      1.903952     -0.438241
50622 H     -1.255376      2.227417      0.899808
50623 H     -2.559605      1.042711      1.106139
50624 C     -1.843063     -0.784920     -0.592798
50625 O     -2.398822     -1.561090      0.086420
50626 H      1.449679     -0.346583     -1.556738
50627 H     -0.738232     -0.404179      1.884323
50628 O      0.829216      0.719570      1.635721
50629 O      1.849549      1.126622      0.733669
50630 H      2.288806      0.300834      0.462004
50631 H      1.544632     -1.658536      1.320805
50632 H     -0.048513     -2.377490      1.034167
50633 Rotational constants (GHz):      1.0920400      0.9813000      0.7685500
50634 Vibrational harmonic frequencies (cm-1):
50635      68.0900      118.8503      139.1770
50636      164.6330      183.9732      202.1795
50637      209.7398      244.7980      260.1757
50638      270.3671      292.5495      310.3284
50639      349.4299      364.2312      373.6086
50640      442.2052      456.3235      487.1120
50641      555.8576      607.2398      636.8584
50642      691.4231      708.1843      782.1367
50643      853.0431      909.7246      948.2830
50644      977.4663     1029.9012     1062.5438
50645     1073.9259     1100.1831     1138.5834
50646     1144.6780     1187.5802     1223.4221
50647     1303.4191     1346.3197     1366.0727
50648     1403.5551     1410.8847     1447.6885
50649     1467.1876     1488.2464     1489.1362
50650     1492.7216     1494.4427     1976.9352
50651     3062.8485     3084.8948     3089.1024
50652     3137.9808     3166.3377     3180.4510
50653     3612.7259     3671.8341     3689.7402
50654 Zero-point correction (Hartree): 0.157083
50655
50656 triHPacyl.mmppttpd
50657 -----
50658 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17455036
50659 Electronic state : 2-A
50660 Cartesian coordinates (Angs):
50661 O     -0.044011      2.090539      0.752536

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50662 O -0.914618 1.552195 -0.225525
50663 C -1.227624 0.216315 0.129065
50664 C -0.032211 -0.744362 -0.012756
50665 C 0.821040 -0.441737 -1.243515
50666 O 1.637385 0.711997 -1.072694
50667 O 2.829497 0.322916 -0.395129
50668 H 0.822374 1.873139 0.371756
50669 C -1.919612 0.115859 1.480066
50670 H -2.837470 0.700827 1.462459
50671 H -1.255998 0.506361 2.245527
50672 H -2.151747 -0.924557 1.701341
50673 C -2.268147 -0.177798 -0.940551
50674 O -2.626740 -1.261612 -1.198357
50675 H 3.495710 0.483105 -1.075345
50676 H -0.434943 -1.757283 -0.108202
50677 O 0.723231 -0.663403 1.178373
50678 O 1.648886 -1.740872 1.166628
50679 H 2.451765 -1.285619 0.872492
50680 H 1.456935 -1.289788 -1.492419
50681 H 0.183674 -0.209922 -2.098118
50682 Rotational constants (GHz): 1.2865300 0.7359900 0.6863600
50683 Vibrational harmonic frequencies (cm-1):
50684 64.7662 96.4132 98.2130
50685 153.8003 167.3719 183.2760
50686 197.0133 213.9678 232.0689
50687 245.7361 260.0195 274.7580
50688 292.2990 329.7103 374.8259
50689 411.4675 449.8524 451.2052
50690 483.6258 501.7408 549.6767
50691 616.0065 716.0147 817.5180
50692 846.0861 892.8483 953.3417
50693 995.7679 1035.3391 1038.2044
50694 1060.6954 1103.4285 1137.3651
50695 1144.3425 1197.0467 1242.6721
50696 1304.6119 1370.7500 1380.8192
50697 1389.7967 1401.8950 1411.3882
50698 1445.0979 1459.2561 1470.9441
50699 1481.3026 1498.7148 1986.5232
50700 3065.3579 3083.2700 3087.4865
50701 3142.1567 3160.6982 3186.4911
50702 3729.9692 3767.0421 3821.6334
50703 Zero-point correction (Hartree): 0.155995
50704
50705 triHPacyl.mmtmptmmmd
50706 -----
50707 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17452124
50708 Electronic state : 2-A
50709 Cartesian coordinates (Angs):
50710 O 1.277401 -2.105805 -0.864575
50711 O 1.250343 -0.729192 -1.192761
50712 C 1.255068 0.068295 -0.017519
50713 C -0.170127 0.379634 0.494209
50714 C -1.069738 0.891084 -0.623383
50715 O -2.344863 1.282233 -0.147519
50716 O -3.165959 0.122298 -0.047929
50717 H 0.351429 -2.278286 -0.623052
50718 C 2.159369 -0.470340 1.080688
50719 H 3.139344 -0.701266 0.668705
50720 H 1.728981 -1.373301 1.502171
50721 H 2.257374 0.281051 1.862496
50722 C 1.865349 1.408194 -0.482996
50723 O 1.887531 2.402806 0.135391
50724 H -3.847725 0.314979 -0.703194
50725 H -0.080025 1.155437 1.258599
50726 O -0.749281 -0.686620 1.224959
50727 O -1.145141 -1.730562 0.347328
50728 H -2.060607 -1.470582 0.152301
50729 H -0.639474 1.805597 -1.035104
50730 H -1.169062 0.163891 -1.428064
50731 Rotational constants (GHz): 1.2531900 0.7729300 0.5857800
50732 Vibrational harmonic frequencies (cm-1):
50733 52.8808 80.3952 91.7436

```

50734	125.7595	164.0462	189.5080		
50735	208.2076	221.8335	243.6229		
50736	263.6597	276.9336	297.3042		
50737	309.4314	313.4990	337.8728		
50738	436.2375	462.5727	484.6582		
50739	516.4839	562.8345	599.7392		
50740	614.7814	667.9631	826.7584		
50741	842.9811	886.1382	953.4787		
50742	982.6661	1004.9269	1056.5356		
50743	1090.0111	1110.1289	1140.2369		
50744	1153.5665	1185.9189	1223.0287		
50745	1296.6132	1325.4110	1386.6437		
50746	1390.1564	1404.8081	1424.8327		
50747	1453.7745	1470.9558	1483.6719		
50748	1484.7040	1492.8392	1978.6859		
50749	3085.9396	3089.1042	3094.6285		
50750	3144.4275	3164.6195	3186.1375		
50751	3690.2418	3714.6124	3826.4668		
50752	Zero-point correction (Hartree): 0.156209				
50753	-----				
50754	triHPacyl.mmtmptmmpd				
50755	-----				
50756	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17540799				
50757	Electronic state : 2-A				
50758	Cartesian coordinates (Angs):				
50759	O	1.358117	-2.090929	-0.840385	
50760	O	1.302218	-0.715652	-1.169667	
50761	C	1.243244	0.082500	0.002658	
50762	C	-0.206137	0.379215	0.447273	
50763	C	-1.075799	0.850532	-0.710034	
50764	O	-2.358406	1.271951	-0.289247	
50765	O	-3.159711	0.113017	-0.064841	
50766	H	0.430679	-2.289439	-0.627168	
50767	C	2.104721	-0.440547	1.142213	
50768	H	3.106145	-0.655084	0.775527	
50769	H	1.672113	-1.350893	1.545144	
50770	H	2.154625	0.312874	1.926672	
50771	C	1.856954	1.431740	-0.435255	
50772	O	1.820551	2.430534	0.175088	
50773	H	-3.299824	0.162708	0.890249	
50774	H	-0.159498	1.169101	1.201418	
50775	O	-0.802301	-0.687038	1.173642	
50776	O	-1.117116	-1.761266	0.299810	
50777	H	-1.993520	-1.493536	-0.026109	
50778	H	-0.633425	1.744360	-1.152352	
50779	H	-1.162014	0.094335	-1.489715	
50780	Rotational constants (GHz): 1.2469800			0.7797800	0.5890200
50781	Vibrational harmonic frequencies (cm-1):				
50782	50.6983	81.7872	93.3135		
50783	122.5944	156.5098	188.3769		
50784	208.1433	226.2867	246.4442		
50785	267.6625	279.9953	304.9782		
50786	316.6772	340.6769	365.9745		
50787	437.6808	464.3825	476.1652		
50788	544.4488	567.9971	612.6692		
50789	647.2460	668.6813	829.1452		
50790	844.2931	887.8250	951.7821		
50791	983.6858	1005.1475	1057.0216		
50792	1091.9251	1113.2323	1134.5994		
50793	1152.3939	1184.1312	1224.7138		
50794	1292.8641	1322.3973	1385.8289		
50795	1401.7582	1404.9588	1420.9782		
50796	1443.9869	1477.2039	1481.8217		
50797	1485.3707	1492.9330	1979.6096		
50798	3085.4519	3088.5440	3093.4860		
50799	3142.7863	3164.8513	3186.3345		
50800	3678.0666	3695.5065	3808.0291		
50801	Zero-point correction (Hartree): 0.156424				
50802	-----				
50803	triHPacyl.mmtpptmmmd				
50804	-----				
50805	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17492646				

```

50806 Electronic state : 2-A
50807 Cartesian coordinates (Angs):
50808 O 1.757738 -1.950256 -0.542326
50809 O 1.516898 -0.645876 -1.036867
50810 C 1.207395 0.235573 0.029761
50811 C -0.297279 0.262946 0.366357
50812 C -1.166574 0.547837 -0.858468
50813 O -2.496171 0.110542 -0.654160
50814 O -3.042537 0.852804 0.425522
50815 H 0.858843 -2.312636 -0.479503
50816 C 2.073043 0.020678 1.262515
50817 H 3.119198 -0.037014 0.970001
50818 H 1.791178 -0.906659 1.751916
50819 H 1.931177 0.852792 1.950015
50820 C 1.552030 1.633111 -0.532479
50821 O 1.303891 2.654938 -0.017073
50822 H -2.885228 0.261196 1.175721
50823 H -0.442652 1.042124 1.117556
50824 O -0.752348 -0.898583 1.051050
50825 O -0.893158 -1.983268 0.143928
50826 H -1.770099 -1.813527 -0.236607
50827 H -1.146589 1.612643 -1.094825
50828 H -0.822020 -0.022203 -1.720973
50829 Rotational constants (GHz): 1.2135300 0.8057700 0.5953700
50830 Vibrational harmonic frequencies (cm-1):
50831 56.7169 77.5930 91.5279
50832 137.9808 141.9283 180.4385
50833 221.7611 227.0421 249.2153
50834 264.7636 279.1068 315.5920
50835 336.4496 348.4319 397.9109
50836 436.0420 457.0685 469.0438
50837 505.0221 576.4025 593.5835
50838 596.3458 718.6465 803.7283
50839 846.0204 903.8284 957.1254
50840 983.4953 1002.5079 1055.0927
50841 1082.8225 1110.9513 1135.6483
50842 1151.2011 1188.3204 1232.4454
50843 1293.7185 1329.0297 1387.8547
50844 1401.6967 1405.2621 1423.2756
50845 1432.6852 1471.3597 1485.5581
50846 1491.7000 1496.1539 1980.9783
50847 3085.8875 3086.1659 3097.6056
50848 3145.3292 3165.3765 3183.3121
50849 3709.1424 3729.7668 3775.5038
50850 Zero-point correction (Hartree): 0.156531
50851
50852 triHPacyl.mtmmptmpmd
50853 -----
50854 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17495686
50855 Electronic state : 2-A
50856 Cartesian coordinates (Angs):
50857 O 2.167092 -0.956618 -1.371868
50858 O 1.968228 -0.683546 0.004441
50859 C 0.561327 -0.645988 0.261895
50860 C -0.078696 0.460994 -0.611090
50861 C -1.379588 1.070919 -0.097239
50862 O -2.395234 0.110095 0.085243
50863 O -2.682749 -0.444329 -1.197249
50864 H 2.253402 -0.061817 -1.732592
50865 C -0.084742 -2.006360 0.058810
50866 H 0.401550 -2.741101 0.697775
50867 H 0.037685 -2.303142 -0.980954
50868 H -1.143437 -1.952836 0.299712
50869 C 0.523801 -0.305326 1.756537
50870 O -0.419307 -0.212947 2.443344
50871 H -3.601094 -0.174419 -1.317543
50872 H -0.258787 0.029679 -1.597484
50873 O 0.859982 1.489413 -0.869908
50874 O 1.248147 2.057110 0.374154
50875 H 2.030803 1.526907 0.595186
50876 H -1.245666 1.520359 0.884547
50877 H -1.696336 1.837519 -0.807384

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50878 Rotational constants (GHz): 1.1459900 0.7681800 0.7577300
50879 Vibrational harmonic frequencies (cm-1):
50880 60.2309 75.0642 115.4993
50881 140.2667 173.5494 177.3661
50882 198.2359 203.4705 210.5969
50883 231.8481 260.3793 265.9792
50884 332.3223 346.5893 389.3754
50885 433.3270 456.8549 458.3006
50886 477.7194 502.6527 545.8178
50887 629.7079 659.8208 774.2796
50888 863.4177 940.8268 950.2771
50889 980.6962 1042.0862 1048.8617
50890 1096.7698 1116.8324 1133.6066
50891 1160.0739 1189.9984 1221.0919
50892 1285.2933 1345.9944 1364.3724
50893 1391.4449 1403.4980 1417.9096
50894 1427.2157 1436.4328 1488.8695
50895 1492.7397 1497.6988 1991.7196
50896 3075.7340 3083.7201 3104.4932
50897 3160.5634 3162.3481 3181.9372
50898 3737.9009 3770.8975 3830.8034
50899 Zero-point correction (Hartree): 0.156090
50900
50901 triHPacyl.mtppmpmpd
50902 -----
50903 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17271628
50904 Electronic state : 2-A
50905 Cartesian coordinates (Angs):
50906 O -2.628071 0.244557 0.778779
50907 O -1.871603 -0.416525 -0.223751
50908 C -0.533789 -0.591741 0.244168
50909 C 0.119618 0.758807 0.547281
50910 C 1.519768 0.669779 1.152020
50911 O 2.373929 -0.296888 0.593295
50912 O 2.823406 0.187857 -0.660647
50913 H -2.565298 1.166390 0.482740
50914 C -0.475097 -1.568529 1.408830
50915 H -1.066749 -2.447154 1.160738
50916 H -0.898205 -1.095733 2.294172
50917 H 0.551678 -1.868132 1.609790
50918 C 0.155729 -1.252488 -0.971589
50919 O -0.330593 -1.994131 -1.731505
50920 H 2.218945 -0.262310 -1.272499
50921 H -0.494668 1.277890 1.286279
50922 O 0.181778 1.564855 -0.620707
50923 O -1.102622 2.146915 -0.832699
50924 H -1.440691 1.615645 -1.566751
50925 H 1.983241 1.655890 1.102934
50926 H 1.424573 0.369420 2.196211
50927 Rotational constants (GHz): 1.1720100 0.8062100 0.6931300
50928 Vibrational harmonic frequencies (cm-1):
50929 19.6865 92.6863 119.2724
50930 143.3188 157.8630 167.3168
50931 184.4271 199.7198 223.9578
50932 259.0256 261.0333 301.2375
50933 331.2678 347.3545 393.7833
50934 410.1165 422.1100 448.8810
50935 488.6456 523.9720 582.2046
50936 609.7056 710.9197 741.2716
50937 880.7593 900.4089 965.4977
50938 985.0229 1030.1068 1032.3334
50939 1065.1946 1126.6546 1140.7368
50940 1155.2996 1183.9843 1252.5352
50941 1311.5970 1367.5955 1375.3126
50942 1399.1098 1413.3933 1413.7196
50943 1432.8562 1436.5988 1461.4598
50944 1494.2832 1497.2367 1995.0387
50945 3077.4012 3078.9399 3088.9427
50946 3135.4827 3158.5061 3167.7624
50947 3714.7431 3745.4620 3793.8386
50948 Zero-point correction (Hartree): 0.155867
50949

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50950 triHPacyl.mttptmpd
50951 -----
50952 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17517081
50953 Electronic state : 2-A
50954 Cartesian coordinates (Angs):
50955 O -1.890764 -1.627191 -1.090695
50956 O -2.072800 -0.513626 -0.233837
50957 C -0.959245 0.363871 -0.390908
50958 C 0.345190 -0.386581 -0.041042
50959 C 1.498901 0.503968 0.395108
50960 O 2.728819 -0.175060 0.272668
50961 O 2.969844 -0.335919 -1.123436
50962 H -1.439796 -2.250284 -0.500823
50963 C -0.913049 0.978685 -1.780147
50964 H -1.810436 1.567076 -1.960232
50965 H -0.857514 0.178538 -2.515220
50966 H -0.040985 1.622663 -1.878760
50967 C -1.266577 1.470241 0.627266
50968 O -0.652647 2.451720 0.804592
50969 H 3.784232 0.169501 -1.231592
50970 H 0.655194 -0.941479 -0.928781
50971 O 0.085352 -1.407678 0.905855
50972 O -0.426696 -0.798121 2.082436
50973 H -1.383625 -0.850438 1.930502
50974 H 1.523739 1.434812 -0.173308
50975 H 1.409002 0.735516 1.455897
50976 Rotational constants (GHz): 1.1281200 0.7281900 0.6849200
50977 Vibrational harmonic frequencies (cm-1):
50978 57.7456 70.6577 117.1560
50979 139.0653 158.9666 176.2516
50980 192.0256 197.3636 207.7092
50981 225.5351 259.3343 291.4468
50982 316.1725 346.1539 379.2590
50983 404.3543 457.7270 461.0773
50984 496.2790 504.8633 573.1571
50985 625.1149 660.2502 804.0729
50986 890.3450 926.8883 950.1325
50987 982.6662 1000.5700 1049.2067
50988 1090.0625 1131.1369 1134.4487
50989 1163.3138 1177.5634 1221.0021
50990 1296.9326 1322.0298 1389.6271
50991 1393.4036 1403.1350 1419.8601
50992 1430.9016 1435.8141 1466.4467
50993 1481.3628 1500.7016 1986.8140
50994 3080.8402 3086.7531 3103.5430
50995 3151.0865 3163.8077 3167.9396
50996 3748.4062 3755.3430 3831.6359
50997 Zero-point correction (Hartree): 0.155953
50998
50999 triHPacyl.pmmmpmmpd
51000 -----
51001 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17516257
51002 Electronic state : 2-A
51003 Cartesian coordinates (Angs):
51004 O 0.765075 0.761767 -1.818596
51005 O 1.415624 0.917542 -0.567252
51006 C 0.510970 0.648798 0.498883
51007 C 0.077209 -0.828645 0.582243
51008 C -0.863754 -1.334649 -0.507881
51009 O -2.024622 -0.535799 -0.583320
51010 O -2.744820 -0.711923 0.635290
51011 H 0.367401 1.637442 -1.942780
51012 C 1.295475 1.039823 1.747756
51013 H 1.618447 2.075960 1.672932
51014 H 2.163901 0.391094 1.837868
51015 H 0.667246 0.922350 2.628009
51016 C -0.700733 1.588435 0.437209
51017 O -0.849079 2.484904 -0.305669
51018 H -3.560756 -1.113273 0.312997
51019 H -0.433296 -0.939435 1.541550
51020 O 1.211683 -1.661610 0.705550
51021 O 1.792035 -1.876542 -0.576216

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51022	H	2.269349	-1.048118	-0.733246	
51023	H	-0.414196	-1.261415	-1.491631	
51024	H	-1.120265	-2.373887	-0.293259	
51025	Rotational constants (GHz):		1.0419500	0.9399600	0.7107600
51026	Vibrational harmonic frequencies (cm-1):				
51027		41.6311	83.1239		132.0794
51028		144.8518	157.0767		157.7043
51029		201.7390	208.3108		214.2577
51030		218.8631	271.6383		289.4082
51031		314.1731	355.3783		373.2239
51032		399.7076	425.3975		435.9424
51033		458.6756	506.4030		588.4560
51034		619.4397	693.1951		793.5669
51035		856.1264	925.6471		949.4658
51036		971.1639	1041.3600		1051.4637
51037		1100.3134	1114.3545		1125.0627
51038		1158.6772	1194.9174		1239.6588
51039		1290.3638	1331.7678		1386.3444
51040		1395.0487	1407.2625		1421.7829
51041		1432.0057	1439.7810		1484.0001
51042		1490.4254	1497.4651		1971.2570
51043		3081.7268	3083.5434		3097.5868
51044		3167.3387	3171.3560		3198.2900
51045		3757.7186	3765.6735		3832.2293
51046	Zero-point correction (Hartree): 0.156090				
51047					
51048	triHPacyl.pmmmpmmpd				
51049	-----				
51050	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17654613				
51051	Electronic state : 2-A				
51052	Cartesian coordinates (Angs):				
51053	O	0.610796	0.827416	-1.823803	
51054	O	1.171624	1.187591	-0.571313	
51055	C	0.337613	0.734743	0.484495	
51056	C	0.261779	-0.801354	0.603750	
51057	C	-0.541654	-1.538318	-0.465449	
51058	O	-1.831993	-0.989327	-0.614276	
51059	O	-2.562896	-1.278737	0.574897	
51060	H	0.072031	1.606202	-2.029575	
51061	C	0.968836	1.334123	1.737413	
51062	H	1.057206	2.412971	1.629786	
51063	H	1.955308	0.896833	1.875503	
51064	H	0.354108	1.108055	2.606192	
51065	C	-1.063859	1.354682	0.364855	
51066	O	-1.387337	2.221607	-0.354437	
51067	H	-2.728588	-0.388304	0.917364	
51068	H	-0.203528	-1.003636	1.571380	
51069	O	1.559356	-1.339860	0.745101	
51070	O	2.181139	-1.448603	-0.529885	
51071	H	2.481783	-0.543146	-0.696175	
51072	H	-0.085552	-1.440408	-1.444071	
51073	H	-0.604570	-2.592522	-0.191058	
51074	Rotational constants (GHz):		1.0562100	0.9385500	0.7160300
51075	Vibrational harmonic frequencies (cm-1):				
51076		57.6908	100.6128		133.1191
51077		152.5215	158.9905		186.7965
51078		204.5237	214.3336		220.1397
51079		271.4911	286.1154		308.5156
51080		324.9184	351.3002		369.7726
51081		383.3583	427.3816		433.7936
51082		451.2775	509.8762		590.5012
51083		622.4298	688.2933		791.2270
51084		849.4328	930.3536		951.4103
51085		971.7012	1040.1676		1050.8104
51086		1100.0365	1118.6560		1128.3332
51087		1154.9260	1191.7566		1244.3970
51088		1286.8450	1335.5990		1384.0577
51089		1404.5571	1409.9414		1424.4978
51090		1428.1640	1436.3814		1485.4741
51091		1489.9174	1496.9444		1976.7105
51092		3082.5819	3088.9479		3092.5840
51093		3167.1319	3170.4423		3198.0181

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51094          3769.1841          3770.0050          3776.9573
51095 Zero-point correction (Hartree): 0.156387
51096
51097 triHPacyl.pmmmpmpmd
51098 -----
51099 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17376323
51100 Electronic state : 2-A
51101 Cartesian coordinates (Angs):
51102 O      -0.791398      0.214674      2.083923
51103 O      -1.378794      0.843009      0.956492
51104 C      -0.460864      0.866960     -0.128038
51105 C      -0.161027     -0.529733     -0.714811
51106 C       0.572429     -1.520792      0.185732
51107 O       1.786881     -0.981022      0.658854
51108 O       2.660378     -0.856755     -0.460688
51109 H      -0.240267      0.925284      2.446250
51110 C      -1.135848      1.756198     -1.165737
51111 H      -1.312594      2.745888     -0.750513
51112 H      -2.083829      1.310876     -1.459360
51113 H      -0.493611      1.842839     -2.039235
51114 C       0.832055      1.583460      0.313947
51115 O       1.705795      1.930161     -0.380728
51116 H       3.372693     -1.456345     -0.208518
51117 H       0.451033     -0.357746     -1.603656
51118 O      -1.348235     -1.102222     -1.228642
51119 O      -2.113822     -1.658933     -0.165160
51120 H      -2.493200     -0.874734      0.259217
51121 H       0.000957     -1.747851      1.077838
51122 H       0.751899     -2.436063     -0.380982
51123 Rotational constants (GHz): 1.1072700      0.8854300      0.7191200
51124 Vibrational harmonic frequencies (cm-1):
51125 41.2327      81.0522      134.5842
51126 138.1075     146.3924     155.7187
51127 174.4142     207.4118     213.9511
51128 226.4842     255.8602     284.9841
51129 289.6384     309.6672     340.4838
51130 377.3260     412.3980     442.0820
51131 476.8055     528.6172     552.5581
51132 618.7866     653.0661     773.9284
51133 853.0746     936.3255     948.4835
51134 969.4847     1041.8769    1053.1000
51135 1096.5435    1116.4703    1116.9654
51136 1144.4949    1191.5650    1235.4259
51137 1291.3038    1330.5630    1378.5827
51138 1395.8637    1407.1337    1421.8657
51139 1425.7295    1443.5247    1484.7663
51140 1488.2341    1495.7702    1994.8663
51141 3084.0838    3084.7332    3092.7881
51142 3168.0622    3172.1742    3201.9797
51143 3753.6269    3759.0844    3834.3037
51144 Zero-point correction (Hartree): 0.155481
51145
51146 triHPacyl.pmmmpmpmd
51147 -----
51148 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17718424
51149 Electronic state : 2-A
51150 Cartesian coordinates (Angs):
51151 O      -0.857215      0.233060      2.049192
51152 O      -1.358607      0.926831      0.918516
51153 C      -0.408418      0.890266     -0.133160
51154 C      -0.188665     -0.523481     -0.721975
51155 C       0.500151     -1.549141      0.176237
51156 O       1.726187     -1.063272      0.674458
51157 O       2.652919     -1.053673     -0.405630
51158 H      -0.371811      0.930019      2.514368
51159 C      -0.981851      1.832556     -1.186863
51160 H      -1.120186      2.826459     -0.767065
51161 H      -1.940636      1.443908     -1.523010
51162 H      -0.301152      1.889558     -2.033236
51163 C       0.916883      1.503762      0.344789
51164 O       1.868230      1.712990     -0.311691
51165 H       2.859578     -0.110318     -0.478535

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51166	H	0.426767	-0.383965	-1.614520		
51167	O	-1.408024	-1.021097	-1.233779		
51168	O	-2.196661	-1.551327	-0.174519		
51169	H	-2.562169	-0.754867	0.238254		
51170	H	-0.092846	-1.770235	1.055571		
51171	H	0.659223	-2.462417	-0.398371		
51172	Rotational constants (GHz):		1.1342100	0.8806600	0.7213800	
51173	Vibrational harmonic frequencies (cm-1):					
51174		52.9102	94.7251		147.0506	
51175		153.5296	172.6375		185.6933	
51176		212.2310	223.8700		230.7444	
51177		254.9350	278.2491		286.7574	
51178		307.3980	335.6596		353.1214	
51179		377.4136	414.7634		440.2913	
51180		477.6897	531.3546		557.6579	
51181		620.7875	653.6242		772.7512	
51182		854.2239	940.1900		952.3986	
51183		971.7431	1041.6916		1053.7471	
51184		1094.2189	1120.2290		1125.9254	
51185		1144.3560	1188.0436		1236.8939	
51186		1291.9222	1333.5419		1377.4315	
51187		1405.7118	1412.2991		1417.8715	
51188		1440.8935	1444.4525		1487.3917	
51189		1491.6936	1495.9827		1966.1071	
51190		3083.3958	3087.4901		3095.6074	
51191		3168.5756	3171.8709		3204.3312	
51192		3769.1394	3773.8373		3776.2125	
51193	Zero-point correction (Hartree): 0.156180					
51194						
51195	triHPacyl.pmpmtmpmd					
51196	-----					
51197	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17624138					
51198	Electronic state : 2-A					
51199	Cartesian coordinates (Angs):					
51200	O	0.270573	-0.931906	1.898180		
51201	O	0.694133	0.351524	1.469525		
51202	C	1.163051	0.281629	0.138758		
51203	C	0.035077	0.232317	-0.919950		
51204	C	-0.877608	-0.993574	-0.949497		
51205	O	-1.748689	-1.154443	0.157428		
51206	O	-2.986071	-0.522798	-0.109887		
51207	H	-0.655838	-0.972606	1.590258		
51208	C	2.024548	1.526655	-0.044426		
51209	H	2.855920	1.499277	0.655797		
51210	H	1.426688	2.417066	0.140334		
51211	H	2.404987	1.569827	-1.063183		
51212	C	2.106755	-0.927112	-0.024284		
51213	O	2.359166	-1.463108	-1.035298		
51214	H	-2.777864	0.405670	0.098306		
51215	H	0.549333	0.226672	-1.885590		
51216	O	-0.655475	1.472909	-0.957953		
51217	O	-1.432985	1.662329	0.220985		
51218	H	-0.779740	1.669441	0.940052		
51219	H	-1.484515	-0.961453	-1.853174		
51220	H	-0.255129	-1.889440	-0.970247		
51221	Rotational constants (GHz):		1.3141600	0.7840200	0.7116000	
51222	Vibrational harmonic frequencies (cm-1):					
51223		56.0005	81.7767		104.5462	
51224		145.5284	165.3471		197.0450	
51225		210.2985	236.8654		248.9726	
51226		270.3000	292.8007		314.6451	
51227		323.6065	376.6841		415.1578	
51228		422.1602	484.8512		510.1423	
51229		580.8566	597.9932		641.4885	
51230		657.3353	676.9148		831.9944	
51231		875.5557	909.6501		950.3589	
51232		954.2013	1017.1257		1048.1013	
51233		1063.5650	1117.4638		1122.3807	
51234		1154.3242	1183.3016		1248.3800	
51235		1319.3576	1352.7464		1367.4953	
51236		1406.2423	1412.1552		1459.7152	
51237		1464.8359	1475.9225		1485.0620	

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51238      1495.5344          1497.3316          1978.1461
51239      3077.9067          3083.8637          3091.2613
51240      3145.2025          3163.8327          3171.9939
51241      3583.0092          3653.7362          3717.1272
51242      Zero-point correction (Hartree): 0.156943
51243
51244      triHPacyl.pmpmtpmd
51245      -----
51246      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17692251
51247      Electronic state : 2-A
51248      Cartesian coordinates (Angs):
51249      O      1.008583      2.006822      -0.656727
51250      O      0.928116      0.747431      -1.309582
51251      C      1.116811      -0.279902      -0.364138
51252      C      -0.145418      -0.641526      0.441477
51253      C      -0.842439      0.499931      1.173296
51254      O      -1.438449      1.467963      0.320030
51255      O      -2.596394      0.915457      -0.289552
51256      H      0.069364      2.226863      -0.545294
51257      C      1.632069      -1.477262      -1.154300
51258      H      2.610491      -1.242351      -1.566680
51259      H      0.940092      -1.694982      -1.963560
51260      H      1.703142      -2.350047      -0.507617
51261      C      2.248654      0.125001      0.609664
51262      O      2.340382      -0.181454      1.736247
51263      H      -2.236218      0.571454      -1.121185
51264      H      0.159936      -1.371737      1.197425
51265      O      -1.016540      -1.273867      -0.485997
51266      O      -2.080121      -1.869830      0.238940
51267      H      -2.743077      -1.161010      0.237208
51268      H      -1.606813      0.103166      1.841002
51269      H      -0.119585      1.061020      1.765840
51270      Rotational constants (GHz):      1.2463000      0.7971200      0.6778300
51271      Vibrational harmonic frequencies (cm-1):
51272      62.9357          65.9257          98.0497
51273      150.2422         170.3235         199.5912
51274      218.7138         227.0930         246.9274
51275      267.2993         278.5398         314.8968
51276      323.0991         387.2429         396.6518
51277      436.3249         469.0420         527.7366
51278      539.6537         569.7192         580.7311
51279      590.8753         703.2630         827.1991
51280      855.5754         898.4328         946.7239
51281      981.2590         1036.4049        1052.2973
51282      1058.6169        1111.4374        1128.2319
51283      1144.9386        1192.9961        1255.4917
51284      1306.8208        1367.1463        1382.3549
51285      1403.5390        1409.7854        1431.7646
51286      1450.7858        1453.8627        1480.2007
51287      1483.3617        1496.3736        1978.9652
51288      3067.1911        3085.0553        3094.0726
51289      3144.3634        3166.9164        3176.7911
51290      3710.4056        3734.1551        3764.4159
51291      Zero-point correction (Hartree): 0.156972
51292
51293      triHPacyl.pmpmpmmd
51294      -----
51295      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17641483
51296      Electronic state : 2-A
51297      Cartesian coordinates (Angs):
51298      O      -0.053201      -0.455212      1.794081
51299      O      1.131108      -0.064973      1.124096
51300      C      0.977101      -0.204213      -0.281421
51301      C      -0.081212      0.784454      -0.869189
51302      C      -1.361184      0.126405      -1.370807
51303      O      -1.908478      -0.808589      -0.474037
51304      O      -2.590797      -0.098268      0.546794
51305      H      0.057932      -1.417025      1.861859
51306      C      2.369129      0.064842      -0.841634
51307      H      3.091884      -0.622411      -0.406065
51308      H      2.649116      1.091657      -0.615594
51309      H      2.355641      -0.067978      -1.921946

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51310	C	0.660084	-1.672003	-0.626467	
51311	O	0.724177	-2.585615	0.104793	
51312	H	-1.870093	0.095771	1.168803	
51313	H	0.379421	1.302897	-1.715670	
51314	O	-0.456569	1.748389	0.086683	
51315	O	0.672959	2.567315	0.353650	
51316	H	1.024514	2.147665	1.152402	
51317	H	-2.095579	0.897127	-1.606872	
51318	H	-1.129951	-0.449009	-2.268285	
51319	Rotational constants (GHz):		1.0597600	1.0240300	0.7519900
51320	Vibrational harmonic frequencies (cm-1):				
51321		81.1281	111.9649		135.9527
51322		156.0557	182.5063		187.7567
51323		223.8826	231.3947		254.0123
51324		261.9476	302.6079		326.8740
51325		344.5666	394.1107		417.4944
51326		434.4702	438.6270		465.0112
51327		480.7062	532.6464		593.5720
51328		618.2636	734.6832		782.6036
51329		872.8609	886.0380		935.9763
51330		989.2417	1038.6062		1055.1789
51331		1068.8613	1124.1375		1147.7638
51332		1161.9663	1190.4232		1225.4510
51333		1316.6247	1356.6568		1378.3591
51334		1402.5104	1410.2110		1430.7272
51335		1435.8359	1460.0869		1467.2758
51336		1491.0010	1497.8127		1977.0164
51337		3053.7801	3078.7826		3080.8511
51338		3134.6463	3161.5951		3168.5589
51339		3701.9625	3746.4906		3780.8628
51340	Zero-point correction (Hartree): 0.157014				
51341					
51342	triHPacyl.pmpptpmmd				
51343	-----				
51344	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17631227				
51345	Electronic state : 2-A				
51346	Cartesian coordinates (Angs):				
51347	O	0.272511	-0.339928	1.934441	
51348	O	-0.990049	-0.462990	1.307872	
51349	C	-1.002525	0.254327	0.085623	
51350	C	-0.023732	-0.361844	-0.972344	
51351	C	1.228192	0.456781	-1.270215	
51352	O	1.899605	0.916842	-0.122366	
51353	O	2.657862	-0.156862	0.411383	
51354	H	0.238663	0.558697	2.300609	
51355	C	-2.452715	0.200898	-0.379564	
51356	H	-3.111856	0.625229	0.375014	
51357	H	-2.728164	-0.834431	-0.569624	
51358	H	-2.550456	0.772030	-1.300925	
51359	C	-0.691874	1.735743	0.391247	
51360	O	-0.720500	2.628738	-0.363703	
51361	H	1.995512	-0.617456	0.952757	
51362	H	-0.581425	-0.465031	-1.908124	
51363	O	0.409303	-1.639845	-0.567600	
51364	O	-0.713936	-2.508541	-0.557334	
51365	H	-0.967819	-2.474971	0.376624	
51366	H	1.902752	-0.137719	-1.886938	
51367	H	0.940357	1.358902	-1.809419	
51368	Rotational constants (GHz):		1.0502100	1.0022600	0.7499400
51369	Vibrational harmonic frequencies (cm-1):				
51370		82.5791	109.6498		149.4011
51371		156.2757	180.2770		190.9104
51372		212.3104	236.2925		248.7477
51373		263.4766	282.8916		315.7029
51374		331.5126	369.6260		402.9728
51375		427.3556	430.9428		472.0791
51376		504.1888	517.3396		536.5112
51377		645.0471	678.2327		785.5158
51378		867.7794	888.1333		941.2916
51379		988.2079	1036.7003		1057.8978
51380		1067.9584	1121.0887		1138.6546
51381		1154.8868	1186.9415		1223.4957

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51382      1315.7686      1351.1293      1374.5141
51383      1401.9312      1408.7828      1427.9125
51384      1428.2047      1465.2257      1468.4798
51385      1488.3713      1496.5108      1991.1272
51386      3058.7553      3079.8635      3090.6873
51387      3145.7152      3163.7813      3169.0300
51388      3721.4896      3734.8195      3779.1637
51389 Zero-point correction (Hartree): 0.156656
51390
51391 triHPacyl.pmtmmtmmmd
51392 -----
51393 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17493445
51394 Electronic state : 2-A
51395 Cartesian coordinates (Angs):
51396 O      -0.735652      -1.185281      1.768026
51397 O      -1.453850      -1.307170      0.551955
51398 C      -1.328896      -0.123399      -0.184193
51399 C      0.132720      0.242680      -0.559154
51400 C      0.974805      0.936348      0.508609
51401 O      2.193840      1.407476      -0.039571
51402 O      3.118742      0.322890      -0.077065
51403 H      0.074609      -1.662275      1.525298
51404 C      -2.150925      -0.379033      -1.443465
51405 H      -3.156318      -0.691651      -1.170474
51406 H      -1.669401      -1.171462      -2.013147
51407 H      -2.204090      0.527151      -2.042978
51408 C      -1.996037      1.055585      0.557561
51409 O      -1.970140      2.177868      0.216039
51410 H      3.818970      0.655782      0.497109
51411 H      0.065253      0.942231      -1.396157
51412 O      0.783371      -0.871319      -1.142285
51413 O      1.249043      -1.756742      -0.132409
51414 H      2.165147      -1.447575      -0.045480
51415 H      0.460496      1.839071      0.835603
51416 H      1.172500      0.313857      1.376571
51417 Rotational constants (GHz):      1.302490      0.7470300      0.6268300
51418 Vibrational harmonic frequencies (cm-1):
51419      78.0459      83.2751      110.2430
51420      133.4470      178.6664      194.6680
51421      206.2823      223.9045      236.9522
51422      255.3569      270.7556      277.1843
51423      307.4001      318.5302      350.0517
51424      377.2637      487.4891      520.8106
51425      535.0224      556.9249      563.7936
51426      593.8680      681.8781      821.2049
51427      864.3140      909.8592      952.5483
51428      975.7499      1008.4060      1051.5455
51429      1084.3003      1108.4180      1127.3982
51430      1153.0193      1175.6959      1253.7510
51431      1307.3655      1334.9797      1375.0022
51432      1392.6776      1399.6448      1423.2612
51433      1449.2328      1468.6454      1473.1448
51434      1487.8431      1499.8493      1970.9456
51435      3081.4391      3086.1223      3115.4562
51436      3167.6789      3169.9159      3172.9973
51437      3723.5600      3750.2692      3828.9512
51438 Zero-point correction (Hartree): 0.156526
51439
51440 triHPacyl.pmtmmtmmpd
51441 -----
51442 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17589244
51443 Electronic state : 2-A
51444 Cartesian coordinates (Angs):
51445 O      0.822616      -1.197297      -1.756042
51446 O      1.473018      -1.311232      -0.501981
51447 C      1.310529      -0.120722      0.213907
51448 C      -0.165319      0.252390      0.512015
51449 C      -0.974099      0.904930      -0.605297
51450 O      -2.193388      1.430355      -0.112822
51451 O      -3.115540      0.353653      0.048814
51452 H      0.013962      -1.698584      -1.566335
51453 C      2.072515      -0.359838      1.513541

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51454	H	3.091421	-0.668432	1.290827	
51455	H	1.570360	-1.150511	2.067542	
51456	H	2.092826	0.551985	2.106509	
51457	C	2.009462	1.053877	-0.507081	
51458	O	1.950847	2.180288	-0.184917	
51459	H	-3.197941	0.315491	1.010973	
51460	H	-0.130970	0.977647	1.329422	
51461	O	-0.843517	-0.848204	1.101193	
51462	O	-1.245721	-1.769935	0.096613	
51463	H	-2.133420	-1.432446	-0.109545	
51464	H	-0.440684	1.778843	-0.976104	
51465	H	-1.170605	0.241156	-1.442662	
51466	Rotational constants (GHz):		1.2937400	0.7528800	0.6315300
51467	Vibrational harmonic frequencies (cm-1):				
51468		78.6043		88.3679	109.3234
51469		130.8667		174.5016	193.9724
51470		210.7349		219.3700	229.8608
51471		260.5023		277.8816	287.9257
51472		322.8174		351.6014	364.8388
51473		382.3816		477.7333	499.0682
51474		539.9777		560.1417	579.1003
51475		620.5798		680.8335	826.4452
51476		868.3434		911.4137	949.8651
51477		976.3432		1006.4024	1052.7877
51478		1087.7963		1109.7067	1123.1861
51479		1151.9008		1173.6734	1255.9493
51480		1304.3504		1336.0330	1372.7485
51481		1399.9641		1402.9809	1418.4579
51482		1442.8619		1461.5357	1477.2905
51483		1487.7477		1499.4781	1972.0231
51484		3080.4347		3083.6639	3119.8173
51485		3167.8749		3169.9599	3173.4903
51486		3723.9465		3746.5515	3808.5706
51487	Zero-point correction (Hartree): 0.156703				
51488	triHPacyl.pmtmptmmpd				
51489	-----				
51491	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17592440				
51492	Electronic state : 2-A				
51493	Cartesian coordinates (Angs):				
51494	O	1.194070	-0.846953	1.954010	
51495	O	1.292534	0.441215	1.363021	
51496	C	1.191636	0.314399	-0.039433	
51497	C	-0.224062	-0.016481	-0.563056	
51498	C	-0.984447	-1.049898	0.258336	
51499	O	-2.231233	-1.356734	-0.336943	
51500	O	-3.153422	-0.321810	-0.007804	
51501	H	2.123926	-1.057937	2.114308	
51502	C	1.697100	1.635703	-0.601037	
51503	H	2.746138	1.768674	-0.345722	
51504	H	1.109600	2.441878	-0.167926	
51505	H	1.574518	1.647809	-1.681938	
51506	C	2.179257	-0.779761	-0.512303	
51507	O	2.178304	-1.322238	-1.548753	
51508	H	-3.188402	0.173206	-0.837948	
51509	H	-0.107432	-0.399898	-1.580129	
51510	O	-0.996973	1.152437	-0.777018	
51511	O	-1.255946	1.779656	0.470460	
51512	H	-2.064802	1.322521	0.754067	
51513	H	-0.438863	-1.992842	0.265120	
51514	H	-1.130249	-0.731753	1.289353	
51515	Rotational constants (GHz):		1.3023700	0.6954300	0.6499800
51516	Vibrational harmonic frequencies (cm-1):				
51517		51.5676		92.7295	100.6613
51518		148.9999		173.0928	191.3450
51519		195.1308		211.6784	250.3525
51520		255.7110		290.2097	296.1440
51521		311.4129		335.3707	378.0544
51522		388.4670		415.0200	477.9554
51523		543.1920		558.0774	575.0642
51524		596.0735		667.4630	816.8602
51525		859.8511		910.1981	950.4762


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51526      981.6624          1004.0819          1043.1887
51527      1088.4593          1112.6799          1124.8774
51528      1156.9711          1178.5825          1248.8951
51529      1302.6267          1318.2824          1392.0784
51530      1404.7377          1407.1122          1409.0938
51531      1419.2968          1448.9891          1471.9834
51532      1481.4613          1498.0436          1988.7980
51533      3084.1541          3088.2202          3102.8130
51534      3155.9816          3169.5155          3174.1172
51535      3723.0962          3796.9047          3798.3366
51536      Zero-point correction (Hartree): 0.156319
51537
51538      triHPacyl.pmtmptpmd
51539      -----
51540      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17339787
51541      Electronic state : 2-A
51542      Cartesian coordinates (Angs):
51543      O      -1.420352      -1.443961      -1.542759
51544      O      -1.627012      -0.047665      -1.385962
51545      C      -1.273371      0.322687      -0.071974
51546      C      0.239038      0.254960      0.212166
51547      C      0.870698      -1.118999      0.025986
51548      O      2.135449      -1.213625      0.666633
51549      O      3.094706      -0.510770      -0.112146
51550      H      -2.316359      -1.786367      -1.420647
51551      C      -1.804183      1.740005      0.097048
51552      H      -2.889423      1.744197      0.020623
51553      H      -1.379276      2.363079      -0.685410
51554      H      -1.502692      2.129706      1.067157
51555      C      -2.030916      -0.567035      0.937548
51556      O      -1.821200      -0.651508      2.085677
51557      H      3.575503      -1.226982      -0.543927
51558      H      0.376162      0.560505      1.251800
51559      O      0.849933      1.221049      -0.626486
51560      O      1.823763      1.934844      0.116627
51561      H      2.605513      1.372279      -0.000663
51562      H      0.276581      -1.885916      0.524080
51563      H      0.964110      -1.367112      -1.030330
51564      Rotational constants (GHz):      1.2491200      0.6779500      0.6238000
51565      Vibrational harmonic frequencies (cm-1):
51566      35.5330          61.5257          90.0068
51567      113.2911          129.7261          158.5167
51568      182.9907          190.0675          207.6206
51569      222.1559          255.1954          277.6100
51570      298.4558          306.3929          342.4380
51571      376.1071          419.6829          433.3018
51572      521.6396          536.5414          554.7858
51573      566.3127          630.1007          810.1798
51574      892.5467          922.8223          967.3857
51575      976.0172          1040.1255          1051.5998
51576      1081.7038          1107.2856          1127.9393
51577      1154.1610          1174.6586          1253.1091
51578      1310.7652          1324.1076          1371.9420
51579      1385.3375          1403.4489          1409.9946
51580      1429.8959          1452.5571          1455.7610
51581      1483.3835          1495.6023          1988.3495
51582      3084.8492          3088.1061          3092.7056
51583      3150.4930          3167.6881          3178.5044
51584      3731.4834          3797.1107          3829.2665
51585      Zero-point correction (Hartree): 0.155145
51586
51587      triHPacyl.ppmmtmmd
51588      -----
51589      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17563671
51590      Electronic state : 2-A
51591      Cartesian coordinates (Angs):
51592      O      -0.806552      -1.818746      -1.107065
51593      O      -0.220896      -1.879252      0.185526
51594      C      0.685732      -0.817261      0.305132
51595      C      -0.009774      0.554650      0.170022
51596      C      -1.298466      0.670835      0.981924
51597      O      -2.391757      0.008218      0.366357

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51598	O	-2.695987	0.709304	-0.837110		
51599	H	-1.667305	-1.419011	-0.902533		
51600	C	1.380746	-1.026974	1.641331		
51601	H	1.881039	-1.993064	1.638433		
51602	H	0.642504	-1.023928	2.441745		
51603	H	2.104761	-0.235683	1.814620		
51604	C	1.771284	-0.925070	-0.796708		
51605	O	2.391686	-0.039502	-1.252526		
51606	H	-3.546848	1.110203	-0.619436		
51607	H	-0.248910	0.743877	-0.875033		
51608	O	0.902033	1.543086	0.619137		
51609	O	1.137273	2.487615	-0.411309		
51610	H	1.875517	2.071112	-0.882238		
51611	H	-1.217548	0.193919	1.958749		
51612	H	-1.526735	1.729688	1.111411		
51613	Rotational constants (GHz):			1.1213200	0.8394200	0.6536900
51614	Vibrational harmonic frequencies (cm-1):					
51615		45.7456	63.0216			93.3929
51616		112.5882	130.6845			173.1807
51617		182.0648	192.8875			213.4221
51618		232.3704	238.5631			284.3501
51619		336.0607	354.4365			370.6496
51620		405.8242	435.5112			445.8592
51621		508.4551	524.4395			556.2597
51622		580.1297	654.2343			731.3515
51623		864.4177	928.4768			954.4709
51624		1008.9049	1032.6207			1062.1966
51625		1084.2253	1111.8884			1131.7099
51626		1167.7605	1192.5465			1257.0442
51627		1286.7053	1342.8474			1362.7884
51628		1392.7819	1402.7439			1419.7662
51629		1425.4817	1444.6917			1472.3891
51630		1488.7148	1499.7038			1971.3002
51631		3080.5676	3085.7040			3127.1675
51632		3143.6015	3159.3761			3181.8863
51633		3727.0311	3757.1263			3823.3598
51634	Zero-point correction (Hartree):			0.155502		
51635	triHPacyl.ppmmtmpmd					
51636	-----					
51637	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17467147					
51638	Electronic state : 2-A					
51639	Cartesian coordinates (Angs):					
51641	O	0.965038	2.052950	-0.921227		
51642	O	0.617544	1.634259	0.387926		
51643	C	-0.400350	0.657301	0.339052		
51644	C	0.028174	-0.550186	-0.533080		
51645	C	1.000305	-1.498904	0.160824		
51646	O	2.129937	-0.832500	0.685902		
51647	O	2.788152	-0.194769	-0.406479		
51648	H	1.839052	1.642096	-1.005649		
51649	C	-0.667159	0.363828	1.811255		
51650	H	-1.016551	1.270394	2.301720		
51651	H	0.263960	0.054115	2.281860		
51652	H	-1.412744	-0.418289	1.914367		
51653	C	-1.686877	1.276730	-0.261235		
51654	O	-2.756227	0.793290	-0.270554		
51655	H	3.653498	-0.620010	-0.385186		
51656	H	0.504198	-0.140189	-1.422183		
51657	O	-1.039703	-1.283915	-1.086960		
51658	O	-1.796661	-1.885573	-0.042118		
51659	H	-2.576895	-1.309712	-0.034066		
51660	H	0.537557	-1.969400	1.027463		
51661	H	1.298724	-2.271551	-0.551140		
51662	Rotational constants (GHz):			1.2702600	0.8409900	0.6491200
51663	Vibrational harmonic frequencies (cm-1):					
51664		75.7001	103.8021			124.3030
51665		161.2284	173.5554			177.5610
51666		188.6907	201.1646			220.2513
51667		245.6725	268.8200			285.6168
51668		292.9986	329.6124			374.5711
51669		418.8865	446.6690			472.8820

51670	485.0476	513.8428	572.6513			
51671	599.2664	651.1160	737.6171			
51672	875.0916	939.6123	948.3576			
51673	977.0854	1009.0254	1062.5050			
51674	1092.8238	1111.4003	1134.5147			
51675	1181.8545	1188.1470	1223.7443			
51676	1279.1804	1351.0956	1370.2970			
51677	1393.3048	1400.7024	1423.1588			
51678	1440.7821	1443.8664	1481.9488			
51679	1489.8236	1513.4451	1970.7320			
51680	3071.6114	3089.2282	3131.9728			
51681	3148.5016	3161.4648	3195.3912			
51682	3746.8711	3766.8494	3837.5606			
51683	Zero-point correction (Hartree): 0.156222					
51684						
51685	triHPacyl.ppmmtppmmd					
51686	-----					
51687	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17563673					
51688	Electronic state : 2-A					
51689	Cartesian coordinates (Angs):					
51690	O	-0.805685	-1.818776	-1.107690		
51691	O	-0.220424	-1.879365	0.185072		
51692	C	0.685929	-0.817113	0.305112		
51693	C	-0.010022	0.554614	0.170189		
51694	C	-1.298736	0.670129	0.982120		
51695	O	-2.391796	0.007550	0.366006		
51696	O	-2.696297	0.709385	-0.836900		
51697	H	-1.666610	-1.419335	-0.903297		
51698	C	1.380590	-1.026993	1.641463		
51699	H	1.882745	-1.992116	1.637864		
51700	H	0.641762	-1.026368	2.441338		
51701	H	2.102960	-0.234498	1.816059		
51702	C	1.771591	-0.924430	-0.796514		
51703	O	2.392046	-0.038734	-1.252043		
51704	H	-3.546982	1.110407	-0.618745		
51705	H	-0.249325	0.743838	-0.874831		
51706	O	0.901485	1.543329	0.619253		
51707	O	1.136830	2.487636	-0.411376		
51708	H	1.875246	2.071106	-0.882017		
51709	H	-1.217825	0.192688	1.958685		
51710	H	-1.527361	1.728831	1.112160		
51711	Rotational constants (GHz):			1.1213300	0.8394000	0.6536900
51712	Vibrational harmonic frequencies (cm-1):					
51713		45.8069	63.0012			93.3924
51714		112.6416	130.6639			173.2017
51715		182.0417	192.8101			213.3849
51716		232.4046	238.5778			284.2976
51717		336.0424	354.4718			370.6764
51718		405.8698	435.5479			445.9970
51719		508.5224	524.4468			556.2791
51720		580.1629	654.2530			731.4208
51721		864.5454	928.4494			954.4370
51722		1008.8997	1032.6572			1062.1803
51723		1084.2467	1111.8688			1131.7545
51724		1167.7975	1192.4996			1256.9741
51725		1286.6972	1342.8692			1362.7459
51726		1392.8313	1402.6764			1419.7810
51727		1425.5176	1444.7329			1472.4026
51728		1488.7069	1499.7336			1971.2698
51729		3080.6110	3085.7227			3127.1548
51730		3143.6418	3159.3518			3181.9754
51731		3726.9885	3757.0680			3823.2835
51732	Zero-point correction (Hartree): 0.155503					
51733						
51734	triHPacyl.ppmmpmmd					
51735	-----					
51736	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17526532					
51737	Electronic state : 2-A					
51738	Cartesian coordinates (Angs):					
51739	O	-1.702691	1.687828	-0.864348		
51740	O	-1.685016	1.180988	0.460550		
51741	C	-1.110867	-0.111381	0.459179		

51742	C	0.279019	-0.116129	-0.209331	
51743	C	1.095263	1.094818	0.230114	
51744	O	2.349883	1.163184	-0.422158	
51745	O	3.226802	0.242450	0.230054	
51746	H	-2.558192	1.365775	-1.186434	
51747	C	-1.096396	-0.542590	1.916152	
51748	H	-2.113136	-0.537777	2.305180	
51749	H	-0.494609	0.148726	2.502031	
51750	H	-0.679991	-1.542696	1.995013	
51751	C	-2.011985	-1.092742	-0.328226	
51752	O	-3.001420	-0.810015	-0.891386	
51753	H	4.018362	0.783419	0.331853	
51754	H	0.173076	-0.098080	-1.294636	
51755	O	0.871983	-1.346306	0.160261	
51756	O	1.730938	-1.776990	-0.880634	
51757	H	2.567587	-1.351901	-0.631806	
51758	H	0.584868	2.006308	-0.077427	
51759	H	1.247993	1.105262	1.310166	
51760	Rotational constants (GHz):		1.4872500	0.6356900	0.5578000
51761	Vibrational harmonic frequencies (cm-1):				
51762		54.4020	65.5271		89.5023
51763		140.8771	159.1522		172.6404
51764		191.3197	206.4212		212.6794
51765		229.4061	268.9089		291.6117
51766		315.9584	329.9028		377.6538
51767		409.1264	433.3437		455.3299
51768		460.6513	515.8573		546.2407
51769		577.5953	709.3019		768.7468
51770		890.2141	898.9007		965.4880
51771		973.4574	1044.9483		1053.0219
51772		1079.5450	1115.0900		1148.9580
51773		1164.2393	1195.8451		1249.5259
51774		1314.8772	1333.0245		1374.9350
51775		1397.0219	1409.4737		1422.2725
51776		1435.5538	1457.9681		1476.2810
51777		1488.3639	1500.3903		1971.3841
51778		3082.2575	3088.2187		3104.0663
51779		3153.1258	3162.2350		3185.3091
51780		3720.6653	3762.3374		3845.5161
51781	Zero-point correction (Hartree): 0.155933				
51782	triHPacyl.ppmpppppd				
51783	-----				
51784	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17739030				
51785	Electronic state : 2-A				
51786	Cartesian coordinates (Angs):				
51787	O	0.372162	-2.133263	-0.873500	
51788	O	0.195037	-1.586073	0.423160	
51789	C	0.554270	-0.208071	0.434446	
51790	C	-0.296002	0.580074	-0.586798	
51791	C	-1.660102	1.004282	-0.052047	
51792	O	-2.354990	-0.063124	0.551730	
51793	O	-2.598605	-1.042655	-0.449073	
51794	H	1.286046	-2.452870	-0.832776	
51795	H	0.410382	0.197568	1.895392	
51796	H	1.118997	-0.363896	2.502093	
51797	H	-0.599304	-0.028583	2.228614	
51798	H	0.600933	1.261428	2.004211	
51799	C	2.049160	-0.049400	0.065204	
51800	O	2.796148	-0.908370	-0.210932	
51801	H	-1.939857	-1.716632	-0.224260	
51802	H	-0.437058	-0.072670	-1.447782	
51803	O	0.386421	1.680585	-1.148485	
51804	O	0.677009	2.621562	-0.119143	
51805	H	1.632273	2.498505	-0.022015	
51806	H	-1.553120	1.748355	0.736794	
51807	H	-2.240605	1.430348	-0.872125	
51808	Rotational constants (GHz):		1.1173300	0.9081300	0.6474600
51809	Vibrational harmonic frequencies (cm-1):				
51810		71.2720	101.3894		115.6246
51811		142.1143	160.5572		190.8758
51812		207.6602	220.7347		237.5499

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51814      270.4884      291.8104      314.3779
51815      330.0966      349.0665      391.7779
51816      402.5643      426.5522      446.0370
51817      472.7082      508.8211      546.3677
51818      629.8219      690.2205      729.3179
51819      877.3938      927.1894      953.7577
51820      976.6058      1020.3340     1048.5197
51821     1103.6308      1122.6773     1130.6052
51822     1165.1390      1189.0883     1234.7317
51823     1282.1706      1348.4491     1382.3834
51824     1401.4977      1410.6982     1419.9018
51825     1425.2117      1429.7583     1484.6121
51826     1493.8453      1511.1087     1981.7250
51827     3079.6616      3087.7721     3125.6759
51828     3146.5935      3165.9231     3188.5252
51829     3769.4031      3773.2945     3774.2856
51830 Zero-point correction (Hartree): 0.156464
51831
51832 triHPacyl.ppmpppppd
51833 -----
51834 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17782661
51835 Electronic state : 2-A
51836 Cartesian coordinates (Angs):
51837 O      0.147057     -1.807437     -1.234280
51838 O     -0.082079     -1.590550      0.150683
51839 C      0.447172     -0.328651      0.531221
51840 C     -0.213599      0.827065     -0.250099
51841 C     -1.630920      1.154858      0.227122
51842 O     -2.439376      0.024042      0.426288
51843 O     -2.639706     -0.585996     -0.840466
51844 H      0.983344     -2.296435     -1.223373
51845 C      0.247265     -0.241263      2.036464
51846 H      0.853345     -0.989984      2.542970
51847 H     -0.801177     -0.416550      2.266404
51848 H      0.542124      0.749192      2.378888
51849 C      1.972984     -0.322120      0.289201
51850 O      2.625351     -1.225748     -0.074139
51851 H     -2.038431     -1.343847     -0.789158
51852 H     -0.219636      0.577193     -1.309346
51853 O      0.491179      2.036426     -0.054778
51854 O      1.535572      2.119079     -1.012377
51855 H      2.316930      1.942083     -0.469124
51856 H     -1.590148      1.642922      1.202117
51857 H     -2.087755      1.837574     -0.490285
51858 Rotational constants (GHz): 1.1459100 0.8500700 0.6585500
51859 Vibrational harmonic frequencies (cm-1):
51860      64.4086      93.9865      94.6775
51861     156.4888     160.3543     182.1203
51862     212.3393     221.1637     250.6499
51863     264.3501     288.6473     319.7596
51864     346.8735     353.0335     382.2052
51865     408.4480     424.8271     451.3017
51866     479.0641     507.1003     518.5367
51867     616.7739     688.7813     734.0696
51868     870.0882     927.3309     958.7698
51869     1014.5985     1023.6803     1046.9127
51870     1096.5285     1135.1283     1141.6770
51871     1164.2943     1194.7069     1239.4822
51872     1291.1574     1340.6050     1386.7231
51873     1401.6549     1412.4387     1416.3221
51874     1421.4582     1423.2100     1482.1266
51875     1492.4179     1512.5444     1975.3257
51876     3079.9434     3082.2479     3125.7723
51877     3139.5431     3160.4913     3174.3333
51878     3772.4999     3776.3564     3779.4810
51879 Zero-point correction (Hartree): 0.156464
51880
51881 triHPacyl.ppmptmpd
51882 -----
51883 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20356538
51884 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.08639611
51885 T1 diagnostic: 0.015734

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51886 E(MP2/Aug-CC-pVTZ) (Hartree): -721.05219627
51887 E(MP3/Aug-CC-pVTZ) (Hartree): -721.06792863
51888 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05451563
51889 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.06921341
51890 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51826714
51891 E(UHF/Aug-CC-pVTZ) (Hartree): -718.51454203
51892 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17835025
51893 Electronic state : 2-A
51894 Cartesian coordinates (Angs):
51895 O 0.731442 2.155786 -0.972502
51896 O 0.651458 1.613527 0.336652
51897 C -0.344713 0.596190 0.370433
51898 C 0.055599 -0.553010 -0.590657
51899 C 1.059918 -1.528534 0.021974
51900 O 2.154742 -0.883866 0.628979
51901 O 2.858789 -0.177133 -0.382891
51902 H 0.114001 2.899367 -0.920418
51903 C -0.468097 0.235434 1.845216
51904 H -0.830746 1.094182 2.407076
51905 H 0.512420 -0.045682 2.222792
51906 H -1.158230 -0.595566 1.960928
51907 C -1.685709 1.221851 -0.067145
51908 O -2.745543 0.723992 -0.066887
51909 H 2.571213 0.732658 -0.214317
51910 H 0.498746 -0.084405 -1.468801
51911 O -1.036496 -1.255030 -1.137007
51912 O -1.722756 -1.940081 -0.092596
51913 H -2.535262 -1.415865 -0.038105
51914 H 0.596143 -2.103213 0.822773
51915 H 1.396634 -2.210620 -0.760828
51916 Rotational constants (GHz): 1.2284200 0.8602800 0.6524200
51917 Vibrational harmonic frequencies (cm-1):
51918 81.0380 113.5137 118.9467
51919 169.8670 177.7743 188.2426
51920 198.6719 214.3119 234.0857
51921 268.5654 271.5792 287.1310
51922 316.6428 339.0072 375.4051
51923 418.7771 424.1145 456.5860
51924 473.8700 510.5907 583.4386
51925 595.1478 653.6644 735.3486
51926 876.1182 930.8647 954.6028
51927 977.4126 1011.4339 1045.9948
51928 1097.2710 1122.9389 1134.5074
51929 1170.0137 1183.7470 1219.3341
51930 1283.1550 1348.3190 1380.1737
51931 1396.6660 1407.9799 1414.8280
51932 1423.3516 1438.9122 1482.0814
51933 1491.0092 1509.0402 1988.6990
51934 3077.8552 3087.3797 3127.4273
51935 3147.3755 3165.2693 3185.9791
51936 3772.2701 3778.8159 3784.3732
51937 Zero-point correction (Hartree): 0.156331
51938
51939 triHPacyl.ppmptmpd
51940 -----
51941 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17671589
51942 Electronic state : 2-A
51943 Cartesian coordinates (Angs):
51944 O -0.495027 -1.751321 -1.460929
51945 O -0.620364 -1.613291 -0.052628
51946 C 0.307328 -0.637113 0.401072
51947 C -0.012420 0.746320 -0.214103
51948 C -1.230561 1.420989 0.428410
51949 O -2.332831 0.572193 0.614122
51950 O -2.800273 0.190284 -0.671071
51951 H 0.140972 -2.477142 -1.536086
51952 C 0.237558 -0.669238 1.919881
51953 H 0.611817 -1.617888 2.299386
51954 H -0.796904 -0.544867 2.232466
51955 H 0.848928 0.140453 2.315213
51956 C 1.720665 -1.116499 0.008355
51957 O 2.751069 -0.642367 0.300765

51958	H	-2.453820	-0.711681	-0.739754	
51959	H	-0.168451	0.623738	-1.283592	
51960	O	1.030677	1.672370	0.006484	
51961	O	1.898925	1.670917	-1.118583	
51962	H	2.699544	1.281060	-0.742594	
51963	H	-0.973015	1.766456	1.430714	
51964	H	-1.501896	2.282847	-0.182712	
51965	Rotational constants (GHz):		1.2343900	0.7984900	0.6641800
51966	Vibrational harmonic frequencies (cm-1):				
51967		52.4384	95.6166		97.8453
51968		157.9745	167.9590		182.5840
51969		197.9620	208.8647		249.2703
51970		255.0764	270.0062		290.4929
51971		313.2078	348.2161		376.0350
51972		397.6490	438.5873		463.5047
51973		472.9970	491.3861		517.3241
51974		599.7900	671.3175		717.7602
51975		871.5833	929.4909		957.3900
51976		1006.4577	1022.2716		1044.2356
51977		1090.2063	1133.8844		1140.5963
51978		1170.3439	1188.6191		1223.9325
51979		1289.2375	1339.4152		1379.5141
51980		1397.0431	1404.6898		1409.9772
51981		1420.0853	1426.7524		1479.6600
51982		1490.5742	1511.5761		1984.2091
51983		3076.9244	3079.7098		3127.1771
51984		3143.7032	3160.1709		3171.0840
51985		3778.9997	3783.6362		3810.2747
51986	Zero-point correction (Hartree): 0.156003				
51987					
51988	triHPacyl.pmpmtpmmd				
51989	-----				
51990	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17596147				
51991	Electronic state : 2-A				
51992	Cartesian coordinates (Angs):				
51993	O	-0.970436	-1.455122	-1.477771	
51994	O	-0.909736	-1.452258	-0.059648	
51995	C	0.246165	-0.753667	0.353080	
51996	C	0.283023	0.689327	-0.196270	
51997	C	-0.979218	1.514767	0.066726	
51998	O	-2.135925	0.955293	-0.537707	
51999	O	-2.941122	0.338533	0.455245	
52000	H	-1.549331	-0.690127	-1.643768	
52001	C	0.243596	-0.830341	1.870935	
52002	H	0.291763	-1.869988	2.188383	
52003	H	-0.675493	-0.387879	2.254317	
52004	H	1.097049	-0.284972	2.265833	
52005	C	1.490509	-1.521334	-0.151348	
52006	O	2.573408	-1.096913	-0.300122	
52007	H	-2.570333	-0.558787	0.481014	
52008	H	0.470337	0.656608	-1.268479	
52009	O	1.350734	1.378881	0.430356	
52010	O	2.319902	1.757094	-0.531713	
52011	H	2.917960	0.994538	-0.510043	
52012	H	-1.157100	1.650091	1.132102	
52013	H	-0.823910	2.493942	-0.387223	
52014	Rotational constants (GHz):		1.2906300	0.7892600	0.6338200
52015	Vibrational harmonic frequencies (cm-1):				
52016		40.4845	78.0863		106.9047
52017		125.4694	174.8068		191.6975
52018		202.2864	211.2137		236.5594
52019		252.9779	276.9204		326.1562
52020		352.2973	362.9350		415.0480
52021		451.6729	456.3835		513.2155
52022		526.1240	543.5781		569.9606
52023		616.2887	658.1481		720.0767
52024		863.8070	929.1967		963.1842
52025		1017.3903	1024.7124		1061.4066
52026		1095.7414	1113.8157		1131.7695
52027		1172.0606	1182.3869		1248.0199
52028		1284.4311	1339.1648		1375.9094
52029		1398.3997	1404.2721		1443.3414

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52030      1451.2731          1471.0545          1482.5295
52031      1489.7693          1504.0343          1978.4035
52032      3079.0577          3090.0004          3115.6292
52033      3149.4552          3155.8117          3176.6185
52034      3683.7853          3723.2044          3758.7828
52035      Zero-point correction (Hartree): 0.156664
52036
52037      triHPacyl.pppmpmpmd
52038      -----
52039      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17455886
52040      Electronic state : 2-A
52041      Cartesian coordinates (Angs):
52042      O      0.450726      2.169220      -1.216614
52043      O      0.548525      1.688907      0.112549
52044      C     -0.354879      0.604084      0.302806
52045      C      0.011504     -0.558320     -0.656684
52046      C      1.180191     -1.441289     -0.207185
52047      O      2.434757     -0.828383     -0.408013
52048      O      2.747954     -0.026712      0.721538
52049      H     -0.233256      2.849305     -1.132161
52050      C     -0.293262      0.314505      1.796980
52051      H     -0.662826      1.174141      2.353317
52052      H      0.737586      0.122130      2.084382
52053      H     -0.899672     -0.557254      2.024796
52054      C     -1.782760      1.109616     -0.003254
52055      O     -2.793676      0.548374      0.179008
52056      H      2.431463      0.846304      0.444005
52057      H      0.291492     -0.100481     -1.606497
52058      O     -1.099766     -1.350781     -1.011098
52059      O     -1.551365     -2.051571      0.144564
52060      H     -2.394826     -1.604397      0.307705
52061      H      1.087050     -1.785397      0.821770
52062      H      1.180991     -2.308364     -0.868775
52063      Rotational constants (GHz):      1.1998300      0.8462200      0.6446000
52064      Vibrational harmonic frequencies (cm-1):
52065      76.1543          100.7310          120.5880
52066      156.1505          180.0981          182.1408
52067      186.3063          218.3356          236.0189
52068      266.5352          288.9581          300.0188
52069      323.3147          346.7362          365.1492
52070      410.5996          419.8841          461.0569
52071      479.3614          513.5047          542.4083
52072      604.3598          643.5141          754.0272
52073      889.5628          931.8871          949.1583
52074      969.6902          1021.7619         1053.0672
52075      1080.4982         1121.9181         1128.1507
52076      1171.7010         1177.9533         1222.2038
52077      1287.0780         1338.8666         1378.4881
52078      1404.2285         1409.2980         1421.3724
52079      1434.8193         1449.1965         1479.8117
52080      1485.9268         1514.2316         1989.4740
52081      3088.6492         3091.6038         3112.8968
52082      3146.9412         3167.8921         3190.0474
52083      3757.9372         3774.7357         3775.8258
52084      Zero-point correction (Hartree): 0.156266
52085
52086      triHPacyl.pppppmpmd
52087      -----
52088      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17480753
52089      Electronic state : 2-A
52090      Cartesian coordinates (Angs):
52091      O      2.357682      -1.243632      -0.981985
52092      O      1.704211     -1.253681      0.274795
52093      C      0.824194     -0.147687      0.383503
52094      C     -0.225249     -0.199721     -0.747802
52095      C     -1.352501     -1.195403     -0.500188
52096      O     -2.246132     -0.855099      0.536868
52097      O     -3.286534     -0.058121     -0.004585
52098      H      3.163261     -0.744860     -0.780911
52099      C      0.305568     -0.240120      1.812750
52100      H      1.141173     -0.138207      2.503570
52101      H     -0.162252     -1.210064      1.963834

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52102	H	-0.435303	0.529940	2.000584	
52103	C	1.617932	1.181319	0.278117	
52104	O	2.775989	1.293122	0.147821	
52105	H	-2.927291	0.836428	0.096506	
52106	H	0.309562	-0.545836	-1.634564	
52107	O	-0.658522	1.084825	-1.162592	
52108	O	-1.242398	1.781496	-0.068903	
52109	H	-0.524975	2.378911	0.190229	
52110	H	-1.915688	-1.340845	-1.422071	
52111	H	-0.902504	-2.147083	-0.206794	
52112	Rotational constants (GHz):		1.5621900	0.6767600	0.6009900
52113	Vibrational harmonic frequencies (cm-1):				
52114		66.6325	85.7999		102.1824
52115		155.5483	177.1708		207.3057
52116		220.1949	238.7186		253.3728
52117		263.6272	287.8580		313.0623
52118		325.6477	348.9211		372.6897
52119		378.6719	423.4167		493.4064
52120		510.6048	523.5643		549.1012
52121		610.1763	709.7683		821.4852
52122		836.0584	921.8672		946.7810
52123		960.3852	1010.4377		1033.8949
52124		1053.7694	1126.0035		1134.5824
52125		1169.7969	1178.6021		1237.1035
52126		1317.8761	1356.3835		1386.2523
52127		1405.9514	1409.3465		1415.7074
52128		1426.9259	1451.4958		1463.1987
52129		1480.4057	1503.2178		1983.8492
52130		3071.2657	3088.2024		3102.9805
52131		3127.6133	3165.0374		3197.3782
52132		3751.9691	3758.6352		3773.0214
52133	Zero-point correction (Hartree): 0.156476				
52134	triHPacyl.pppppppmmd				
52135	-----				
52137	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17506389				
52138	Electronic state : 2-A				
52139	Cartesian coordinates (Angs):				
52140	O	2.013890	-1.120916	-1.394863	
52141	O	1.455501	-1.441797	-0.130873	
52142	C	0.775108	-0.315997	0.386493	
52143	C	-0.334871	0.149495	-0.578853	
52144	C	-1.421291	-0.905622	-0.773323	
52145	O	-2.312004	-0.977751	0.321999	
52146	O	-3.367576	-0.051859	0.113868	
52147	H	2.915931	-0.867412	-1.150575	
52148	C	0.274719	-0.745863	1.756883	
52149	H	1.120547	-0.936993	2.415017	
52150	H	-0.315546	-1.653515	1.658195	
52151	H	-0.352386	0.034806	2.180296	
52152	C	1.770164	0.844697	0.613839	
52153	O	2.932428	0.808398	0.472200	
52154	H	-2.949490	0.793145	0.336503	
52155	H	0.113184	0.377912	-1.544717	
52156	O	-0.965292	1.317170	-0.074087	
52157	O	-0.292418	2.467530	-0.554029	
52158	H	0.310890	2.670283	0.177216	
52159	H	-1.988480	-0.696929	-1.679278	
52160	H	-0.953860	-1.887772	-0.856620	
52161	Rotational constants (GHz):		1.3865000	0.6905500	0.5864000
52162	Vibrational harmonic frequencies (cm-1):				
52163		44.0522	69.9361		91.8200
52164		130.0172	150.7350		170.1407
52165		196.6611	203.4731		246.1744
52166		272.1674	275.7110		290.3680
52167		324.1546	351.2013		388.3456
52168		402.8391	422.5628		433.3096
52169		491.6076	508.6623		539.8749
52170		612.7779	718.3939		765.4186
52171		863.9616	911.5779		935.3529
52172		1003.4893	1014.7204		1050.1392
52173		1070.4195	1124.4719		1140.5519

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52174      1164.4000      1171.9962      1243.5966
52175      1312.4790      1353.8523      1375.7458
52176      1397.9659      1411.3477      1423.0133
52177      1431.3972      1454.9410      1469.2520
52178      1481.4709      1499.6103      1980.2517
52179      3084.5446      3087.7213      3124.5264
52180      3143.2513      3164.7295      3178.6469
52181      3745.9438      3769.3556      3778.1246
52182      Zero-point correction (Hartree): 0.155971
52183
52184      triHPacyl.pppppptpmd
52185      -----
52186      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17686176
52187      Electronic state : 2-A
52188      Cartesian coordinates (Angs):
52189      O      1.937556      -1.211321      -1.248907
52190      O      1.547931      -1.232226      0.115282
52191      C      0.919936      -0.010188      0.440672
52192      C      -0.235004      0.303080      -0.534297
52193      C      -1.108482      -0.904890      -0.853943
52194      O      -1.851579      -1.382220      0.250757
52195      O      -2.947754      -0.498158      0.470101
52196      H      2.837795      -0.857623      -1.190147
52197      C      0.513167      -0.147764      1.898965
52198      H      1.399958      -0.335403      2.502203
52199      H      -0.176777      -0.980982      2.006236
52200      H      0.042617      0.772715      2.234866
52201      C      1.940013      1.153236      0.336385
52202      O      3.058292      1.055360      -0.001665
52203      H      -2.626299      0.030399      1.214013
52204      H      0.179616      0.672590      -1.475391
52205      O      -0.965403      1.347888      0.086304
52206      O      -1.892002      1.853074      -0.858787
52207      H      -2.662735      1.285474      -0.696380
52208      H      -1.788360      -0.665510      -1.672693
52209      H      -0.479939      -1.741679      -1.154073
52210      Rotational constants (GHz):      1.4643700      0.6816400      0.6054000
52211      Vibrational harmonic frequencies (cm-1):
52212      50.9273      69.6401      92.4066
52213      153.6253      163.0631      188.4863
52214      213.7054      233.2488      239.1607
52215      256.0967      295.6857      313.6660
52216      326.3343      370.8312      392.5987
52217      411.2278      424.4920      455.5929
52218      485.8654      545.8991      568.1011
52219      650.0037      713.9674      809.1070
52220      836.2988      899.1781      938.7557
52221      973.4134      1026.8696      1046.8727
52222      1059.5449      1110.5733      1147.8626
52223      1160.6315      1204.4446      1257.3621
52224      1304.1093      1363.4270      1384.7036
52225      1401.0970      1411.3043      1418.6146
52226      1422.2335      1452.9754      1478.1632
52227      1491.3358      1503.1320      1974.0168
52228      3075.4748      3085.6036      3089.5479
52229      3152.2924      3163.5955      3181.7537
52230      3727.7228      3770.3277      3787.4999
52231      Zero-point correction (Hartree): 0.156566
52232
52233      triHPacyl.pppppptppd
52234      -----
52235      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17570490
52236      Electronic state : 2-A
52237      Cartesian coordinates (Angs):
52238      O      1.913869      -1.274171      -1.227165
52239      O      1.537475      -1.248888      0.141249
52240      C      0.944165      -0.001750      0.442952
52241      C      -0.216204      0.318299      -0.524225
52242      C      -1.113604      -0.881134      -0.809587
52243      O      -1.868793      -1.308455      0.309472
52244      O      -2.988233      -0.435750      0.449752
52245      H      2.816711      -0.924301      -1.188068

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52246	C	0.549893	-0.089928	1.907970	
52247	H	1.438062	-0.287510	2.506052	
52248	H	-0.168730	-0.893433	2.042539	
52249	H	0.101807	0.848899	2.220674	
52250	C	1.993506	1.128254	0.294762	
52251	O	3.104632	0.992617	-0.056041	
52252	H	-3.719680	-1.050629	0.315261	
52253	H	0.196069	0.648066	-1.482154	
52254	O	-0.903353	1.391535	0.082371	
52255	O	-1.878738	1.860180	-0.832072	
52256	H	-2.661417	1.387568	-0.509509	
52257	H	-1.785662	-0.649738	-1.636191	
52258	H	-0.498556	-1.737913	-1.080358	
52259	Rotational constants (GHz):		1.4833600	0.6713100	0.5948600
52260	Vibrational harmonic frequencies (cm-1):				
52261		41.6000	64.5897		87.1579
52262		153.6611	171.0482		187.1634
52263		201.3924	205.2157		232.4864
52264		250.6881	267.2169		295.2399
52265		308.3163	325.3190		371.4039
52266		400.5289	422.0721		453.8893
52267		485.8692	501.4323		566.1878
52268		650.4479	715.7077		802.0274
52269		835.9809	896.1314		938.1362
52270		977.8149	1025.8270		1047.6626
52271		1057.4388	1109.3254		1149.5089
52272		1162.2713	1207.1310		1257.6998
52273		1306.7730	1366.5449		1384.7044
52274		1396.9694	1410.8807		1420.6816
52275		1424.1639	1452.7201		1471.1256
52276		1488.4321	1497.2319		1970.8851
52277		3063.7217	3088.7948		3091.9178
52278		3152.3899	3169.6736		3189.7809
52279		3761.6771	3765.8069		3825.7824
52280	Zero-point correction (Hartree): 0.156114				
52281	triHPacyl.ppppmpmd				
52282	-----				
52284	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17581685				
52285	Electronic state : 2-A				
52286	Cartesian coordinates (Angs):				
52287	O	2.468439	-1.377890	-0.897649	
52288	O	1.785648	-1.311092	0.342963	
52289	C	0.955867	-0.161178	0.367050	
52290	C	-0.108396	-0.295054	-0.751232	
52291	C	-1.190072	-1.322391	-0.424662	
52292	O	-2.086509	-0.956511	0.600541	
52293	O	-3.168023	-0.241571	0.026036	
52294	H	3.301081	-0.931252	-0.689684	
52295	C	0.451266	-0.105420	1.804276	
52296	H	1.293806	0.045697	2.477007	
52297	H	-0.032637	-1.048179	2.049310	
52298	H	-0.272938	0.693902	1.920230	
52299	C	1.834560	1.086457	0.137049	
52300	O	1.510192	2.212421	0.153151	
52301	H	-2.840886	0.671185	0.050777	
52302	H	0.426547	-0.673766	-1.624379	
52303	O	-0.600129	0.938704	-1.235095	
52304	O	-1.224882	1.668306	-0.185745	
52305	H	-0.559574	2.348770	-0.002803	
52306	H	-1.756189	-1.546027	-1.329089	
52307	H	-0.696435	-2.233743	-0.079865	
52308	Rotational constants (GHz):		1.3369100	0.7710400	0.6284600
52309	Vibrational harmonic frequencies (cm-1):				
52310		77.3709	88.0964		112.1674
52311		170.1989	184.8452		189.1949
52312		211.4432	235.1819		246.6258
52313		271.8008	276.7381		280.8172
52314		310.6246	343.9074		351.5742
52315		411.8419	450.6464		465.2088
52316		505.8470	519.3526		532.2204
52317		643.4169	668.1704		831.9004

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52318      834.8963          922.7394          940.3424
52319      960.5444          1005.3149         1031.0336
52320     1051.7158         1127.8092         1129.0530
52321     1174.1786         1182.4193         1222.7471
52322     1318.7246         1346.1442         1386.1558
52323     1404.1475         1408.6967         1414.3468
52324     1425.1199         1458.8393         1462.3076
52325     1478.2178         1496.3251         1985.1385
52326     3072.9382         3087.9964         3102.7450
52327     3127.6447         3163.4892         3198.2030
52328     3743.6538         3758.1186         3788.3422
52329 Zero-point correction (Hartree): 0.156258
52330
52331 triHPacyl.ppppptommd
52332 -----
52333 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17463355
52334 Electronic state : 2-A
52335 Cartesian coordinates (Angs):
52336 O      2.001558      -1.456153      -1.313535
52337 O      1.468210      -1.609599      -0.005682
52338 C      0.910648      -0.377914      0.394938
52339 C     -0.211860      0.056506     -0.575949
52340 C     -1.299922     -1.006410     -0.726205
52341 O     -2.161953     -1.046851      0.393045
52342 O     -3.219772     -0.121705      0.189853
52343 H      2.945040     -1.354909     -1.127624
52344 C      0.458230     -0.583682      1.832202
52345 H      1.321982     -0.755065      2.472105
52346 H     -0.201901     -1.446702      1.879049
52347 H     -0.083643      0.295648      2.171248
52348 C      2.027702      0.688362      0.408189
52349 O      1.917787      1.846047      0.557466
52350 H     -2.782340      0.727198      0.353545
52351 H      0.223840      0.259933     -1.552219
52352 O     -0.812790      1.248396     -0.082537
52353 O     -0.476391      2.350143     -0.908083
52354 H      0.265419      2.735210     -0.418503
52355 H     -1.888778     -0.811859     -1.622078
52356 H     -0.841600     -1.992849     -0.798783
52357 Rotational constants (GHz): 1.1833200 0.7862900 0.6166500
52358 Vibrational harmonic frequencies (cm-1):
52359 30.9136 61.0433 73.8458
52360 114.8844 154.3927 174.8115
52361 190.6650 205.8042 237.1803
52362 261.4513 267.4759 281.5261
52363 288.8578 347.0485 378.0648
52364 418.4728 434.6185 450.6590
52365 466.7791 507.4045 516.5944
52366 635.7973 670.1876 776.0324
52367 863.0832 908.1692 941.9859
52368 996.1902 1007.3108 1049.5941
52369 1068.8603 1118.7740 1131.1742
52370 1158.6232 1180.9636 1241.5105
52371 1306.6777 1349.6024 1360.3666
52372 1395.9564 1405.9801 1408.9385
52373 1439.8620 1455.5888 1468.9358
52374 1483.6105 1496.6363 1980.4099
52375 3084.3209 3088.1747 3130.9412
52376 3144.5960 3164.3994 3179.1959
52377 3765.7117 3770.5438 3799.8623
52378 Zero-point correction (Hartree): 0.155578
52379
52380 triHPacyl.ppppptommd
52381 -----
52382 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17433693
52383 Electronic state : 2-A
52384 Cartesian coordinates (Angs):
52385 O      1.882285      -1.512995      -1.269841
52386 O      1.478700      -1.492479      0.092241
52387 C      0.996784      -0.204149      0.388935
52388 C     -0.158882      0.185286     -0.561043
52389 C     -1.146580     -0.943558     -0.826202

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52390	O	-1.823198	-1.346073	0.345915	
52391	O	-2.947862	-0.498269	0.534867	
52392	H	2.835472	-1.366838	-1.193269	
52393	C	0.648966	-0.231081	1.869571	
52394	H	1.543559	-0.465976	2.443511	
52395	H	-0.107003	-0.992575	2.043960	
52396	H	0.268949	0.740252	2.175028	
52397	C	2.145036	0.819063	0.185300	
52398	O	2.063292	1.985137	0.216784	
52399	H	-2.543182	0.318759	0.860997	
52400	H	0.261335	0.514704	-1.513863	
52401	O	-0.791266	1.292101	0.069977	
52402	O	-1.564837	1.967164	-0.912555	
52403	H	-1.062324	2.786300	-1.013990	
52404	H	-1.873661	-0.623796	-1.573188	
52405	H	-0.612003	-1.820882	-1.187654	
52406	Rotational constants (GHz):		1.2042600	0.7910700	0.6283700
52407	Vibrational harmonic frequencies (cm-1):				
52408		48.3034	50.0233		69.6913
52409		93.5990	145.9638		158.5293
52410		198.7992	218.7258		229.4602
52411		246.2233	271.3426		274.4294
52412		291.2820	311.1994		348.5983
52413		367.5983	401.6431		420.1278
52414		471.0596	514.7725		530.2216
52415		634.5513	681.9159		805.1001
52416		844.3198	899.7327		948.1015
52417		981.0051	1019.3662		1045.0287
52418		1056.3854	1114.7390		1138.1732
52419		1152.0071	1203.2788		1255.4031
52420		1301.4513	1365.3200		1369.0238
52421		1398.8060	1405.4417		1407.4006
52422		1414.9888	1435.5955		1469.2912
52423		1489.4319	1498.6501		1990.3939
52424		3078.8713	3086.1078		3092.8716
52425		3151.6810	3166.3923		3182.4177
52426		3774.3108	3792.3772		3807.7905
52427	Zero-point correction (Hartree): 0.155187				
52428					
52429	triHPacyl.ppppttpmd				
52430	-----				
52431	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17615700				
52432	Electronic state : 2-A				
52433	Cartesian coordinates (Angs):				
52434	O	1.855592	-1.647531	-1.162518	
52435	O	1.527735	-1.435922	0.201648	
52436	C	1.025403	-0.126733	0.352416	
52437	C	-0.156180	0.127937	-0.609269	
52438	C	-1.128586	-1.044177	-0.699656	
52439	O	-1.831060	-1.295963	0.501338	
52440	O	-2.847936	-0.307216	0.641753	
52441	H	2.769796	-1.330191	-1.200520	
52442	C	0.704040	0.016213	1.830924	
52443	H	1.606898	-0.153869	2.414583	
52444	H	-0.046694	-0.719526	2.110662	
52445	H	0.337636	1.020949	2.025297	
52446	C	2.152616	0.877656	-0.014735	
52447	O	2.156134	2.030371	0.168468	
52448	H	-2.440759	0.304099	1.271677	
52449	H	0.230813	0.317390	-1.613759	
52450	O	-0.777438	1.306188	-0.125526	
52451	O	-1.720954	1.729498	-1.093548	
52452	H	-2.517976	1.255024	-0.806679	
52453	H	-1.840471	-0.873043	-1.508413	
52454	H	-0.579584	-1.961600	-0.903841	
52455	Rotational constants (GHz):		1.2418700	0.7748300	0.6301700
52456	Vibrational harmonic frequencies (cm-1):				
52457		50.2119	71.2324		85.6512
52458		140.7758	165.8422		172.9630
52459		207.7362	235.5712		240.2327
52460		251.0374	270.4795		279.0354
52461		313.8197	347.5723		369.9412

52462	399.3200	416.6035	466.8708		
52463	501.9195	533.5346	550.9200		
52464	640.7310	686.8088	807.8636		
52465	833.0271	897.5072	946.1206		
52466	972.1876	1022.3529	1048.3868		
52467	1057.3398	1109.3573	1138.7038		
52468	1161.4086	1212.9603	1251.4039		
52469	1301.9105	1362.4137	1379.6853		
52470	1399.3358	1410.4368	1411.1429		
52471	1416.6766	1453.0674	1477.2819		
52472	1490.9391	1502.6689	2001.8839		
52473	3074.8584	3084.6261	3089.1621		
52474	3155.6327	3163.3413	3179.3348		
52475	3729.2407	3774.3406	3784.9226		
52476	Zero-point correction (Hartree): 0.156055				
52477	-----				
52478	triHPacyl.pppppttpd				
52479	-----				
52480	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17484627				
52481	Electronic state : 2-A				
52482	Cartesian coordinates (Angs):				
52483	O	1.797673	-1.709930	-1.154454	
52484	O	1.481360	-1.476561	0.209397	
52485	C	1.040212	-0.143577	0.355461	
52486	C	-0.136042	0.162580	-0.598871	
52487	C	-1.143587	-0.978834	-0.697259	
52488	O	-1.854073	-1.216189	0.503660	
52489	O	-2.884102	-0.234596	0.610190	
52490	H	2.716323	-1.406360	-1.201071	
52491	C	0.733199	0.025255	1.833784	
52492	H	1.626335	-0.198536	2.414307	
52493	H	-0.066980	-0.653909	2.116311	
52494	H	0.422758	1.049027	2.021954	
52495	C	2.212468	0.800903	-0.026338	
52496	O	2.274410	1.954830	0.138123	
52497	H	-3.671100	-0.792878	0.602963	
52498	H	0.252403	0.336730	-1.606801	
52499	O	-0.700680	1.356019	-0.101684	
52500	O	-1.685332	1.791293	-1.022102	
52501	H	-2.484257	1.436381	-0.603057	
52502	H	-1.847809	-0.777593	-1.504913	
52503	H	-0.619225	-1.909751	-0.905394	
52504	Rotational constants (GHz): 1.2570800			0.7629300	0.6183000
52505	Vibrational harmonic frequencies (cm-1):				
52506		44.0297	65.6750	80.0892	
52507		142.1778	165.0404	178.1574	
52508		187.8783	206.7786	230.3236	
52509		247.0379	266.4240	275.9243	
52510		290.8500	308.2895	350.5710	
52511		367.6335	408.0553	470.0254	
52512		487.1162	505.9961	535.0334	
52513		640.9287	686.3516	801.2640	
52514		832.1553	894.2838	944.8592	
52515		976.0235	1021.9044	1049.1188	
52516		1055.2203	1108.4590	1138.3910	
52517		1163.9162	1214.6105	1251.4122	
52518		1304.7127	1365.0893	1379.9680	
52519		1395.4227	1406.0940	1409.8247	
52520		1422.0889	1452.0683	1470.9676	
52521		1486.8420	1495.5164	2002.3730	
52522		3062.7366	3089.0514	3092.3327	
52523		3155.4277	3169.8367	3188.1367	
52524		3755.0788	3769.3800	3826.1892	
52525	Zero-point correction (Hartree): 0.155579				
52526	-----				
52527	triHPacyl.pptmppmpd				
52528	-----				
52529	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17663300				
52530	Electronic state : 2-A				
52531	Cartesian coordinates (Angs):				
52532	O	-1.702611	1.913064	-0.002349	
52533	O	-1.628112	0.840871	0.924399	

52534	C	-1.060076	-0.291396	0.289922	
52535	C	0.292716	0.067254	-0.366049	
52536	C	1.170098	0.914258	0.545878	
52537	O	2.315754	1.401096	-0.125786	
52538	O	3.258705	0.340186	-0.261344	
52539	H	-2.586391	1.784540	-0.378236	
52540	C	-1.020860	-1.360447	1.368124	
52541	H	-2.022162	-1.474245	1.781445	
52542	H	-0.338012	-1.069365	2.162609	
52543	H	-0.689184	-2.302872	0.944445	
52544	C	-1.999792	-0.790000	-0.836333	
52545	O	-3.023362	-0.304978	-1.140430	
52546	H	3.200459	0.150793	-1.207562	
52547	H	0.094964	0.652692	-1.265973	
52548	O	0.951606	-1.074035	-0.885288	
52549	O	1.523148	-1.835534	0.169712	
52550	H	2.396844	-1.418997	0.245889	
52551	H	0.625007	1.813350	0.826782	
52552	H	1.464934	0.380733	1.450048	
52553	Rotational constants (GHz):		1.5033400	0.6614700	0.5617200
52554	Vibrational harmonic frequencies (cm-1):				
52555		55.5271	71.3248		102.1723
52556		134.3823	174.0644		195.7795
52557		212.8223	228.2095		258.6453
52558		276.8494	296.2451		302.3022
52559		326.1005	348.2262		377.6248
52560		381.2715	422.4745		465.4636
52561		510.6804	552.4447		577.0292
52562		635.2355	724.0917		756.2452
52563		849.8882	911.9998		947.1889
52564		967.5584	1002.2899		1048.4895
52565		1092.7278	1114.8224		1148.8349
52566		1171.5044	1176.3034		1248.7808
52567		1302.8042	1339.8404		1377.8859
52568		1405.1688	1415.3881		1421.3815
52569		1423.2646	1456.4615		1475.2713
52570		1484.4574	1496.4391		1972.8903
52571		3085.7757	3091.6347		3100.8340
52572		3160.1747	3162.9638		3192.1336
52573		3726.7323	3768.0830		3804.6097
52574	Zero-point correction (Hartree): 0.156578				
52575	triHPacyl.pptmpppppd				
52576	-----				
52577	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17541334				
52578	Electronic state : 2-A				
52579	Cartesian coordinates (Angs):				
52580	O	1.658355	-1.478613	-1.310884	
52581	O	1.532088	-1.433564	0.100348	
52582	C	0.958208	-0.200865	0.484498	
52583	C	-0.401707	0.029372	-0.207573	
52584	C	-1.406560	-1.058686	0.147730	
52585	O	-2.592141	-0.907708	-0.597905	
52586	O	-3.463054	-0.036411	0.107966	
52587	H	2.565224	-1.162904	-1.437419	
52588	C	0.866568	-0.255790	2.001835	
52589	H	1.862234	-0.238905	2.440818	
52590	H	0.372334	-1.177743	2.300148	
52591	H	0.296739	0.597010	2.364162	
52592	C	1.910827	0.962386	0.123817	
52593	O	2.957064	0.873027	-0.394946	
52594	H	-3.085194	0.834032	-0.084027	
52595	H	-0.271310	0.044433	-1.288273	
52596	O	-0.964752	1.269777	0.194978	
52597	O	-0.491332	2.295852	-0.664736	
52598	H	0.241156	2.671486	-0.154021	
52599	H	-0.986030	-2.024846	-0.132653	
52600	H	-1.648998	-1.059955	1.210864	
52601	Rotational constants (GHz):		1.3915400	0.6559600	0.5626000
52602	Vibrational harmonic frequencies (cm-1):				
52603		37.1966	60.5998		93.6410
52604		120.0351	148.7769		171.0823

52606	194.2785	212.3066	237.9574		
52607	261.2812	273.4435	299.9921		
52608	337.6627	350.1919	364.4924		
52609	399.0786	401.1465	424.6956		
52610	476.5404	508.2437	556.1636		
52611	580.0350	712.0724	742.9911		
52612	869.1011	900.3090	956.6015		
52613	977.8237	1045.8604	1051.4377		
52614	1094.3703	1131.8066	1140.6358		
52615	1176.5054	1181.4691	1243.6888		
52616	1310.6939	1335.3527	1376.8679		
52617	1408.5926	1412.7674	1425.6509		
52618	1429.0707	1446.0958	1467.5416		
52619	1487.4917	1506.5312	1981.3327		
52620	3081.2240	3085.0085	3128.0372		
52621	3143.1664	3162.0275	3173.5862		
52622	3758.5135	3777.6455	3779.0338		
52623	Zero-point correction (Hartree): 0.155849				
52624					
52625	triHPacyl.pptmptmmmd				
52626	-----				
52627	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17453679				
52628	Electronic state : 2-A				
52629	Cartesian coordinates (Angs):				
52630	O	-1.500647	2.217508	-0.363134	
52631	O	-1.526887	1.339093	0.751403	
52632	C	-1.165434	0.040045	0.319921	
52633	C	0.202514	0.058841	-0.405640	
52634	C	1.201991	0.967108	0.303189	
52635	O	2.399253	1.106501	-0.439499	
52636	O	3.224571	-0.031475	-0.205168	
52637	H	-2.391653	2.105912	-0.726073	
52638	C	-1.252280	-0.831215	1.560155	
52639	H	-2.249920	-0.741308	1.986970	
52640	H	-0.518949	-0.510207	2.296692	
52641	H	-1.057549	-1.865138	1.292440	
52642	C	-2.227220	-0.448477	-0.699109	
52643	O	-2.338099	-1.522757	-1.142755	
52644	H	3.991587	0.377593	0.213103	
52645	H	0.059741	0.456980	-1.412021	
52646	O	0.683353	-1.242120	-0.658284	
52647	O	1.213885	-1.811243	0.531646	
52648	H	2.151363	-1.586893	0.425337	
52649	H	0.791836	1.974127	0.343744	
52650	H	1.422681	0.627063	1.315036	
52651	Rotational constants (GHz):		1.3257100	0.7218500	0.5758200
52652	Vibrational harmonic frequencies (cm-1):				
52653	50.9890		78.8791		88.1069
52654	146.9373		156.5679		186.0752
52655	220.9270		227.4040		244.7665
52656	259.0228		268.0873		277.8029
52657	294.8264		318.7271		331.7691
52658	350.7991		420.9508		478.1426
52659	488.4819		515.4527		558.5291
52660	620.1038		675.6794		768.9363
52661	844.3673		909.6212		948.8061
52662	965.1374		1002.7735		1047.1300
52663	1081.1341		1112.3183		1155.3698
52664	1165.2415		1186.8882		1239.7841
52665	1306.9240		1341.0442		1381.1537
52666	1393.4501		1408.6875		1411.0532
52667	1423.6941		1463.7751		1465.6000
52668	1484.9952		1494.7595		2000.7644
52669	3085.3046		3093.0816		3102.1959
52670	3159.8622		3163.5848		3191.1231
52671	3747.5140		3770.8858		3827.7438
52672	Zero-point correction (Hartree): 0.155835				
52673					
52674	triHPacyl.pptmptmmpd				
52675	-----				
52676	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17603390				
52677	Electronic state : 2-A				


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52678 Cartesian coordinates (Angs):
52679 O -1.516669 2.191679 -0.413291
52680 O -1.569694 1.326374 0.710533
52681 C -1.165526 0.030632 0.310613
52682 C 0.228002 0.079018 -0.361370
52683 C 1.196102 0.989536 0.384955
52684 O 2.398556 1.183274 -0.334493
52685 O 3.203890 0.012683 -0.217962
52686 H -2.401645 2.082114 -0.790703
52687 C -1.286703 -0.825655 1.558724
52688 H -2.300165 -0.739218 1.947336
52689 H -0.584348 -0.485897 2.316718
52690 H -1.072906 -1.861363 1.314354
52691 C -2.173717 -0.494205 -0.744527
52692 O -2.226116 -1.570579 -1.194138
52693 H 3.122426 -0.366425 -1.103603
52694 H 0.111059 0.483231 -1.368948
52695 O 0.748202 -1.213091 -0.609182
52696 O 1.214962 -1.795828 0.600194
52697 H 2.131870 -1.476223 0.617287
52698 H 0.765817 1.986328 0.454387
52699 H 1.413880 0.625405 1.389518
52700 Rotational constants (GHz): 1.3102900 0.7327600 0.5840500
52701 Vibrational harmonic frequencies (cm-1):
52702 42.6025 80.4296 95.4943
52703 142.1578 154.2748 195.3377
52704 208.4123 228.6172 245.9274
52705 261.6849 268.4587 288.9837
52706 315.7724 335.6383 342.3745
52707 373.4545 420.9898 471.4179
52708 491.1977 560.7254 585.8767
52709 620.3328 675.7776 771.9023
52710 848.9534 912.6029 948.1368
52711 962.9458 1001.6783 1047.3924
52712 1084.5427 1113.6220 1149.6798
52713 1163.9360 1186.2434 1240.9751
52714 1301.1467 1337.6653 1378.8094
52715 1404.4149 1409.1592 1411.4677
52716 1417.2793 1459.7216 1472.3993
52717 1484.6911 1496.1853 1999.6677
52718 3085.7395 3089.9257 3099.4540
52719 3160.4471 3164.2348 3192.3654
52720 3713.7098 3775.5524 3804.1129
52721 Zero-point correction (Hartree): 0.156047
52722
52723 triHPacyl.pptmptmppd
52724 -----
52725 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17549373
52726 Electronic state : 2-A
52727 Cartesian coordinates (Angs):
52728 O 1.935090 -1.829196 -1.052815
52729 O 1.733231 -1.452009 0.297991
52730 C 1.106754 -0.182576 0.343784
52731 C -0.283674 -0.276862 -0.330005
52732 C -1.325870 -0.914552 0.579137
52733 O -2.507655 -1.179839 -0.143545
52734 O -3.320605 -0.016352 -0.116660
52735 H 2.833701 -1.509748 -1.216127
52736 C 1.112032 0.181623 1.824102
52737 H 2.136542 0.304342 2.170123
52738 H 0.652385 -0.625202 2.392129
52739 H 0.554358 1.099446 1.984988
52740 C 1.997438 0.843187 -0.390038
52741 O 1.838247 2.000720 -0.472434
52742 H -2.908090 0.543826 -0.790221
52743 H -0.169523 -0.904619 -1.214195
52744 O -0.741778 0.939307 -0.889972
52745 O -0.939992 1.894732 0.148939
52746 H -0.197345 2.494704 -0.017420
52747 H -0.956211 -1.883078 0.920222
52748 H -1.558206 -0.283494 1.436595
52749 Rotational constants (GHz): 1.3092900 0.7298900 0.5827800

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52750 Vibrational harmonic frequencies (cm-1):
52751      70.7575      90.1037      111.7753
52752     133.9966     179.6106     191.6933
52753     198.8439     214.6303     233.6451
52754     256.0258     266.2799     291.8020
52755     314.7452     329.0397     343.9580
52756     414.2760     429.2349     450.5166
52757     484.5668     519.8758     565.9834
52758     591.8033     673.7070     767.6495
52759     866.7601     930.4861     950.7494
52760     968.8326     998.2370    1050.7448
52761    1085.8069    1126.0466    1140.5142
52762    1169.9242    1179.8579    1222.4272
52763    1307.4098    1321.3322    1389.6819
52764    1403.8898    1413.6042    1415.7745
52765    1433.7697    1438.2304    1470.7957
52766    1486.0896    1502.3456    1986.5120
52767    3081.6018    3086.6966    3117.8292
52768    3142.5021    3158.5618    3190.2434
52769    3763.4385    3779.1541    3787.7843
52770 Zero-point correction (Hartree): 0.156037
52771
52772 triHPacyl.pptmptmpd
52773 -----
52774 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17477151
52775 Electronic state : 2-A
52776 Cartesian coordinates (Angs):
52777 O      1.546833     -1.821626     -1.271580
52778 O      1.522030     -1.618990      0.133203
52779 C      1.094908     -0.299140      0.385112
52780 C     -0.289207     -0.034103     -0.250671
52781 C     -1.293215     -1.119822      0.131457
52782 O     -2.540792     -0.872183     -0.473444
52783 O     -3.305508     -0.037693      0.383743
52784 H      2.483826     -1.691461     -1.473201
52785 C      1.118337     -0.144954      1.898225
52786 H      2.140821     -0.207382      2.265631
52787 H      0.538627     -0.945907      2.352427
52788 H      0.690463      0.816460      2.170252
52789 C      2.131407      0.686115     -0.197827
52790 O      2.093355      1.857312     -0.164043
52791 H     -2.922147      0.835008      0.214084
52792 H     -0.210120     -0.005743     -1.335573
52793 O     -0.798616      1.218817      0.187669
52794 O     -0.653873      2.188076     -0.840313
52795 H      0.166757      2.632408     -0.583129
52796 H     -0.944657     -2.074453     -0.261262
52797 H     -1.424392     -1.197203      1.211127
52798 Rotational constants (GHz):  1.2184200   0.7422800   0.5799600
52799 Vibrational harmonic frequencies (cm-1):
52800      38.5475      61.1020      69.5822
52801     112.9659     149.5571     170.4342
52802     191.9923     201.5193     217.1841
52803     249.7282     251.8672     282.5797
52804     300.7118     323.2197     361.5182
52805     392.2081     426.7324     433.5126
52806     477.3354     501.7851     548.3938
52807     567.4718     649.7533     769.3177
52808     869.6434     897.3086     953.5309
52809     977.2528    1043.2662    1049.9258
52810    1084.4211    1130.2840    1133.4299
52811    1172.7627    1184.6337    1237.3922
52812    1305.8812    1332.7199    1369.2582
52813    1402.3434    1407.3522    1408.9173
52814    1435.9250    1443.9871    1466.7994
52815    1485.6132    1501.3425    1980.5360
52816    3083.2783    3088.4481    3129.6150
52817    3147.9286    3161.4846    3180.0328
52818    3771.4993    3780.3879    3794.5511
52819 Zero-point correction (Hartree): 0.155282
52820
52821 triHPacyl.pptmptmpd

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52822 -----
52823 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17435768
52824 Electronic state : 2-A
52825 Cartesian coordinates (Angs):
52826 O 1.687732 -1.733858 -1.184658
52827 O 1.725068 -1.435863 0.203785
52828 C 1.214424 -0.137335 0.386538
52829 C -0.218282 -0.010749 -0.169801
52830 C -1.097452 -1.201560 0.189302
52831 O -2.355264 -1.131154 -0.445058
52832 O -3.211633 -0.300895 0.324941
52833 H 2.605483 -1.572064 -1.443529
52834 C 1.334304 0.137375 1.876962
52835 H 2.378594 0.074299 2.176480
52836 H 0.765653 -0.609642 2.427898
52837 H 0.945348 1.126237 2.103036
52838 C 2.116090 0.871635 -0.370272
52839 O 1.865734 1.984305 -0.631364
52840 H -3.075233 0.569072 -0.078396
52841 H -0.181829 0.080896 -1.255612
52842 O -0.715704 1.208818 0.368713
52843 O -1.575609 1.813456 -0.581917
52844 H -1.023403 2.531689 -0.918904
52845 H -0.636562 -2.112397 -0.191724
52846 H -1.235144 -1.282770 1.268826
52847 Rotational constants (GHz): 1.2778400 0.7275300 0.5803400
52848 Vibrational harmonic frequencies (cm-1):
52849 32.5973 59.7583 66.9439
52850 107.4005 146.7030 165.8084
52851 192.0014 206.1343 211.2390
52852 246.6740 255.9837 261.6107
52853 289.5577 309.8870 341.6808
52854 397.1890 403.3760 431.5039
52855 483.4443 515.7081 545.1281
52856 551.8548 640.3411 781.5174
52857 894.9165 898.0423 967.0102
52858 975.1185 1041.4242 1052.1505
52859 1085.9127 1124.6610 1137.9673
52860 1162.3556 1194.2859 1254.7436
52861 1308.1349 1329.2787 1374.8063
52862 1398.6272 1405.1358 1407.8012
52863 1422.5191 1447.6594 1458.1727
52864 1488.3473 1497.8486 1987.0800
52865 3079.3806 3084.7976 3105.8484
52866 3145.7999 3159.8231 3182.3348
52867 3769.7284 3797.4932 3800.3331
52868 Zero-point correction (Hartree): 0.155106
52869 triHPacyl.pptmptpmd
52870 -----
52871 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17449527
52872 Electronic state : 2-A
52873 Cartesian coordinates (Angs):
52874 O 1.546215 -1.922337 -1.069597
52875 O 1.642360 -1.481984 0.275446
52876 C 1.210690 -0.138925 0.348943
52877 C -0.209284 0.028296 -0.232352
52878 O -1.113597 -1.117066 0.214147
52879 O -2.402876 -1.039588 -0.365492
52880 O -3.148216 -0.063265 0.364603
52881 H 2.389794 -1.622697 -1.439993
52882 C 1.336603 0.249833 1.811967
52883 H 2.369189 0.129327 2.133779
52884 H 0.703265 -0.391145 2.422496
52885 H 1.033737 1.285788 1.935006
52886 C 2.172653 0.736007 -0.494049
52887 O 2.240551 1.901053 -0.507556
52888 H -3.981569 -0.529771 0.496626
52889 H -0.168650 0.042545 -1.322341
52890 O -0.659114 1.291042 0.215355
52891 O -1.522152 1.846871 -0.760826
52892 H -2.383264 1.496870 -0.480807

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52894      H      -0.713313      -2.060772      -0.152736
52895      H      -1.205716      -1.153355      1.300581
52896      Rotational constants (GHz):      1.2999900      0.7144200      0.5678100
52897      Vibrational harmonic frequencies (cm-1):
52898          56.8922          60.5297          77.7606
52899          144.3903          161.2913          171.7122
52900          185.1120          198.6244          212.5502
52901          226.2623          251.3684          277.6163
52902          288.3057          312.4140          356.3421
52903          399.2015          407.3135          436.9728
52904          497.7781          519.5139          534.9451
52905          559.4093          647.7160          779.6310
52906          893.9716          898.7716          963.2674
52907          970.7509          1044.4509          1052.0485
52908          1073.2790          1113.5664          1148.9594
52909          1159.2864          1204.5368          1245.1179
52910          1313.3306          1329.1141          1374.7123
52911          1396.3975          1407.3205          1413.4121
52912          1431.4275          1456.5719          1475.0644
52913          1487.7666          1498.5970          2003.0701
52914          3081.9190          3086.5444          3100.9500
52915          3155.4299          3159.6681          3183.8327
52916          3718.6981          3766.3115          3843.9519
52917      Zero-point correction (Hartree): 0.155407
52918
52919      triHPacyl.pptpppmmmd
52920      -----
52921      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17637872
52922      Electronic state : 2-A
52923      Cartesian coordinates (Angs):
52924      O      -1.509663      -1.935958      -0.339099
52925      O      -1.553126      -0.708185      -1.050081
52926      C      -1.064591      0.329130      -0.218333
52927      C      0.338959      -0.027820      0.311365
52928      C      1.209891      -0.673778      -0.767606
52929      O      2.580127      -0.563232      -0.429091
52930      O      2.793665      -1.283381      0.775841
52931      H      -2.394244      -1.965109      0.054999
52932      C      -1.155736      1.588612      -1.061022
52933      H      -2.184181      1.708767      -1.398818
52934      H      -0.502756      1.512520      -1.926778
52935      H      -0.860695      2.450488      -0.470254
52936      C      -1.995306      0.515377      1.004120
52937      O      -2.971510      -0.094337      1.227258
52938      H      2.715886      -0.584804      1.441738
52939      H      0.229234      -0.729456      1.139036
52940      O      0.991440      1.066984      0.928492
52941      O      1.491512      1.957452      -0.062251
52942      H      2.363637      1.572305      -0.238201
52943      H      0.926388      -1.716488      -0.901135
52944      H      1.127864      -0.152095      -1.720285
52945      Rotational constants (GHz):      1.4106900      0.6836600      0.5854100
52946      Vibrational harmonic frequencies (cm-1):
52947          62.4908          76.6103          95.5779
52948          145.3838          164.1583          185.1721
52949          208.9026          249.9717          259.9486
52950          286.7464          294.8245          311.1358
52951          349.6759          353.9605          380.9538
52952          419.2333          425.5422          467.1584
52953          493.6008          516.4849          545.6989
52954          699.5231          712.9120          759.3361
52955          840.9102          917.9649          955.2001
52956          973.7552          995.3664          1048.3227
52957          1077.4794          1124.3415          1145.4437
52958          1178.1497          1179.9966          1255.5840
52959          1298.1315          1349.2101          1387.0458
52960          1409.5096          1415.4769          1423.3558
52961          1426.3023          1441.8945          1481.4061
52962          1484.4960          1499.0120          1974.8429
52963          3086.7161          3102.2617          3106.0712
52964          3157.3211          3164.4680          3189.2251
52965          3752.8477          3769.4382          3776.3850

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52966 Zero-point correction (Hartree): 0.156859
52967
52968 triHPacyl.pptppptpmd
52969 -----
52970 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17633426
52971 Electronic state : 2-A
52972 Cartesian coordinates (Angs):
52973 O -1.409231 1.924913 -0.406000
52974 O -1.628493 1.054607 0.692482
52975 C -1.148044 -0.232611 0.367029
52976 C 0.327254 -0.178575 -0.073533
52977 C 1.141213 0.760850 0.810352
52978 O 2.528305 0.622115 0.564998
52979 O 2.795701 1.141418 -0.729121
52980 H -2.241799 1.838142 -0.894077
52981 C -1.396685 -1.078604 1.604518
52982 H -2.457845 -1.055755 1.846243
52983 H -0.837326 -0.679440 2.447722
52984 H -1.088201 -2.103220 1.417528
52985 C -1.970977 -0.834338 -0.798994
52986 O -2.859791 -0.308009 -1.353005
52987 H 2.692674 0.355187 -1.287426
52988 H 0.384378 0.143151 -1.114440
52989 O 0.794215 -1.515536 0.013195
52990 O 1.943685 -1.649124 -0.811893
52991 H 2.652502 -1.566381 -0.157403
52992 H 0.831955 1.794269 0.659177
52993 H 1.031972 0.490661 1.861185
52994 Rotational constants (GHz): 1.3942200 0.6602900 0.5828200
52995 Vibrational harmonic frequencies (cm-1):
52996 64.6756 69.0775 101.9694
52997 148.0394 167.8891 178.4831
52998 195.7089 205.7053 227.6760
52999 265.3516 271.7428 302.7855
53000 345.7723 372.3386 397.3135
53001 419.4154 421.9943 453.6889
53002 478.3541 522.6802 537.4924
53003 595.0910 708.9536 771.8675
53004 885.6638 909.4448 961.3807
53005 977.5541 1032.8111 1053.7007
53006 1079.7642 1130.4271 1144.3461
53007 1164.7721 1197.9655 1255.0763
53008 1305.7171 1350.7657 1373.3640
53009 1411.9600 1421.2616 1423.1660
53010 1429.2918 1442.4778 1468.1210
53011 1487.5729 1499.5087 1975.9749
53012 3085.7930 3091.2345 3097.9682
53013 3150.3718 3163.0190 3184.4617
53014 3750.0042 3767.2940 3779.7432
53015 Zero-point correction (Hartree): 0.156456
53016
53017 triHPacyl.pptpmtmmmd
53018 -----
53019 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17589196
53020 Electronic state : 2-A
53021 Cartesian coordinates (Angs):
53022 O -1.263960 2.283105 -0.219523
53023 O -1.455508 1.323287 0.809070
53024 C -1.164115 0.041218 0.288627
53025 C 0.270713 0.017695 -0.281841
53026 C 1.245380 0.805599 0.597722
53027 O 2.577881 0.401213 0.342592
53028 O 2.878284 0.707812 -1.010855
53029 H -2.145936 2.327287 -0.616431
53030 C -1.450141 -0.930124 1.419615
53031 H -2.482656 -0.803564 1.741106
53032 H -0.788946 -0.733071 2.260382
53033 H -1.293607 -1.947945 1.075023
53034 C -2.148934 -0.263656 -0.868061
53035 O -2.217790 -1.251845 -1.487229
53036 H 2.682256 -0.131174 -1.452806
53037 H 0.256526 0.466028 -1.276069

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53038	O	0.742812	-1.289358	-0.544806	
53039	O	1.112633	-1.926784	0.672413	
53040	H	2.036514	-1.646000	0.758160	
53041	H	1.124394	1.873819	0.425453	
53042	H	1.099206	0.590794	1.655513	
53043	Rotational constants (GHz):		1.2556500	0.7410000	0.6171700
53044	Vibrational harmonic frequencies (cm-1):				
53045		51.8572	83.0427		89.9244
53046		124.8457	165.3299		170.5825
53047		214.0555	245.4769		252.2828
53048		266.3858	277.7385		295.3987
53049		311.2500	349.2855		357.6270
53050		400.9002	429.4023		474.0212
53051		487.6781	496.5805		554.2576
53052		635.3535	716.9006		763.7407
53053		841.4906	926.1073		955.2198
53054		967.3583	992.6071		1047.2713
53055		1073.7269	1123.2951		1141.7365
53056		1174.4438	1187.1235		1246.5220
53057		1296.2001	1347.3192		1387.4978
53058		1405.3549	1410.3738		1412.8878
53059		1424.7737	1439.7376		1480.2689
53060		1482.5836	1496.7398		1997.4547
53061		3085.7794	3102.3284		3107.0762
53062		3157.8670	3161.9426		3188.4330
53063		3758.8266	3775.1768		3777.7861
53064	Zero-point correction (Hartree): 0.156253				
53065	triHPacyl.pptpptommd				
53066	-----				
53067	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17500567				
53068	Electronic state : 2-A				
53069	Cartesian coordinates (Angs):				
53070	O	1.328599	-1.843753	-1.228097	
53071	O	1.627235	-1.495632	0.116758	
53072	C	1.232732	-0.160519	0.318374	
53073	C	-0.266012	0.031716	0.022122	
53074	C	-1.127506	-1.094711	0.584735	
53075	O	-2.493613	-0.755949	0.548314	
53076	O	-2.870362	-0.606699	-0.814020	
53077	H	2.199196	-1.777558	-1.643912	
53078	C	1.639208	0.172624	1.744466	
53079	H	2.716078	0.058581	1.851983	
53080	H	1.145368	-0.512020	2.431626	
53081	H	1.350849	1.192749	1.982197	
53082	C	2.033213	0.761143	-0.638027	
53083	O	1.767177	1.861486	-0.935312	
53084	H	-2.844436	0.357459	-0.906928	
53085	H	-0.413057	0.089952	-1.055110	
53086	O	-0.622541	1.279948	0.597159	
53087	O	-1.537315	1.939983	-0.261050	
53088	H	-0.955331	2.563240	-0.718201	
53089	H	-0.937995	-2.017148	0.033735	
53090	H	-0.923928	-1.251835	1.644583	
53091	Rotational constants (GHz):		1.2189900	0.7577400	0.6126200
53092	Vibrational harmonic frequencies (cm-1):				
53093		39.6043	63.3296		81.4334
53094		95.4859	144.6454		161.9571
53095		188.3234	199.4794		227.2315
53096		243.4037	258.5936		274.5727
53097		285.3755	347.4414		352.2366
53098		393.1218	403.4307		444.5100
53099		473.9691	521.9384		544.5505
53100		595.0054	638.8448		783.4035
53101		883.8875	915.8539		963.4566
53102		972.4034	1036.5449		1052.1267
53103		1077.7623	1132.4022		1144.1535
53104		1167.8510	1194.8648		1259.3814
53105		1299.7912	1343.9859		1378.4600
53106		1403.3715	1407.5955		1414.2442
53107		1416.7259	1448.1862		1470.7838
53108		1488.2952	1499.1682		1984.6001
53109					

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53110      3079.1826      3085.2601      3120.2284
53111      3139.1251      3160.3382      3182.4581
53112      3763.8192      3786.4904      3799.0018
53113 Zero-point correction (Hartree): 0.155448
53114
53115 triHPacyl.pptpmtmd
53116 -----
53117 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17570136
53118 Electronic state : 2-A
53119 Cartesian coordinates (Angs):
53120 O      1.154105      -2.085713      -0.932742
53121 O      1.524950      -1.522990      0.315596
53122 C      1.238699      -0.142301      0.290672
53123 C      -0.245381      0.101747      -0.049703
53124 C      -1.152145      -0.892412      0.670945
53125 O      -2.512348      -0.518573      0.556905
53126 O      -2.904556      -0.710948      -0.793954
53127 H      1.970198      -1.990302      -1.445195
53128 C      1.667788      0.388605      1.647956
53129 H      2.722726      0.171248      1.803316
53130 H      1.092531      -0.094754      2.435288
53131 H      1.507022      1.462331      1.685713
53132 C      2.104217      0.529675      -0.806103
53133 O      2.210980      1.673406      -1.014639
53134 H      -2.713427      0.155549      -1.184771
53135 H      -0.388437      0.024136      -1.128663
53136 O      -0.512985      1.435183      0.349386
53137 O      -1.654716      1.899016      -0.358718
53138 H      -2.346986      1.779106      0.307488
53139 H      -1.003229      -1.899811      0.284734
53140 H      -0.962898      -0.874429      1.744812
53141 Rotational constants (GHz):      1.2599100      0.7324400      0.5905800
53142 Vibrational harmonic frequencies (cm-1):
53143      51.4530      78.9996      90.1448
53144      136.8654      166.7066      174.3620
53145      184.6519      207.0698      233.2296
53146      250.6704      271.7103      281.7579
53147      295.2847      346.5429      387.4002
53148      402.6092      415.4580      466.2926
53149      500.1272      526.0806      543.8060
53150      577.7127      647.3262      785.5725
53151      888.0925      915.4450      960.7020
53152      970.4731      1032.5621      1052.5920
53153      1075.0096      1129.5699      1143.9487
53154      1159.0000      1206.2391      1249.0935
53155      1306.9438      1348.2456      1373.1034
53156      1408.4880      1411.1388      1421.0812
53157      1427.2577      1441.9482      1468.3153
53158      1487.7163      1498.6180      2001.5531
53159      3084.6718      3090.8142      3097.7242
53160      3152.1151      3160.8855      3184.1745
53161      3744.2567      3774.7741      3780.9028
53162 Zero-point correction (Hartree): 0.155985
53163
53164 triHPacyl.ptmmmmmpmd
53165 -----
53166 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17389545
53167 Electronic state : 2-A
53168 Cartesian coordinates (Angs):
53169 O      2.464052      0.175087      -0.903106
53170 O      1.454947      -0.799697      -1.137256
53171 C      0.394469      -0.690491      -0.197069
53172 C      -0.452495      0.570350      -0.447448
53173 C      -1.537652      0.866704      0.588934
53174 O      -2.514391      -0.143970      0.697856
53175 O      -3.148383      -0.264688      -0.572893
53176 H      2.242684      0.838876      -1.571198
53177 C      -0.411568      -1.965694      -0.436134
53178 H      0.252799      -2.822105      -0.341046
53179 H      -0.827269      -1.941063      -1.441992
53180 H      -1.223471      -2.042984      0.279815
53181 C      0.898089      -0.772879      1.255182

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53182	O	1.967982	-1.064657	1.626629	
53183	H	-4.045500	0.024094	-0.366312	
53184	H	-0.912940	0.451957	-1.430334	
53185	O	0.341380	1.734123	-0.606767	
53186	O	0.988912	2.005505	0.630030	
53187	H	1.839734	1.552376	0.505728	
53188	H	-1.110001	0.936405	1.587508	
53189	H	-1.997088	1.820890	0.321097	
53190	Rotational constants (GHz):		1.3374700	0.7357200	0.6427100
53191	Vibrational harmonic frequencies (cm-1):				
53192		36.2566	78.7890		97.5530
53193		151.0400	159.7812		174.3127
53194		184.1181	205.2957		226.9755
53195		238.3617	261.6633		277.4020
53196		326.2929	343.0023		372.2088
53197		406.3343	441.3404		455.4260
53198		535.0346	561.8520		605.9305
53199		610.0271	708.2987		742.3260
53200		868.5849	920.1418		948.8238
53201		977.4502	1039.8481		1040.8745
53202		1099.4624	1113.7703		1133.1569
53203		1153.7530	1188.4303		1230.4054
53204		1284.3220	1339.4658		1375.8595
53205		1390.0535	1408.2337		1421.5300
53206		1425.9946	1440.6522		1479.4479
53207		1487.9672	1497.0430		1991.1340
53208		3071.0608	3085.9323		3100.8659
53209		3152.7329	3162.2890		3194.1465
53210		3710.0181	3790.9434		3830.5548
53211	Zero-point correction (Hartree):		0.156179		
53212	triHPacyl.ptmmmtmpmd				
53213	-----				
53214	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17516037				
53215	Electronic state : 2-A				
53216	Cartesian coordinates (Angs):				
53217	O	2.673878	-0.092449	-0.705471	
53218	O	1.595701	-0.950739	-1.057499	
53219	C	0.483927	-0.764049	-0.195658	
53220	C	-0.224413	0.575191	-0.501848	
53221	C	-1.377686	0.970687	0.420414	
53222	O	-2.457764	0.065137	0.391916	
53223	O	-2.956725	0.036072	-0.943071	
53224	H	2.579467	0.608698	-1.365399	
53225	C	-0.410801	-1.961174	-0.498650	
53226	H	0.156921	-2.877299	-0.351475	
53227	H	-0.741736	-1.908389	-1.534769	
53228	H	-1.278013	-1.951683	0.153900	
53229	C	0.935011	-0.872069	1.273581	
53230	O	0.234335	-0.939901	2.210254	
53231	H	-3.842346	0.399160	-0.822265	
53232	H	-0.598040	0.490978	-1.525083	
53233	O	0.685446	1.656367	-0.583578	
53234	O	1.228317	1.882376	0.710999	
53235	H	2.031567	1.335074	0.683034	
53236	H	-1.066546	0.986636	1.462673	
53237	H	-1.703009	1.970399	0.123947	
53238	Rotational constants (GHz):		1.2555900	0.7576700	0.6964700
53239	Vibrational harmonic frequencies (cm-1):				
53240		39.0808	79.5357		121.5916
53241		152.3925	170.4856		181.9224
53242		201.9558	214.5578		225.6560
53243		241.6525	265.4824		273.5930
53244		313.1021	324.4807		343.7342
53245		419.5265	436.3912		476.3664
53246		491.7690	551.2883		573.1826
53247		631.9193	672.9893		744.3659
53248		868.3573	930.3287		948.6951
53249		977.3920	1037.8635		1043.1259
53250		1099.8608	1116.9941		1138.1020
53251		1154.3524	1190.0703		1215.6552
53252		1284.3383	1338.0855		1369.9213


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53254      1391.5215          1407.9671          1418.9463
53255      1425.7154          1442.8246          1485.6951
53256      1488.1632          1497.4114          1980.1099
53257      3074.0708          3085.0867          3094.4291
53258      3161.0986          3163.1387          3193.1529
53259      3711.1773          3788.5249          3829.9605
53260 Zero-point correction (Hartree): 0.156053
53261
53262 triHPacyl.ptmmpmmpmd
53263 -----
53264 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17580051
53265 Electronic state : 2-A
53266 Cartesian coordinates (Angs):
53267 O      2.510363      0.175592      -0.789074
53268 O      1.478349      -0.737149      -1.130664
53269 C      0.378948      -0.655503      -0.229012
53270 C      -0.478176      0.597666      -0.493239
53271 C      -1.554831      0.894373      0.552773
53272 O      -2.483645      -0.149660      0.744820
53273 O      -3.150974      -0.360269      -0.496924
53274 H      3.087073      -0.388126      -0.253030
53275 C      -0.402325      -1.937003      -0.516992
53276 H      0.249656      -2.794390      -0.362786
53277 H      -0.730314      -1.918053      -1.554898
53278 H      -1.271322      -2.008661      0.128798
53279 C      0.844788      -0.759096      1.227619
53280 O      1.911367      -1.066082      1.609668
53281 H      -4.045574      -0.066745      -0.285926
53282 H      -0.945176      0.456597      -1.469653
53283 O      0.292609      1.763386      -0.675149
53284 O      0.971903      2.039250      0.543684
53285 H      1.854458      1.706382      0.316541
53286 H      -1.105016      1.038068      1.533809
53287 H      -2.063983      1.811756      0.249359
53288 Rotational constants (GHz):      1.3550200      0.7404500      0.6390200
53289 Vibrational harmonic frequencies (cm-1):
53290      49.5541          77.9883          112.3093
53291      151.6561         179.3440         186.8618
53292      199.1710         206.7267         237.3918
53293      238.0029         266.8820         285.8019
53294      333.7648         343.3279         371.3631
53295      410.4421         426.6131         457.2284
53296      519.1848         552.6961         569.8613
53297      609.8330         714.3697         754.1844
53298      870.3675         919.0355         949.3725
53299      978.4974         1041.9004        1043.3805
53300      1099.0223        1114.8036        1134.9948
53301      1152.8483        1188.3931        1232.2054
53302      1284.6422        1338.0337        1378.2155
53303      1389.3923        1405.7319        1421.1158
53304      1426.0073        1447.7823        1481.7953
53305      1491.3652        1497.6015        1971.0800
53306      3072.1402        3086.3847        3104.4596
53307      3150.8171        3161.3023        3198.9154
53308      3740.6064        3774.9099        3829.3420
53309 Zero-point correction (Hartree): 0.156353
53310
53311 triHPacyl.ptmmpppmmd
53312 -----
53313 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17445146
53314 Electronic state : 2-A
53315 Cartesian coordinates (Angs):
53316 O      2.310045      0.594059      -0.917265
53317 O      1.402687      -0.438540      -1.259243
53318 C      0.472790      -0.691262      -0.211221
53319 C      -0.449141      0.501879      0.079955
53320 C      -1.649145      0.170349      0.970520
53321 O      -2.634734      -0.612812      0.333265
53322 O      -3.145366      0.141500      -0.759398
53323 H      2.973534      0.120443      -0.392498
53324 C      -0.268022      -1.929392      -0.701797
53325 H      0.462079      -2.675545      -1.008940

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53326	H	-0.896304	-1.663217	-1.549682	
53327	H	-0.899005	-2.336736	0.082242	
53328	C	1.218831	-1.069037	1.083714	
53329	O	2.376055	-1.208398	1.211909	
53330	H	-4.033751	0.355907	-0.449209	
53331	H	-0.807802	0.894766	-0.871650	
53332	O	0.249760	1.520012	0.777469	
53333	O	0.597474	2.566031	-0.111020	
53334	H	1.421094	2.220427	-0.492607	
53335	H	-1.348349	-0.422595	1.836545	
53336	H	-2.070747	1.116510	1.313034	
53337	Rotational constants (GHz):		1.2762200	0.7216100	0.5970200
53338	Vibrational harmonic frequencies (cm-1):				
53339		34.9692	45.8457		100.5542
53340		120.6538	142.6446		192.9152
53341		218.3126	229.6571		249.7052
53342		254.3498	271.1499		278.5245
53343		326.0027	336.9496		379.8258
53344		393.2043	425.6297		458.2012
53345		515.1947	564.9548		577.0218
53346		604.7180	647.0798		726.8844
53347		862.4539	929.8844		956.5863
53348		1014.4308	1034.5431		1051.6568
53349		1109.0388	1115.2407		1136.3608
53350		1167.2621	1178.7936		1230.2633
53351		1282.1092	1324.6557		1370.8402
53352		1391.3004	1413.0272		1416.7022
53353		1425.2534	1461.1334		1482.1650
53354		1482.4054	1499.9544		1979.1475
53355		3071.0332	3084.9341		3113.4788
53356		3129.0960	3163.1546		3184.2118
53357		3704.7937	3756.5934		3824.6138
53358	Zero-point correction (Hartree): 0.155923				
53359	triHPacyl.ptmmpmpmd				
53360	-----				
53362	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17495959				
53363	Electronic state : 2-A				
53364	Cartesian coordinates (Angs):				
53365	O	2.697825	-0.125839	-0.597822	
53366	O	1.613353	-0.939434	-1.020066	
53367	C	0.469869	-0.741782	-0.198112	
53368	C	-0.239841	0.581978	-0.570082	
53369	C	-1.386121	1.021910	0.341151	
53370	O	-2.430721	0.080233	0.449105	
53371	O	-2.969625	-0.110296	-0.857064	
53372	H	3.201233	-0.749311	-0.056668	
53373	C	-0.404146	-1.956315	-0.496239	
53374	H	0.143602	-2.865192	-0.255977	
53375	H	-0.650796	-1.960201	-1.556877	
53376	H	-1.319887	-1.908837	0.084367	
53377	C	0.879689	-0.826798	1.279925	
53378	O	0.178328	-0.774333	2.215758	
53379	H	-3.854365	0.260447	-0.754331	
53380	H	-0.619098	0.439052	-1.584534	
53381	O	0.655970	1.657999	-0.714869	
53382	O	1.240773	1.923040	0.554190	
53383	H	2.098829	1.485795	0.433971	
53384	H	-1.041279	1.162314	1.363352	
53385	H	-1.762167	1.971011	-0.047017	
53386	Rotational constants (GHz):		1.2834900	0.7606900	0.6932600
53387	Vibrational harmonic frequencies (cm-1):				
53388		53.3217	78.4951		126.7666
53389		147.5125	180.6313		188.3381
53390		191.7827	206.5186		232.6850
53391		242.7513	266.4068		276.7818
53392		314.1936	333.3303		346.5746
53393		378.3575	433.9231		473.6865
53394		493.9764	521.5947		553.8948
53395		629.7701	669.1102		747.1710
53396		868.8052	929.1289		948.7870
53397		978.3065	1040.0461		1043.8797

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53398      1098.9639      1118.8199      1136.3506
53399      1153.7915      1188.5119      1216.5203
53400      1285.4199      1337.5174      1373.7520
53401      1389.1206      1406.5387      1413.3330
53402      1423.9725      1443.9784      1488.0254
53403      1490.7582      1496.9031      1987.0387
53404      3073.7964      3084.4904      3096.6267
53405      3158.9391      3163.0027      3196.1637
53406      3738.7723      3796.2699      3830.3630
53407 Zero-point correction (Hartree): 0.156019
53408
53409 triHPacyl.ptppmttmd
53410 -----
53411 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17547523
53412 Electronic state : 2-A
53413 Cartesian coordinates (Angs):
53414 O      2.354800      1.292758      0.583388
53415 O      2.285660      0.299514     -0.428798
53416 C      1.104643     -0.460651     -0.262343
53417 C     -0.092083      0.310428     -0.860437
53418 C     -1.333385     -0.510140     -1.180651
53419 O     -1.878976     -1.230711     -0.102414
53420 O     -2.465713     -0.290610      0.791577
53421 H      1.687567      1.940008      0.305962
53422 C      1.353587     -1.774781     -0.987085
53423 H      2.292517     -2.194265     -0.635118
53424 H      1.423743     -1.596626     -2.059759
53425 H      0.547176     -2.478336     -0.787600
53426 C      0.986804     -0.787802      1.246671
53427 O      0.049262     -0.793585      1.947670
53428 H     -1.802276     -0.285069      1.502011
53429 H      0.264450      0.721975     -1.813282
53430 O     -0.331964      1.385094      0.042755
53431 O     -1.413989      2.165879     -0.426141
53432 H     -2.157884      1.733953      0.026102
53433 H     -2.091554      0.138288     -1.620749
53434 H     -1.073781     -1.268964     -1.918807
53435 Rotational constants (GHz):      1.2633900      0.8295600      0.7234600
53436 Vibrational harmonic frequencies (cm-1):
53437      58.4207      100.0973      135.5066
53438      150.4061      176.6641      190.0525
53439      198.7365      233.9535      256.3738
53440      267.6112      297.5851      342.1941
53441      358.7550      379.7801      385.5633
53442      419.3409      476.7557      506.9540
53443      519.0503      576.6794      577.5008
53444      591.2492      690.3026      793.3199
53445      869.1032      909.9507      938.2740
53446      977.3435      1041.0481     1045.2927
53447      1060.7270     1125.8914     1143.0428
53448      1183.0271     1207.7399     1222.0041
53449      1298.7050     1362.5818     1378.1819
53450      1403.3657     1412.2513     1443.7275
53451      1454.0046     1460.9095     1480.1165
53452      1497.6167     1503.1977     1990.7772
53453      3027.9398     3076.9101     3092.7229
53454      3137.4424     3156.3936     3172.5931
53455      3710.4002     3723.6112     3748.0408
53456 Zero-point correction (Hartree): 0.157052
53457
53458 triHPacyl.tmmmmmpmd
53459 -----
53460 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17543228
53461 Electronic state : 2-A
53462 Cartesian coordinates (Angs):
53463 O     -2.562114     -0.557712     -0.894624
53464 O     -1.327801      0.128832     -0.801072
53465 C     -0.688200     -0.168864      0.434814
53466 C      0.564042      0.726354      0.477605
53467 C      1.523317      0.513176     -0.689675
53468 O      2.043554     -0.798504     -0.674660
53469 O      2.842238     -0.927806      0.498919

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53470	H	-2.279400	-1.424323	-1.226212	
53471	C	-1.588162	0.084462	1.636173	
53472	H	-2.464023	-0.556860	1.599939	
53473	H	-1.899276	1.126832	1.628716	
53474	H	-1.035866	-0.115686	2.552726	
53475	C	-0.271141	-1.652381	0.480043	
53476	O	-0.663876	-2.502114	-0.228093	
53477	H	3.709307	-1.105443	0.115084	
53478	H	1.086179	0.485934	1.405386	
53479	O	0.214419	2.085986	0.620566	
53480	O	-0.131255	2.629906	-0.647960	
53481	H	-1.011892	2.258571	-0.809169	
53482	H	1.013758	0.589748	-1.646994	
53483	H	2.320754	1.256044	-0.637846	
53484	Rotational constants (GHz):			1.0594900	0.9071300 0.6247200
53485	Vibrational harmonic frequencies (cm-1):				
53486		36.4159	74.7206		120.7768
53487		145.6113	155.5495		167.0794
53488		184.3952	199.2377		214.2619
53489		224.8165	252.0517		288.8179
53490		320.2582	361.1858		365.9936
53491		407.9040	424.6440		441.3462
53492		463.3441	507.2598		582.4768
53493		597.0816	691.9646		770.2605
53494		877.1479	912.2522		951.1841
53495		973.1176	1023.2568		1064.8146
53496		1106.5482	1121.0343		1129.6950
53497		1152.4440	1193.6689		1228.0173
53498		1287.6850	1328.3568		1381.9828
53499		1397.1673	1405.2588		1420.7514
53500		1444.0407	1450.6816		1480.0302
53501		1485.2900	1498.1881		1970.3255
53502		3086.8312	3087.1677		3107.3642
53503		3165.2970	3168.3969		3180.9649
53504		3750.7655	3758.8402		3831.7288
53505	Zero-point correction (Hartree):			0.155867	
53506	triHPacyl.tmmmmmmppd				
53507	-----				
53508	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17663283				
53509	Electronic state : 2-A				
53510	Cartesian coordinates (Angs):				
53511	O	-2.509694	-0.622957	-0.910588	
53512	O	-1.298413	0.101943	-0.808617	
53513	C	-0.650527	-0.184038	0.421664	
53514	C	0.554397	0.772327	0.492275	
53515	C	1.544193	0.617459	-0.658397	
53516	O	2.041070	-0.700265	-0.733989	
53517	O	2.845684	-0.927158	0.419399	
53518	H	-2.206565	-1.464355	-1.285207	
53519	C	-1.563598	-0.012139	1.627890	
53520	H	-2.409424	-0.690634	1.569113	
53521	H	-1.920201	1.015462	1.650717	
53522	H	-1.004682	-0.212872	2.540512	
53523	C	-0.155668	-1.646817	0.432510	
53524	O	-0.567925	-2.526622	-0.224095	
53525	H	2.359980	-1.644876	0.850720	
53526	H	1.069780	0.548876	1.428259	
53527	O	0.135486	2.109551	0.651843	
53528	O	-0.220612	2.663727	-0.608711	
53529	H	-1.088590	2.269036	-0.780479	
53530	H	1.065457	0.778991	-1.620577	
53531	H	2.356697	1.333857	-0.530656	
53532	Rotational constants (GHz):			1.0393200	0.9360400 0.6308100
53533	Vibrational harmonic frequencies (cm-1):				
53534		50.5110	96.7021		123.6784
53535		146.3319	158.9599		165.2205
53536		186.5546	214.3615		224.1088
53537		250.3251	288.5272		295.1561
53538		317.5590	354.0445		361.0394
53539		391.8140	404.4687		429.7610
53540		459.5913	506.8915		589.8220

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53542      595.7699      682.8062      765.0947
53543      872.5640      914.5352      952.8732
53544      974.0492     1022.6216     1065.2236
53545     1111.3276     1122.3602     1131.1678
53546     1150.9423     1192.6325     1232.6928
53547     1286.4931     1330.6606     1386.3187
53548     1403.2350     1410.2508     1428.1458
53549     1441.2398     1447.2510     1483.1976
53550     1486.1759     1497.1192     1972.5266
53551     3086.3881     3092.2928     3102.6362
53552     3163.7049     3171.8626     3182.9772
53553     3758.5418     3767.0729     3775.5868
53554 Zero-point correction (Hartree): 0.155999
53555
53556 triHPacyl.tmmmtmmpd
53557 -----
53558 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17509250
53559 Electronic state : 2-A
53560 Cartesian coordinates (Angs):
53561 O      1.823764     -1.659529      1.365174
53562 O      1.151063     -0.446328      1.078854
53563 C      0.619494     -0.518787     -0.225814
53564 C     -0.148291      0.795525     -0.486467
53565 C     -1.019578      1.210811      0.693202
53566 O     -1.955170      0.198973      1.000370
53567 O     -2.948125      0.214014     -0.018095
53568 H      1.122049     -2.180276      1.780916
53569 C      1.679579     -0.776440     -1.285025
53570 H      2.132645     -1.753090     -1.140232
53571 H      2.441793     -0.005328     -1.194563
53572 H      1.231188     -0.725396     -2.275874
53573 C     -0.402221     -1.680604     -0.280980
53574 O     -1.196034     -1.878329     -1.124502
53575 H     -2.802552     -0.638732     -0.454238
53576 H     -0.787762      0.613094     -1.353305
53577 O      0.679454      1.838817     -0.938999
53578 O      1.547017      2.215225      0.133002
53579 H      1.433866      3.173229      0.126790
53580 H     -0.426291      1.327425      1.596488
53581 H     -1.534588      2.143299      0.458077
53582 Rotational constants (GHz): 1.0582900 0.8897500 0.6686900
53583 Vibrational harmonic frequencies (cm-1):
53584      57.1264      100.9190      108.8881
53585     127.3036     156.7815     167.9026
53586     178.5845     185.7489     199.8287
53587     224.4218     242.5917     273.9307
53588     289.0627     302.5049     352.2003
53589     367.8055     401.6078     433.2989
53590     473.4488     515.6790     574.6821
53591     595.5838     651.9583     756.6867
53592     865.0780     929.1267     956.8638
53593     977.1640     1024.5568    1058.0323
53594    1108.5174     1124.0761    1125.2449
53595    1153.7881     1196.1590    1226.5528
53596    1287.4014     1336.3053    1381.5802
53597    1400.0885     1401.5468    1417.4514
53598    1432.9900     1444.0856    1478.9043
53599    1485.7864     1499.4015    1960.0682
53600    3084.4683     3087.0842    3099.1621
53601    3164.9561     3169.5550    3179.5710
53602    3770.9963     3784.5363    3835.6152
53603 Zero-point correction (Hartree): 0.155337
53604
53605 triHPacyl.tmmmtmmpd
53606 -----
53607 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20334596
53608 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.08635494
53609 T1 diagnostic: 0.015872
53610 E(MP2/Aug-CC-pVTZ) (Hartree): -721.05208687
53611 E(MP3/Aug-CC-pVTZ) (Hartree): -721.06779146
53612 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05437612
53613 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.06903069

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53614 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.52044989
53615 E(UHF/Aug-CC-pVTZ) (Hartree): -718.51671428
53616 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17806134
53617 Electronic state : 2-A
53618 Cartesian coordinates (Angs):
53619 O -2.096784 -1.408162 -1.287512
53620 O -1.349195 -0.256608 -0.937497
53621 C -0.610511 -0.519991 0.242542
53622 C 0.186923 0.768997 0.540666
53623 C 1.073120 1.221739 -0.615997
53624 O 1.993120 0.215438 -0.976722
53625 O 2.961345 0.125162 0.060893
53626 H -1.491789 -1.855856 -1.896238
53627 C -1.503844 -0.916770 1.409141
53628 H -2.038136 -1.835656 1.184685
53629 H -2.218804 -0.116921 1.591814
53630 H -0.896556 -1.061576 2.300831
53631 C 0.372639 -1.678997 -0.011237
53632 O 1.184655 -2.077225 0.739079
53633 H 2.820398 -0.777470 0.383782
53634 H 0.814647 0.550278 1.407320
53635 O -0.659992 1.801532 0.994076
53636 O -1.306918 2.417295 -0.112429
53637 H -1.991921 1.774883 -0.351200
53638 H 0.490142 1.394780 -1.516251
53639 H 1.592217 2.138212 -0.334528
53640 Rotational constants (GHz): 1.0767800 0.8924400 0.6527300
53641 Vibrational harmonic frequencies (cm-1):
53642 53.2076 110.2449 130.0823
53643 142.6752 172.8109 175.3621
53644 183.0644 210.6525 216.2126
53645 244.1876 283.3002 290.3661
53646 308.2307 343.3005 356.6134
53647 383.6416 397.9087 425.4471
53648 478.4949 517.7142 578.3481
53649 604.3103 659.9820 752.2698
53650 874.8335 929.2512 956.8165
53651 975.2632 1021.9796 1058.9558
53652 1107.7297 1123.8579 1128.8768
53653 1152.7457 1190.8215 1212.9366
53654 1287.7723 1330.2673 1380.3628
53655 1404.6028 1411.3825 1421.1123
53656 1443.5941 1446.8579 1482.2935
53657 1485.0940 1497.6160 1961.3345
53658 3085.3527 3098.1553 3099.7782
53659 3164.3933 3175.7451 3178.9592
53660 3763.2549 3765.0784 3780.8685
53661 Zero-point correction (Hartree): 0.155864
53662
53663 triHPacyl.tmmmtppmd
53664 -----
53665 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17482962
53666 Electronic state : 2-A
53667 Cartesian coordinates (Angs):
53668 O -1.617272 -2.181817 -1.043383
53669 O -0.958181 -0.933259 -1.149396
53670 C -0.645501 -0.464256 0.143767
53671 C 0.060026 0.890333 -0.062488
53672 C 1.172707 0.811983 -1.105856
53673 O 2.101327 -0.201004 -0.789867
53674 O 2.911914 0.284165 0.272526
53675 H -0.876383 -2.800966 -1.108393
53676 C -1.870936 -0.370201 1.042257
53677 H -2.259250 -1.361331 1.260570
53678 H -2.638355 0.191912 0.512728
53679 H -1.615420 0.137724 1.969539
53680 C 0.342892 -1.439611 0.818198
53681 O 0.956307 -1.244511 1.801897
53682 H 2.649422 -0.290675 1.007194
53683 H 0.475674 1.202794 0.896964
53684 O -0.823991 1.884459 -0.530234
53685 O -1.349438 2.577337 0.599772

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53686	H	-2.294792	2.556674	0.407880	
53687	H	0.766437	0.534359	-2.076713	
53688	H	1.672208	1.777075	-1.175549	
53689	Rotational constants (GHz):		0.9906700	0.8765200	0.6633600
53690	Vibrational harmonic frequencies (cm-1):				
53691		59.9990	80.7255		115.1999
53692		141.3968	163.3032		173.2486
53693		181.0086	189.4524		202.4584
53694		248.9761	263.1613		278.2109
53695		292.4101	329.1605		349.8269
53696		379.6224	390.5222		402.5336
53697		458.9329	525.3140		577.3328
53698		591.4098	639.7818		732.3922
53699		872.4033	929.6904		958.8238
53700		1019.9739	1022.3009		1061.7419
53701		1110.3317	1117.2036		1137.9098
53702		1146.3801	1195.4908		1225.4746
53703		1289.1321	1331.8237		1389.6465
53704		1399.2224	1405.9908		1416.0932
53705		1420.0728	1447.7085		1479.6011
53706		1484.1965	1506.4802		1958.1802
53707		3083.4996	3098.6317		3101.7910
53708		3161.5529	3164.1577		3176.4209
53709		3761.8740	3784.6049		3832.9240
53710	Zero-point correction (Hartree): 0.155503				
53711					
53712	triHPacyl.tmpmmtpmd				
53713	-----				
53714	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17531859				
53715	Electronic state : 2-A				
53716	Cartesian coordinates (Angs):				
53717	O	2.068794	-0.154628	1.633639	
53718	O	0.794406	-0.154280	1.024157	
53719	C	0.845094	0.539286	-0.210378	
53720	C	-0.597542	0.563048	-0.739627	
53721	C	-1.171428	-0.801148	-1.113834	
53722	O	-1.083821	-1.798964	-0.124803	
53723	O	-1.843808	-1.372431	0.998734	
53724	H	2.462401	-0.960258	1.265287	
53725	C	1.429017	1.939651	-0.074869	
53726	H	2.457830	1.890150	0.269832	
53727	H	0.831765	2.495314	0.643910	
53728	H	1.397302	2.443733	-1.039051	
53729	C	1.707439	-0.240462	-1.230021	
53730	O	2.462496	-1.102163	-0.985145	
53731	H	-1.153870	-0.961268	1.544403	
53732	H	-0.596888	1.159228	-1.659776	
53733	O	-1.316486	1.248839	0.272661	
53734	O	-2.692153	1.252314	-0.049673	
53735	H	-2.991618	0.458241	0.422404	
53736	H	-2.204074	-0.675700	-1.441357	
53737	H	-0.593756	-1.201187	-1.949834	
53738	Rotational constants (GHz):		1.3271700	0.7664800	0.6773000
53739	Vibrational harmonic frequencies (cm-1):				
53740		50.0833	86.6111		107.5058
53741		131.1597	148.8780		192.1240
53742		197.8681	212.4185		238.8236
53743		255.7872	283.2856		329.7868
53744		340.1218	372.8690		404.0985
53745		407.2732	431.4013		471.7647
53746		504.7990	547.9288		564.0391
53747		655.8554	726.9367		801.4396
53748		845.2813	891.8982		942.0908
53749		975.8505	1040.5866		1052.8355
53750		1073.3391	1128.8804		1136.7123
53751		1161.6814	1197.6728		1236.4457
53752		1301.7297	1364.3803		1380.1588
53753		1402.4521	1416.5073		1435.8548
53754		1442.7447	1451.1116		1484.2987
53755		1487.1658	1499.1686		1982.2204
53756		3039.4133	3079.9015		3089.6152
53757		3124.3743	3169.5338		3183.4988

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53758          3730.8918          3738.8228          3761.9333
53759 Zero-point correction (Hartree): 0.156537
53760
53761 triHPacyl.tmpmttmd
53762 -----
53763 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17515102
53764 Electronic state : 2-A
53765 Cartesian coordinates (Angs):
53766 O      1.839661      1.501314      -1.337898
53767 O      0.635721      0.865967      -0.956681
53768 C      0.943874     -0.287567     -0.194524
53769 C     -0.403419     -0.833955      0.313158
53770 C     -1.107469      0.042638      1.346479
53771 O     -1.237917      1.402309      1.004001
53772 O     -2.058369      1.484189     -0.154408
53773 H      1.969216      2.128825     -0.611760
53774 C      1.723964     -1.311852     -1.005841
53775 H      2.655076     -0.876940     -1.359443
53776 H      1.118500     -1.613247     -1.857734
53777 H      1.944891     -2.179504     -0.386928
53778 C      1.786975      0.116282      1.036663
53779 O      2.146123     -0.601718      1.887977
53780 H     -1.387314      1.498267     -0.856417
53781 H     -0.205985     -1.797233      0.797177
53782 O     -1.143600     -1.042237     -0.881869
53783 O     -2.462537     -1.434810     -0.558311
53784 H     -2.914560     -0.575531     -0.561110
53785 H     -2.081709     -0.389428      1.576078
53786 H     -0.514329      0.051413      2.262027
53787 Rotational constants (GHz):      1.2114000      0.7487900      0.7249700
53788 Vibrational harmonic frequencies (cm-1):
53789      56.8504          82.7131          107.3478
53790      117.9229         137.9263         182.8621
53791      201.4303         218.5199         235.9365
53792      244.3626         273.3120         307.7759
53793      326.2272         351.0960         363.5825
53794      401.6327         468.6195         479.4405
53795      508.4207         548.0226         569.1594
53796      621.5300         710.6818         806.0015
53797      847.8460         903.3647         949.3866
53798      972.9758        1040.7353        1047.8468
53799     1069.8858        1123.7612        1128.1422
53800     1162.1392        1191.6491        1227.9634
53801     1302.1555        1362.0193        1377.3587
53802     1399.9413        1413.4639        1424.5854
53803     1435.6396        1447.7098        1485.9082
53804     1489.6367        1499.6768        1989.0110
53805     3046.4721        3085.6114        3089.5993
53806     3134.1708        3167.6865        3177.3807
53807     3730.4907        3739.0218        3774.6785
53808 Zero-point correction (Hartree): 0.156190
53809
53810 triHPacyl.tmtmmmmmpd
53811 -----
53812 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17579209
53813 Electronic state : 2-A
53814 Cartesian coordinates (Angs):
53815 O      2.497117      0.487327      1.392333
53816 O      1.154359      0.190560      1.058883
53817 C      1.008156      0.173854     -0.346042
53818 C     -0.482358     -0.088807     -0.639101
53819 C     -1.106431     -1.072970      0.341666
53820 O     -2.427019     -1.411065     -0.031864
53821 O     -3.284183     -0.346811      0.371573
53822 H      2.887988     -0.397732      1.441222
53823 C      1.509196      1.435821     -1.026617
53824 H      2.583827      1.534257     -0.903151
53825 H      1.009031      2.288943     -0.574480
53826 H      1.266836      1.399259     -2.087168
53827 C      1.797602     -1.035974     -0.928558
53828 O      2.544861     -1.721165     -0.340775
53829 H     -3.452927      0.094881     -0.472033

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53830      H      -0.541395      -0.511471      -1.645291
53831      O      -1.240191      1.096372      -0.771156
53832      O      -1.293907      1.764667      0.479578
53833      H      -2.072848      1.353200      0.887872
53834      H      -0.555213      -2.014840      0.313245
53835      H      -1.090575      -0.697115      1.363119
53836      Rotational constants (GHz):      1.5172100      0.6441700      0.5629900
53837      Vibrational harmonic frequencies (cm-1):
53838          60.3091          69.7285          93.6705
53839          145.6278          166.9028          181.8316
53840          190.8970          227.5936          236.2975
53841          263.2165          294.5280          306.0600
53842          334.3709          354.7506          380.8157
53843          402.6362          414.3154          440.2423
53844          507.8935          539.0978          564.6711
53845          621.5236          685.1252          794.5640
53846          861.0234          893.8442          951.3159
53847          991.1011          1005.8728          1048.1432
53848          1102.9859          1116.2643          1131.0227
53849          1159.6950          1188.4227          1232.1425
53850          1303.0320          1322.4587          1397.4670
53851          1405.5192          1409.9877          1421.3873
53852          1436.1490          1445.7163          1477.2255
53853          1478.5409          1498.6966          1974.4884
53854          3085.1447          3089.1096          3089.6152
53855          3148.1199          3169.6779          3183.3117
53856          3736.5601          3768.4090          3799.0772
53857      Zero-point correction (Hartree): 0.156278
53858
53859      triHPacyl.tmtmmtmmpd
53860      -----
53861      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17551484
53862      Electronic state : 2-A
53863      Cartesian coordinates (Angs):
53864      O      -2.455800      -1.049022      1.400817
53865      O      -1.111336      -0.737302      1.082729
53866      C      -1.088222      -0.042272      -0.145965
53867      C      0.381712      0.333968      -0.430547
53868      C      1.138454      0.723758      0.832458
53869      O      2.436731      1.196433      0.535352
53870      O      3.271287      0.067183      0.293673
53871      H      -2.719041      -0.280566      1.927027
53872      C      -1.717249      -0.820907      -1.288006
53873      H      -2.777937      -0.969160      -1.106266
53874      H      -1.220592      -1.786302      -1.356916
53875      H      -1.579438      -0.276199      -2.220270
53876      C      -1.873757      1.290445      0.031365
53877      O      -1.936840      2.163878      -0.743483
53878      H      3.343541      0.084312      -0.670607
53879      H      0.369856      1.185952      -1.114873
53880      O      1.064924      -0.643000      -1.189532
53881      O      1.191999      -1.831403      -0.424855
53882      H      2.023226      -1.670405      0.049993
53883      H      0.634275      1.564893      1.312589
53884      H      1.192748      -0.096614      1.545883
53885      Rotational constants (GHz):      1.3662900      0.6584300      0.5875100
53886      Vibrational harmonic frequencies (cm-1):
53887          56.6115          85.9587          90.9171
53888          116.3946          160.3059          171.2033
53889          192.1805          201.7455          226.1778
53890          253.7856          262.0728          279.6845
53891          304.9778          323.6905          376.9029
53892          381.7142          411.4637          485.9012
53893          494.2833          529.2076          561.8161
53894          621.1841          648.3987          798.2132
53895          860.0088          897.9230          954.1767
53896          991.1351          1006.7620          1043.5715
53897          1102.6072          1112.7813          1126.5333
53898          1162.0644          1186.8019          1221.5165
53899          1303.6834          1323.7942          1399.3050
53900          1403.6610          1409.7408          1418.9314
53901          1420.5123          1444.9110          1477.2273

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53902      1477.8449      1497.8578      1989.9852
53903      3086.7035      3087.1123      3092.5751
53904      3146.4818      3168.7175      3180.5621
53905      3743.7234      3781.5992      3796.4241
53906 Zero-point correction (Hartree): 0.155717
53907
53908 triHPacyl.tmtmmttmd
53909 -----
53910 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17311731
53911 Electronic state : 2-A
53912 Cartesian coordinates (Angs):
53913 O      -2.717711      0.034591      -1.629654
53914 O      -1.333048      0.010029      -1.334398
53915 C      -1.160310      0.158745      0.058926
53916 C      0.357678      0.117496      0.300885
53917 C      1.005577      -1.067323      -0.405948
53918 O      2.323927      -1.322738      0.047915
53919 O      3.191344      -0.365718      -0.548117
53920 H      -2.946877      -0.904590      -1.584677
53921 C      -1.808676      1.414311      0.617423
53922 H      -2.890584      1.352147      0.540185
53923 H      -1.450417      2.268802      0.049256
53924 H      -1.525242      1.531206      1.662058
53925 C      -1.789414      -1.067619      0.777059
53926 O      -1.696119      -1.329026      1.912860
53927 H      3.721083      -0.913372      -1.139382
53928 H      0.514764      0.036050      1.378469
53929 O      0.888585      1.352819      -0.139368
53930 O      1.940120      1.732888      0.732543
53931 H      2.704368      1.299895      0.320563
53932 H      0.465893      -1.986452      -0.165167
53933 H      1.001101      -0.920094      -1.485627
53934 Rotational constants (GHz):      1.3503700      0.6056600      0.5785700
53935 Vibrational harmonic frequencies (cm-1):
53936      39.9999      57.2050      86.6536
53937      101.3042      112.6739      142.9665
53938      157.8136      185.1281      208.3207
53939      225.1467      256.0118      272.2913
53940      290.2637      309.3994      345.0488
53941      373.9144      408.2094      441.5775
53942      488.8133      512.5437      537.5658
53943      583.5357      633.9472      797.6864
53944      882.2577      902.4501      970.7782
53945      986.4483      1043.8584      1050.2056
53946      1091.9941      1116.8748      1120.8568
53947      1166.9657      1176.9606      1227.8422
53948      1307.9446      1328.7369      1381.3551
53949      1384.3277      1402.3438      1417.2129
53950      1429.1201      1456.2957      1458.9018
53951      1480.2971      1496.1989      1991.3824
53952      3073.1329      3088.1663      3094.1206
53953      3136.4811      3169.8049      3182.8420
53954      3736.2248      3782.2150      3833.4885
53955 Zero-point correction (Hartree): 0.154770
53956
53957 triHPacyl.tmtmptmmpd
53958 -----
53959 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17404843
53960 Electronic state : 2-A
53961 Cartesian coordinates (Angs):
53962 O      2.448063      -1.027641      -1.409805
53963 O      1.097007      -0.780510      -1.050321
53964 C      1.090274      -0.004462      0.127976
53965 C      -0.381236      0.363927      0.410743
53966 C      -1.154382      0.689944      -0.860217
53967 O      -2.456110      1.158915      -0.571258
53968 O      -3.272475      0.030821      -0.267376
53969 H      2.522143      -1.974965      -1.237539
53970 C      1.743024      -0.699719      1.310423
53971 H      2.808670      -0.825755      1.135728
53972 H      1.268734      -1.669182      1.452323
53973 H      1.601945      -0.100804      2.208095

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53974	C	1.837973	1.332393	-0.140717	
53975	O	1.976335	2.196380	0.636945	
53976	H	-3.347320	0.101582	0.694137	
53977	H	-0.374308	1.244200	1.058566	
53978	O	-1.042615	-0.589889	1.219406	
53979	O	-1.176637	-1.807776	0.503111	
53980	H	-2.014332	-1.664629	0.033140	
53981	H	-0.663465	1.514418	-1.380770	
53982	H	-1.204528	-0.159766	-1.538555	
53983	Rotational constants (GHz):			1.3684400	0.6581800 0.5865200
53984	Vibrational harmonic frequencies (cm-1):				
53985		47.3090	76.3638		88.1084
53986		114.2929	157.7713		182.2884
53987		194.1104	217.6735		233.7077
53988		250.8417	266.5279		280.8742
53989		314.5555	316.6582		364.1705
53990		394.7622	410.2203		482.1287
53991		494.5970	544.0443		565.4252
53992		625.5221	654.5601		800.3152
53993		864.9444	898.4728		952.5779
53994		988.6360	1006.1794		1044.3405
53995		1102.3102	1111.7836		1125.4187
53996		1162.5870	1184.9875		1221.1316
53997		1302.8813	1322.4624		1395.9909
53998		1398.7492	1409.6182		1413.5035
53999		1421.6911	1447.8395		1476.8740
54000		1482.4739	1500.2190		1982.0402
54001		3082.8757	3089.4410		3092.0749
54002		3147.4843	3165.3397		3170.9706
54003		3738.2134	3800.4858		3816.3516
54004	Zero-point correction (Hartree): 0.155822				
54005	triHPacyl.tmtpttpmd				
54006	-----				
54007	-----				
54008	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17489898				
54009	Electronic state : 2-A				
54010	Cartesian coordinates (Angs):				
54011	O	-2.934429	-0.493226	1.209777	
54012	O	-1.522334	-0.535342	1.116739	
54013	C	-1.140270	-0.085047	-0.165084	
54014	C	0.393078	-0.129502	-0.194461	
54015	C	1.012802	0.540827	1.025115	
54016	O	2.421094	0.427797	1.030093	
54017	O	2.927257	1.170348	-0.068707	
54018	H	-3.080635	0.379054	1.602408	
54019	C	-1.775812	-0.881933	-1.293603	
54020	H	-2.850815	-0.726037	-1.307976	
54021	H	-1.564126	-1.936538	-1.136767	
54022	H	-1.351691	-0.564052	-2.244368	
54023	C	-1.563291	1.402458	-0.327934	
54024	O	-1.292932	2.101813	-1.224485	
54025	H	2.988463	0.490651	-0.757244	
54026	H	0.703601	0.374202	-1.112590	
54027	O	0.767048	-1.495303	-0.277170	
54028	O	2.079826	-1.558664	-0.822949	
54029	H	2.613378	-1.659054	-0.021537	
54030	H	0.719213	1.593577	1.074421	
54031	H	0.699321	0.027989	1.933061	
54032	Rotational constants (GHz):			1.3498500	0.6352700 0.5784900
54033	Vibrational harmonic frequencies (cm-1):				
54034		54.8519	74.9089		97.0987
54035		126.1936	138.3064		161.6981
54036		182.8755	203.1697		208.9094
54037		250.6519	260.2454		273.5873
54038		318.5715	346.7762		365.2841
54039		391.1435	410.8884		464.3629
54040		485.9781	498.8120		552.8882
54041		582.4464	640.0984		808.0282
54042		885.8772	905.6824		961.2349
54043		995.0009	1036.3439		1049.6849
54044		1088.2532	1111.4413		1146.7994
54045		1169.4003	1182.3002		1235.1176

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54046      1302.6751      1343.9112      1388.1850
54047      1403.1865      1418.1796      1419.5251
54048      1428.1264      1436.9447      1471.6528
54049      1480.0717      1498.0678      1992.7480
54050      3058.4391      3087.9791      3090.7852
54051      3147.6479      3170.6500      3182.5271
54052      3752.0651      3784.2978      3785.3714
54053 Zero-point correction (Hartree): 0.155617
54054
54055 triHPacyl.tpmmmmmpd
54056 -----
54057 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17586875
54058 Electronic state : 2-A
54059 Cartesian coordinates (Angs):
54060 O      1.505408      -2.223934      0.240940
54061 O      0.554524      -1.386113      -0.386040
54062 C      0.582548      -0.086443      0.192972
54063 C     -0.570355      0.637270      -0.545749
54064 C     -1.926321      0.502324      0.139754
54065 O     -2.231674      -0.832393      0.470698
54066 O     -2.330703      -1.570907      -0.739840
54067 H      2.285832      -2.080878      -0.315671
54068 C      0.498651      -0.119709      1.711986
54069 H      1.408745      -0.540460      2.131721
54070 H     -0.344497      -0.741044      2.003723
54071 H      0.358995      0.888821      2.092606
54072 C      1.916377      0.611017      -0.185295
54073 O      2.836214      0.105695      -0.704866
54074 H     -1.477700      -2.031124      -0.748611
54075 H     -0.628479      0.191906      -1.540916
54076 O     -0.286755      1.988359      -0.833566
54077 O     -0.147056      2.702689      0.389173
54078 H      0.813771      2.819461      0.425967
54079 H     -1.930533      1.033876      1.090666
54080 H     -2.691199      0.925513      -0.513477
54081 Rotational constants (GHz):      1.0804500      0.9119900      0.6067500
54082 Vibrational harmonic frequencies (cm-1):
54083      74.3068      94.4135      114.8554
54084      148.0148      161.4026      164.4588
54085      205.8970      216.7626      258.7463
54086      267.8364      305.6215      311.2692
54087      348.4076      361.3023      384.0229
54088      409.3267      433.2905      442.4957
54089      460.3050      520.2624      549.4507
54090      624.9217      685.8678      737.1816
54091      892.8235      909.3315      953.4951
54092      978.7146      1024.6456      1049.2658
54093      1109.2426      1121.0144      1136.3421
54094      1158.2098      1189.3212      1237.9812
54095      1282.8071      1343.7427      1383.8157
54096      1403.1463      1414.0290      1429.3880
54097      1437.4435      1441.2662      1484.4426
54098      1496.2352      1508.9996      1982.3621
54099      3081.1891      3095.7885      3099.1519
54100      3147.2502      3176.2158      3183.9319
54101      3758.5940      3764.2834      3766.8428
54102 Zero-point correction (Hartree): 0.156560
54103
54104 triHPacyl.tpmmmmmpd
54105 -----
54106 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17662246
54107 Electronic state : 2-A
54108 Cartesian coordinates (Angs):
54109 O      0.704593      -2.549262      -0.105218
54110 O      0.095935      -1.348501      -0.536979
54111 C      0.486966      -0.269586      0.296858
54112 C     -0.376898      0.917992      -0.187616
54113 C     -1.803279      0.910524      0.370543
54114 O     -2.429369      -0.344524      0.326247
54115 O     -2.605160      -0.691029      -1.039812
54116 H      1.534463      -2.538850      -0.606417
54117 C      0.347690      -0.556214      1.783467

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54118	H	1.092822	-1.274842	2.113921	
54119	H	-0.643736	-0.961983	1.971981	
54120	H	0.481573	0.373555	2.335079	
54121	C	1.982289	0.039347	0.034009	
54122	O	2.742439	-0.656271	-0.525513	
54123	H	-1.869654	-1.309637	-1.167477	
54124	H	-0.395685	0.911342	-1.277849	
54125	O	0.147882	2.146863	0.265224	
54126	O	1.119174	2.605806	-0.661028	
54127	H	1.945649	2.411935	-0.195159	
54128	H	-1.782823	1.174931	1.428739	
54129	H	-2.387174	1.656504	-0.169756	
54130	Rotational constants (GHz):		1.0638800	0.8998000	0.5996400
54131	Vibrational harmonic frequencies (cm-1):				
54132		65.4864		85.6706	97.3038
54133		152.9601		158.4969	184.0029
54134		204.4083		223.9230	250.1105
54135		268.2723		283.3695	297.7572
54136		316.2780		352.7992	383.2850
54137		405.1493		437.7563	453.0568
54138		470.1919		502.8241	546.8924
54139		597.5979		685.2821	730.2468
54140		886.0795		908.8153	960.0320
54141		1018.9762		1024.9259	1052.8451
54142		1095.6620		1133.1397	1148.3833
54143		1165.5896		1191.7090	1241.8371
54144		1292.1064		1337.9435	1386.8678
54145		1402.9109		1414.1457	1421.7565
54146		1437.8388		1444.4129	1481.1169
54147		1493.5521		1508.5098	1973.7241
54148		3080.8396		3083.1045	3106.1045
54149		3136.4338		3163.3592	3174.9089
54150		3753.4297		3761.5281	3764.4541
54151	Zero-point correction (Hartree):		0.156283		
54152	triHPacyl.tpmmmtmppd				
54153	-----				
54155	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17647267		
54156	Electronic state : 2-A				
54157	Cartesian coordinates (Angs):				
54158	O	0.309889	2.799006	-0.009615	
54159	O	0.602991	1.493720	-0.471235	
54160	C	-0.344343	0.578720	0.064964	
54161	C	0.099550	-0.773903	-0.559351	
54162	C	1.169971	-1.499631	0.254122	
54163	O	2.244902	-0.667094	0.616309	
54164	O	2.888883	-0.239727	-0.576588	
54165	H	-0.235024	3.142792	-0.732068	
54166	C	-0.402157	0.634950	1.584872	
54167	H	-0.800828	1.591881	1.911006	
54168	H	0.605559	0.519475	1.978185	
54169	H	-1.036882	-0.165855	1.955273	
54170	C	-1.738669	0.957549	-0.489619	
54171	O	-2.769212	0.469204	-0.223004	
54172	H	2.545641	0.663082	-0.658377	
54173	H	0.496657	-0.542337	-1.549207	
54174	O	-0.968636	-1.642923	-0.853537	
54175	O	-1.577505	-2.065068	0.362471	
54176	H	-2.407757	-1.566499	0.333967	
54177	H	0.757085	-1.849884	1.199056	
54178	H	1.518949	-2.355709	-0.326189	
54179	Rotational constants (GHz):		1.1318600	0.9084200	0.6046200
54180	Vibrational harmonic frequencies (cm-1):				
54181		78.7257		104.8114	111.9491
54182		148.5422		164.6964	178.4778
54183		201.4729		217.1273	233.2569
54184		251.0230		285.4459	309.3789
54185		318.2601		338.4067	371.6309
54186		408.1663		421.2204	467.9235
54187		471.1337		484.2509	581.7041
54188		595.4167		682.5715	721.6727
54189		883.3446		924.0247	952.9382

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54190          977.5567              1018.5901              1047.2305
54191          1099.4576             1120.4961              1138.7214
54192          1167.6163             1185.8016              1219.1242
54193          1285.0325             1343.5972              1377.1769
54194          1399.3515             1413.8232              1420.7936
54195          1440.7434             1442.1391              1482.1929
54196          1491.8823             1506.9854              1987.7245
54197          3079.6955             3092.4605              3103.3850
54198          3148.9953             3174.7437              3181.4248
54199          3753.7689             3764.7283              3778.5954
54200 Zero-point correction (Hartree): 0.156172
54201
54202 triHPacyl.tpmmtmpmd
54203 -----
54204 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17529099
54205 Electronic state : 2-A
54206 Cartesian coordinates (Angs):
54207 O          0.415170          2.701479          -0.447255
54208 O          0.622342          1.316312          -0.652636
54209 C         -0.288258          0.584957          0.150219
54210 C          0.016482         -0.896343          -0.196049
54211 C          1.242011         -1.451806          0.539217
54212 O          2.351448         -0.593861          0.544456
54213 O          2.797661         -0.455900          -0.796907
54214 H         -0.194155          2.915866          -1.168476
54215 C         -0.181983          0.907813          1.631655
54216 H         -0.538405          1.914483          1.832650
54217 H          0.858630          0.830759          1.939506
54218 H         -0.793946          0.199080          2.188394
54219 C         -1.719073          0.947655          -0.315398
54220 O         -2.729030          0.645156          0.195310
54221 H          2.427489          0.411129          -1.023275
54222 H          0.153086         -0.976000          -1.274190
54223 O         -1.026290         -1.754453          0.208784
54224 O         -1.942142         -1.902508          -0.868245
54225 H         -2.734993         -1.483564          -0.506982
54226 H          0.998304         -1.600298          1.592064
54227 H          1.495649         -2.414906          0.094398
54228 Rotational constants (GHz):      1.1327500          0.8606900          0.5984900
54229 Vibrational harmonic frequencies (cm-1):
54230          58.7091              92.1935              98.9551
54231          139.2177             166.6582             182.7904
54232          198.0907             221.8549             223.8972
54233          269.1106             274.8193             287.5695
54234          313.0822             338.3746             375.7605
54235          383.4279             435.3643             457.8581
54236          485.2751             487.9076             521.2383
54237          627.2542             652.1421             718.5935
54238          885.6255             916.2640             959.5886
54239          1013.7957            1019.9759            1050.5162
54240          1087.7176            1132.8285            1147.0218
54241          1172.4726            1188.4029            1220.6238
54242          1289.4069            1336.4655            1379.1933
54243          1397.7585            1411.2541            1422.4781
54244          1425.2398            1444.7453            1477.9669
54245          1490.0980            1508.0204            1982.0818
54246          3079.7879            3082.8618            3112.8781
54247          3136.2954            3164.6826            3175.3761
54248          3753.5678            3779.2370            3803.1034
54249 Zero-point correction (Hartree): 0.155958
54250
54251 triHPacyl.ttmmtmpmd
54252 -----
54253 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17472892
54254 Electronic state : 2-A
54255 Cartesian coordinates (Angs):
54256 O          2.628505          -1.090987          -0.753812
54257 O          1.611568          -0.125441          -0.942216
54258 C          0.477379          -0.448232          -0.146234
54259 C         -0.605685          0.544973          -0.610390
54260 C         -1.743190          0.780830          0.383401
54261 O         -2.413213          -0.392391          0.784388

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54262	O	-3.014544	-0.951176	-0.381489		
54263	H	3.064267	-0.771227	0.051104		
54264	C	0.032861	-1.894937	-0.318150		
54265	H	0.817471	-2.570300	0.010670		
54266	H	-0.164566	-2.069860	-1.374713		
54267	H	-0.872145	-2.078669	0.252674		
54268	C	0.829125	-0.245727	1.344641		
54269	O	1.912053	-0.178124	1.795104		
54270	H	-3.952579	-0.855245	-0.176852		
54271	H	-1.006650	0.174925	-1.555121		
54272	O	-0.061372	1.802604	-0.959358		
54273	O	0.638557	2.304927	0.171454		
54274	H	1.552936	2.104773	-0.077028		
54275	H	-1.353026	1.202369	1.308901		
54276	H	-2.441068	1.486494	-0.071820		
54277	Rotational constants (GHz):			1.2848900	0.7399300	0.6309200
54278	Vibrational harmonic frequencies (cm-1):					
54279		52.0460	85.7332			112.6579
54280		131.0819	147.6860			168.5872
54281		183.4136	200.3655			214.4435
54282		231.9342	274.0335			285.7044
54283		335.2671	360.1822			370.3056
54284		406.7919	430.4899			441.7262
54285		478.0729	492.5394			573.6653
54286		593.7298	726.2959			737.7638
54287		872.3845	908.5136			950.1525
54288		977.6671	1040.8319			1053.2025
54289		1098.7996	1118.4837			1133.1688
54290		1159.0987	1186.1611			1240.0503
54291		1285.0581	1340.0336			1376.7402
54292		1388.9712	1405.9234			1412.1161
54293		1425.8955	1445.4358			1482.8284
54294		1486.8879	1502.0184			1964.0545
54295		3074.2504	3090.9681			3109.3349
54296		3148.0582	3171.2189			3196.1877
54297		3756.1253	3775.7902			3829.4278
54298	Zero-point correction (Hartree):			0.155919		
54299	triHPacyl.tttmmmpmmd					
54300	-----					
54302	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17419332					
54303	Electronic state : 2-A					
54304	Cartesian coordinates (Angs):					
54305	O	2.580632	-0.769821	-1.150572		
54306	O	1.472467	0.091268	-0.977684		
54307	C	0.534109	-0.472164	-0.064874		
54308	C	-0.589133	0.573041	-0.018740		
54309	C	-1.757364	0.213669	0.898985		
54310	O	-2.547324	-0.845526	0.406952		
54311	O	-3.127450	-0.416898	-0.819578		
54312	H	3.137599	-0.536169	-0.391765		
54313	C	0.075588	-1.858415	-0.483205		
54314	H	0.942800	-2.484472	-0.674218		
54315	H	-0.522254	-1.777223	-1.389948		
54316	H	-0.535517	-2.308425	0.294396		
54317	C	1.174763	-0.549368	1.340112		
54318	O	2.313582	-0.439899	1.597188		
54319	H	-4.059426	-0.347912	-0.578591		
54320	H	-0.961731	0.724426	-1.032726		
54321	O	-0.082154	1.795562	0.485265		
54322	O	0.378658	2.600995	-0.586750		
54323	H	1.227335	2.187359	-0.804966		
54324	H	-1.405944	-0.137938	1.870210		
54325	H	-2.357932	1.114331	1.035373		
54326	Rotational constants (GHz):			1.2510200	0.6904600	0.5949800
54327	Vibrational harmonic frequencies (cm-1):					
54328		18.4013	58.8148			88.1131
54329		124.7106	164.5078			172.0335
54330		184.2790	205.0766			218.9281
54331		224.1525	256.2514			301.9559
54332		310.7341	343.2326			384.4856
54333		398.3489	411.4655			432.3641

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54334      449.4038      506.4052      565.4752
54335      615.3729      642.0859      725.9816
54336      879.9601      907.5853      954.4651
54337      1014.5490     1037.5904     1048.7335
54338      1114.6647     1122.0043     1139.6500
54339      1157.2212     1187.0267     1239.0077
54340      1289.7133     1330.0640     1376.7461
54341      1392.4317     1410.9227     1420.1160
54342      1444.8612     1454.3395     1479.2005
54343      1483.6182     1498.9303     1979.4973
54344      3075.2055     3087.7092     3110.4397
54345      3134.2261     3167.7755     3182.9337
54346      3751.1531     3764.6807     3823.2610
54347 Zero-point correction (Hartree): 0.155514
54348
54349 triHPacyl.ttpmmpmmd
54350 -----
54351 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17496438
54352 Electronic state : 2-A
54353 Cartesian coordinates (Angs):
54354 O      2.932464      -0.389541      -0.198594
54355 O      1.795470      0.413849      -0.448640
54356 C      0.604933     -0.366161     -0.378897
54357 C     -0.504847      0.635476     -0.733328
54358 C     -1.858840     -0.004807     -1.032684
54359 O     -2.252329     -1.042853     -0.168550
54360 O     -2.668390     -0.463438      1.056411
54361 H      2.980614     -0.380239      0.769813
54362 C      0.648167     -1.583900     -1.285046
54363 H      1.534834     -2.174078     -1.072818
54364 H      0.690495     -1.249360     -2.321595
54365 H     -0.238389     -2.194668     -1.132342
54366 C      0.399023     -0.813204      1.090188
54367 O      1.214193     -0.827469      1.932666
54368 H     -1.878391     -0.572917      1.608299
54369 H     -0.190264      1.170482     -1.633140
54370 O     -0.652045      1.579818      0.313978
54371 O      0.220099      2.675509      0.079430
54372 H      1.082686      2.325396      0.346363
54373 H     -2.613588      0.782145     -1.045432
54374 H     -1.814320     -0.478179     -2.014153
54375 Rotational constants (GHz):      1.2248900      0.7713300      0.6707000
54376 Vibrational harmonic frequencies (cm-1):
54377      58.4405      83.9547      111.8432
54378      143.7830     149.7761     168.7285
54379      195.4413     210.6219     233.8390
54380      269.3998     302.4248     311.3915
54381      336.5699     362.9040     378.8936
54382      390.1686     411.1358     431.2171
54383      450.8403     472.5800     580.6931
54384      584.8432     705.1121     780.1905
54385      868.4580     907.0495     933.3961
54386      991.1520     1024.8900     1053.0507
54387      1071.4008     1141.1556     1143.3326
54388      1149.8528     1190.3396     1239.8939
54389      1308.8239     1355.0725     1363.1813
54390      1402.0456     1409.7951     1428.0477
54391      1442.6545     1450.0900     1460.9841
54392      1492.5026     1506.7793     1977.0634
54393      3076.8554     3081.6693     3086.6366
54394      3136.9798     3162.5910     3184.1083
54395      3738.4420     3755.3761     3774.9612
54396 Zero-point correction (Hartree): 0.155903
54397
54398 triHPacyl.ttpmmpmmd
54399 -----
54400 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17671595
54401 Electronic state : 2-A
54402 Cartesian coordinates (Angs):
54403 O      -3.121321     -0.360725     -0.277916
54404 O     -1.828270     -0.757298     -0.689980
54405 C     -0.875720      0.222101     -0.311609

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54406      C      0.446770      -0.322279      -0.866522
54407      C      1.551153      0.715732      -1.005644
54408      O      1.814525      1.464375      0.160971
54409      O      2.420545      0.598007      1.112674
54410      H      -3.177665      -0.754720      0.605237
54411      C      -1.234079      1.609444      -0.821609
54412      H      -2.235887      1.867539      -0.491149
54413      H      -1.216291      1.603300      -1.911255
54414      H      -0.529314      2.347107      -0.444752
54415      C      -0.764841      0.281530      1.236884
54416      O      -1.550440      -0.116215      2.008998
54417      H      1.668348      0.400791      1.693608
54418      H      0.246125      -0.732542      -1.862173
54419      O      0.773843      -1.381510      0.024324
54420      O      2.011548      -1.948984      -0.349687
54421      H      2.624454      -1.444383      0.208635
54422      H      2.463022      0.233344      -1.357214
54423      H      1.254074      1.459201      -1.745013
54424      Rotational constants (GHz):      1.4043800      0.6944600      0.6566200
54425      Vibrational harmonic frequencies (cm-1):
54426          70.4931          93.3145          111.0477
54427          136.3458          164.7018          198.0429
54428          207.0573          227.1894          253.4445
54429          274.3097          295.7002          331.6311
54430          360.3349          378.0153          402.1076
54431          410.5975          438.5090          462.3774
54432          484.0530          536.2437          570.5685
54433          643.1546          694.5456          781.6524
54434          864.0501          908.2232          934.3403
54435          979.6047          1039.2448          1048.2316
54436          1058.7655          1126.3205          1142.7416
54437          1161.2645          1196.6610          1239.8881
54438          1297.5861          1361.5431          1376.7935
54439          1400.0818          1410.5994          1424.2887
54440          1440.3957          1449.2658          1480.1601
54441          1499.2303          1508.3174          1980.8841
54442          3056.9564          3081.4001          3095.9566
54443          3141.5894          3162.5374          3182.7689
54444          3730.6481          3743.0381          3771.3278
54445      Zero-point correction (Hartree): 0.156784
54446
54447      triHPacyl.ttpmttpmd
54448      -----
54449      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17604036
54450      Electronic state : 2-A
54451      Cartesian coordinates (Angs):
54452      O      3.257893      0.388639      0.190623
54453      O      2.038625      0.926947      -0.284419
54454      C      1.036566      -0.075463      -0.227442
54455      C      -0.235247      0.671506      -0.667426
54456      C      -1.306794      -0.189812      -1.318892
54457      O      -1.744703      -1.288402      -0.553106
54458      O      -2.516794      -0.787849      0.532786
54459      H      3.237310      0.646950      1.122709
54460      C      1.395632      -1.278989      -1.085712
54461      H      2.353469      -1.678272      -0.763921
54462      H      1.485163      -0.959232      -2.123889
54463      H      0.632956      -2.049541      -0.997012
54464      C      0.902999      -0.551295      1.242722
54465      O      0.107222      -1.277613      1.702366
54466      H      -1.908972      -0.943158      1.272549
54467      H      0.074893      1.419998      -1.406274
54468      O      -0.675315      1.332357      0.511299
54469      O      -1.847314      2.066375      0.225020
54470      H      -2.531436      1.420368      0.464275
54471      H      -2.154723      0.437131      -1.595117
54472      H      -0.904501      -0.633549      -2.229387
54473      Rotational constants (GHz):      1.4068500      0.7317900      0.6574100
54474      Vibrational harmonic frequencies (cm-1):
54475          78.3687          113.8862          126.8874
54476          148.6345          154.3497          182.8635
54477          203.1641          228.3844          250.1761

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54478	265.3403	287.8741	298.3090			
54479	340.8383	349.9989	380.0904			
54480	398.7724	478.5641	486.5867			
54481	488.7324	523.9890	567.2445			
54482	632.1311	682.3916	778.3213			
54483	864.6413	911.2760	936.5812			
54484	983.0692	1035.7150	1047.3616			
54485	1058.5522	1128.7556	1134.8494			
54486	1169.7395	1195.3175	1233.2820			
54487	1298.5156	1356.4052	1377.6343			
54488	1398.5518	1410.8016	1420.8930			
54489	1432.9995	1450.3347	1478.3589			
54490	1497.9612	1506.8508	1985.6057			
54491	3043.0292	3076.7915	3093.9719			
54492	3139.9172	3158.2991	3179.0009			
54493	3740.0424	3750.0944	3788.9650			
54494	Zero-point correction (Hartree): 0.156579					
54495						
54496						
54497						
54498	CO elimination from (2R,3R)-2-Me-2,3,4-triOOH-1-oxo-butyl (D, R,R-di-HPALD-I)					
54499	=====					
54500						
54501	TS.triHPacyl.COelim.mmpppmmpmd					
54502	-----					
54503	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16086863					
54504	Electronic state : 2-A					
54505	Cartesian coordinates (Angs):					
54506	O	-0.175920	0.349154	1.970846		
54507	O	0.862688	-0.342465	1.235132		
54508	C	1.009741	0.264600	0.009043		
54509	C	-0.087793	0.062349	-1.019523		
54510	C	-0.894826	-1.218101	-0.833577		
54511	O	-1.673529	-1.282261	0.350840		
54512	O	-2.989966	-0.834069	0.072726		
54513	H	-0.917248	-0.261098	1.791984		
54514	C	1.714826	1.582659	0.019040		
54515	H	2.626468	1.508483	0.608453		
54516	H	1.082037	2.354049	0.466422		
54517	H	1.952784	1.900184	-0.995295		
54518	C	2.418516	-1.016263	-0.644488		
54519	O	3.453035	-0.921094	-0.179649		
54520	H	-2.866801	0.132436	0.044081		
54521	H	0.413138	-0.033566	-1.988850		
54522	O	-0.850502	1.247294	-1.236071		
54523	O	-1.681878	1.543426	-0.122531		
54524	H	-1.063236	1.686514	0.614204		
54525	H	-1.554079	-1.372029	-1.686379		
54526	H	-0.187271	-2.046318	-0.767930		
54527	Rotational constants (GHz):			1.4382300	0.6719800	0.6317900
54528	Vibrational harmonic frequencies (cm-1):					
54529	i405.2782		41.6306			84.9068
54530	106.3869		138.8295			152.7652
54531	168.3275		173.1424			210.7980
54532	225.3462		239.4257			255.1508
54533	269.5507		304.3138			321.1331
54534	357.1824		371.8754			478.3625
54535	499.9347		522.2216			577.8620
54536	628.9909		697.1336			715.1250
54537	822.7990		878.0857			906.8291
54538	949.1748		969.6706			1021.5987
54539	1029.3876		1057.8214			1121.2816
54540	1149.3145		1203.7425			1261.6078
54541	1316.3516		1353.1291			1367.3719
54542	1402.3602		1411.3169			1432.9770
54543	1460.3123		1463.2160			1471.9082
54544	1483.6917		1487.8712			2094.6714
54545	3052.6914		3060.3289			3085.2929
54546	3122.0141		3143.4944			3163.1655
54547	3620.1811		3642.5924			3701.6216
54548	Zero-point correction (Hartree): 0.153203					
54549						

```

54550 TS.triHPacyl.COelim.mmpppmpmd
54551 -----
54552 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15987403
54553 Electronic state : 2-A
54554 Cartesian coordinates (Angs):
54555 O -0.502942 1.463516 1.480221
54556 O 0.635394 0.575696 1.457569
54557 C 1.024823 0.412991 0.147031
54558 C 0.150822 -0.444668 -0.749363
54559 C -0.694581 -1.472587 -0.003611
54560 O -1.690429 -0.936743 0.852229
54561 O -2.920494 -0.862136 0.150596
54562 H -1.212016 0.798481 1.566876
54563 C 1.724907 1.577002 -0.476863
54564 H 2.503803 1.938795 0.191889
54565 H 1.027850 2.399764 -0.657830
54566 H 2.157948 1.295042 -1.435696
54567 C 2.602106 -0.833749 0.532590
54568 O 2.958504 -1.483414 -0.333097
54569 H -2.784856 -0.068555 -0.398690
54570 H 0.822384 -1.012605 -1.403162
54571 O -0.544925 0.333123 -1.723404
54572 O -1.567731 1.122216 -1.131746
54573 H -1.098480 1.709058 -0.514022
54574 H -1.175321 -2.145772 -0.711657
54575 H -0.028796 -2.046216 0.644647
54576 Rotational constants (GHz): 1.3029200 0.7123700 0.6711500
54577 Vibrational harmonic frequencies (cm-1):
54578 i403.8184 23.5388 83.8138
54579 104.8163 130.1717 148.5530
54580 170.8791 185.2697 213.3369
54581 216.8206 244.3276 245.6307
54582 263.8030 306.3972 338.6786
54583 343.3412 370.7776 475.8785
54584 499.2854 521.3738 570.9549
54585 620.3817 692.9464 711.2367
54586 822.1908 903.5965 920.0237
54587 949.3231 968.0000 1020.7363
54588 1029.9030 1053.5439 1119.5153
54589 1149.6237 1205.6959 1259.8243
54590 1321.7884 1355.1352 1374.4672
54591 1404.4859 1411.6395 1437.8494
54592 1460.8506 1461.1317 1473.7370
54593 1478.4105 1489.5598 2085.3785
54594 3052.1382 3054.5253 3079.1621
54595 3120.4165 3141.2496 3159.7993
54596 3613.7762 3643.2154 3699.6367
54597 Zero-point correction (Hartree): 0.153099
54598
54599 TS.triHPacyl.COelim.mmtmpmmrmd
54600 -----
54601 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16135982
54602 Electronic state : 2-A
54603 Cartesian coordinates (Angs):
54604 O -1.245317 1.919491 -1.155839
54605 O -1.160657 0.485562 -1.073727
54606 C -1.059227 0.082226 0.235232
54607 C 0.328822 -0.329219 0.664610
54608 C 1.065221 -1.107242 -0.416785
54609 O 2.378700 -1.457177 -0.020354
54610 O 3.228701 -0.338570 -0.260130
54611 H -0.325398 2.165693 -0.954795
54612 C -1.901485 0.800851 1.238903
54613 H -2.893855 0.980952 0.831114
54614 H -1.450460 1.757670 1.502945
54615 H -1.979869 0.201002 2.145880
54616 C -2.017321 -1.695523 0.134039
54617 O -3.060669 -1.661457 -0.322594
54618 H 3.810785 -0.687457 -0.946186
54619 H 0.247685 -0.948795 1.561031
54620 O 1.077089 0.786822 1.139427
54621 O 1.315943 1.676445 0.056667

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54622	H	2.180720	1.358215	-0.250379	
54623	H	0.554940	-2.058333	-0.572640	
54624	H	1.089051	-0.564433	-1.360562	
54625	Rotational constants (GHz):			1.3436400	0.6648000 0.5441500
54626	Vibrational harmonic frequencies (cm-1):				
54627	i375.3708		40.9033		67.7273
54628	83.5016		106.1716		143.6327
54629	166.7024		187.0561		203.7996
54630	225.9144		230.9476		251.9149
54631	267.8833		279.3867		312.9005
54632	321.1750		330.7666		438.6314
54633	492.3972		510.0728		557.5670
54634	581.9053		602.3967		687.1066
54635	835.4068		887.3782		928.6811
54636	952.1602		989.9905		1003.4941
54637	1047.5246		1097.6813		1110.7958
54638	1136.5285		1207.7690		1267.6359
54639	1308.0368		1331.7875		1365.2821
54640	1390.2236		1408.8826		1426.5249
54641	1442.2412		1450.8912		1472.1543
54642	1475.1031		1486.5653		2086.3247
54643	3066.9946		3089.7927		3094.1255
54644	3133.1213		3146.7752		3161.4419
54645	3697.0475		3710.2594		3825.5669
54646	Zero-point correction (Hartree):				0.152921
54647	TS.triHPacyl.COelim.mmtmpmmmpd				
54648	-----				
54649	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16270065				
54650	Electronic state : 2-A				
54651	Cartesian coordinates (Angs):				
54652	O	-1.325422	1.926870	-1.111354	
54653	O	-1.194792	0.496810	-1.053702	
54654	C	-1.042347	0.074872	0.244080	
54655	C	0.360912	-0.343580	0.608321	
54656	C	1.068475	-1.089143	-0.513096	
54657	O	2.375340	-1.489848	-0.151087	
54658	O	3.235682	-0.357952	-0.266507	
54659	H	-0.406532	2.198610	-0.944228	
54660	C	-1.840773	0.779004	1.293142	
54661	H	-2.850861	0.960521	0.932357	
54662	H	-1.382581	1.734517	1.549423	
54663	H	-1.877218	0.166724	2.194467	
54664	C	-1.997613	-1.698512	0.164314	
54665	O	-3.052272	-1.667091	-0.265627	
54666	H	3.420029	-0.165126	0.662801	
54667	H	0.315666	-0.982505	1.493845	
54668	O	1.129545	0.769231	1.077515	
54669	O	1.301901	1.690432	0.008416	
54670	H	2.095564	1.334172	-0.426677	
54671	H	0.537441	-2.021010	-0.708781	
54672	H	1.096711	-0.509358	-1.435006	
54673	Rotational constants (GHz):			1.3449400	0.6688400 0.5446200
54674	Vibrational harmonic frequencies (cm-1):				
54675	i378.0998		40.3300		64.8405
54676	86.7174		103.8570		132.9695
54677	166.5623		198.4923		204.7509
54678	208.6557		232.2033		257.3999
54679	282.2631		305.8529		319.9922
54680	328.9512		396.7564		442.0995
54681	481.1700		515.8997		558.8110
54682	604.2422		623.9904		686.9317
54683	840.8970		885.9549		935.0452
54684	949.5196		991.2537		1001.5921
54685	1047.5651		1100.3704		1110.1236
54686	1130.7939		1207.2266		1269.5401
54687	1302.5994		1330.6507		1363.9628
54688	1403.6745		1409.4847		1422.9061
54689	1437.9288		1443.8466		1472.5110
54690	1480.0307		1486.9093		2086.6427
54691	3067.5470		3088.2716		3095.6237
54692	3133.2040		3145.4875		3162.9791

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54694          3670.8261          3696.6542          3802.7241
54695 Zero-point correction (Hartree): 0.153134
54696
54697 TS.triHPacyl.COelim.mmtmptmmpd
54698 -----
54699 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16166371
54700 Electronic state : 2-A
54701 Cartesian coordinates (Angs):
54702 O      1.338424      -2.204776      -0.915783
54703 O      1.190573      -0.798682      -1.150965
54704 C      1.162531      -0.113158      0.038026
54705 C     -0.206870      0.380045      0.445462
54706 C     -1.040388      0.861185      -0.733621
54707 O     -2.311663      1.334970      -0.335626
54708 O     -3.156481      0.207756      -0.112333
54709 H      0.445849      -2.434723      -0.606618
54710 C      2.074025      -0.579820      1.125498
54711 H      3.052676      -0.819329      0.714794
54712 H      1.673622      -1.471775      1.608317
54713 H      2.171033      0.200726      1.879885
54714 C      2.069044      1.645251      -0.492236
54715 O      1.926358      2.503623      0.247031
54716 H     -3.248933      0.228713      0.849867
54717 H     -0.094843      1.192104      1.168560
54718 O     -0.901238      -0.606472      1.219104
54719 O     -1.165559      -1.735563      0.397192
54720 H     -2.008374      -1.479693      -0.015376
54721 H     -0.556160      1.724994      -1.190639
54722 H     -1.148216      0.091128      -1.496510
54723 Rotational constants (GHz):      1.1546000      0.7655100      0.5672500
54724 Vibrational harmonic frequencies (cm-1):
54725      1375.0238      37.1731      67.3878
54726      90.3396      112.6533      135.3617
54727      165.1483      193.2819      206.1331
54728      222.1481      235.2027      266.4020
54729      290.7423      297.1661      321.0156
54730      357.5763      386.8576      439.1631
54731      477.6387      510.1158      551.9991
54732      605.7029      617.7350      679.3080
54733      839.8270      884.5605      947.5261
54734      966.7182      990.6828      1002.3208
54735      1043.4655      1098.8995      1109.8906
54736      1131.1065      1209.4933      1267.3080
54737      1304.6519      1332.8147      1371.8825
54738      1402.8570      1409.4540      1424.0626
54739      1439.7861      1445.3199      1472.4967
54740      1480.4666      1487.8464      2068.0917
54741      3066.9511      3088.8728      3095.3679
54742      3132.3758      3144.8472      3160.5739
54743      3701.9571      3720.2375      3802.8375
54744 Zero-point correction (Hartree): 0.153348
54745
54746 TS.triHPacyl.COelim.mmtppmmmd
54747 -----
54748 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16171993
54749 Electronic state : 2-A
54750 Cartesian coordinates (Angs):
54751 O      -1.561332      1.975724      -0.813989
54752 O      -1.340102      0.559807      -0.940074
54753 C      -1.028427      0.016308      0.281039
54754 C      0.435613      -0.267115      0.500702
54755 C      1.120875      -0.893964      -0.716361
54756 O      2.498069      -0.575066      -0.747951
54757 O      3.106011      -1.141580      0.403302
54758 H     -0.644556      2.296947      -0.778247
54759 C     -1.821353      0.488681      1.457075
54760 H     -2.867205      0.600128      1.179149
54761 H     -1.448457      1.451310      1.808166
54762 H     -1.733839      -0.230020      2.272123
54763 C     -1.764653      -1.845811      0.037431
54764 O     -2.836514      -1.901108      -0.344039
54765 H      3.057185      -0.406950      1.032646

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54766	H	0.528585	-0.922468	1.369031	
54767	O	1.146806	0.900082	0.930701	
54768	O	1.208226	1.827847	-0.144512	
54769	H	1.983101	1.508816	-0.634630	
54770	H	0.976474	-1.974361	-0.712316	
54771	H	0.727071	-0.477647	-1.642734	
54772	Rotational constants (GHz):		1.2890200	0.6864300	0.5501700
54773	Vibrational harmonic frequencies (cm-1):				
54774	i382.6450		42.8439		65.2359
54775	75.5272		105.8158		137.3686
54776	149.6387		189.8509		211.9208
54777	217.9149		233.6949		256.6145
54778	279.7927		314.0718		338.0404
54779	349.2749		408.5663		440.2634
54780	468.1242		492.1129		553.4208
54781	570.5053		620.0079		743.4288
54782	805.7440		898.8203		928.3887
54783	959.8437		983.0297		1011.0166
54784	1047.1982		1081.3408		1099.3039
54785	1147.9062		1214.8123		1273.9195
54786	1294.3556		1341.6253		1366.4395
54787	1403.5193		1411.3043		1422.3121
54788	1428.0066		1436.6092		1474.9056
54789	1487.5432		1493.6458		2088.0551
54790	3065.9747		3091.8552		3096.4235
54791	3131.7572		3150.2136		3161.6806
54792	3714.7825		3734.5032		3770.6122
54793	Zero-point correction (Hartree): 0.153278				
54794					
54795	TS.triHPacyl.COelim.mmtpptmmd				
54796	-----				
54797	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16089500				
54798	Electronic state : 2-A				
54799	Cartesian coordinates (Angs):				
54800	O	1.751255	-2.067147	-0.640972	
54801	O	1.417736	-0.728581	-1.034751	
54802	C	1.160618	0.034774	0.077200	
54803	C	-0.301744	0.258318	0.377286	
54804	C	-1.134125	0.569538	-0.869491	
54805	O	-2.478529	0.167202	-0.701376	
54806	O	-3.033158	0.924086	0.364105	
54807	H	0.867941	-2.431122	-0.462486	
54808	C	2.086710	-0.119919	1.238939	
54809	H	3.113862	-0.201199	0.889173	
54810	H	1.843545	-1.020498	1.804083	
54811	H	1.990844	0.738364	1.903453	
54812	C	1.673685	1.896416	-0.611923	
54813	O	1.439445	2.752868	0.104973	
54814	H	-2.879318	0.340209	1.121418	
54815	H	-0.386505	1.066205	1.107339	
54816	O	-0.873016	-0.843552	1.097145	
54817	O	-0.949619	-1.972490	0.237648	
54818	H	-1.789879	-1.813483	-0.221556	
54819	H	-1.081532	1.633873	-1.103062	
54820	H	-0.782723	-0.006195	-1.724605	
54821	Rotational constants (GHz):		1.1208800	0.7910100	0.5708900
54822	Vibrational harmonic frequencies (cm-1):				
54823	i377.8301		39.0425		58.7448
54824	80.3176		117.2975		134.1737
54825	146.8305		175.5216		200.9801
54826	218.9693		226.9612		255.5237
54827	283.2473		312.5783		347.6810
54828	354.5063		420.5027		441.4141
54829	463.7126		494.8408		558.3460
54830	571.6867		603.2480		741.1812
54831	804.2552		898.5302		956.3035
54832	964.8655		983.2292		1004.5774
54833	1042.9295		1077.4984		1098.4311
54834	1149.8007		1214.4201		1270.2419
54835	1298.1574		1345.1984		1377.3883
54836	1403.7923		1410.5965		1423.1060
54837	1429.4880		1442.4880		1473.7877

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54838      1487.1910          1492.4730          2071.7958
54839      3066.1701          3086.6171          3096.5585
54840      3131.8858          3149.4210          3160.5891
54841      3710.5954          3736.8522          3770.1824
54842      Zero-point correction (Hartree): 0.153268
54843
54844      TS.triHPacyl.COelim.pmpmmmpmd
54845      -----
54846      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16092404
54847      Electronic state : 2-A
54848      Cartesian coordinates (Angs):
54849      O      0.595352      -1.465908      1.255207
54850      O      0.843925      -0.066285      1.307419
54851      C      0.954134      0.475845      0.056032
54852      C     -0.231060      0.481417     -0.884229
54853      C     -0.998624     -0.813701     -1.125784
54854      O     -1.717696     -1.332245     -0.018755
54855      O     -3.024688     -0.792183      0.001463
54856      H     -0.378393     -1.506922      1.212874
54857      C      1.713971      1.763610      0.151662
54858      H      2.653939      1.597295      0.673866
54859      H      1.148997      2.528487      0.692195
54860      H      1.915522      2.152068     -0.845765
54861      C      2.297372     -0.750041     -0.927630
54862      O      3.276017     -0.895008     -0.364212
54863      H     -2.881786      0.053127      0.458825
54864      H      0.179036      0.757454     -1.860896
54865      O     -1.080103      1.602172     -0.603710
54866      O     -1.657260      1.450618      0.684873
54867      H     -0.953514      1.715938      1.293783
54868      H     -1.702515     -0.662538     -1.942926
54869      H     -0.280430     -1.586987     -1.400555
54870      Rotational constants (GHz):      1.4139700      0.7124400      0.6074800
54871      Vibrational harmonic frequencies (cm-1):
54872      i324.5551          45.8113          71.9229
54873      96.9545          108.1866          148.6446
54874      167.1485          180.5247          194.3316
54875      223.8441          233.3637          256.8361
54876      262.0186          275.6696          288.8095
54877      330.8379          359.0992          425.6516
54878      487.6864          530.4321          577.6146
54879      602.4179          618.0984          725.6317
54880      832.3028          918.9813          946.5815
54881      951.9876          1014.6310          1037.3108
54882      1051.5822          1060.1279          1108.2833
54883      1146.3962          1199.2285          1295.8988
54884      1322.5265          1352.9582          1381.7454
54885      1399.3916          1410.9589          1420.5489
54886      1461.6280          1464.0864          1473.6941
54887      1481.9144          1487.7764          2094.5948
54888      3045.3046          3068.0108          3091.1722
54889      3118.2069          3146.7207          3161.3005
54890      3624.6936          3704.5517          3783.7205
54891      Zero-point correction (Hartree): 0.153253
54892
54893      TS.triHPacyl.COelim.pmpmtmpmd
54894      -----
54895      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16014788
54896      Electronic state : 2-A
54897      Cartesian coordinates (Angs):
54898      O      0.485291      -1.118235      1.759106
54899      O      0.695952      0.270610      1.538691
54900      C      1.006574      0.526448      0.234399
54901      C     -0.008901      0.267210     -0.860933
54902      C     -0.787658     -1.044279     -0.870276
54903      O     -1.663286     -1.259683      0.223960
54904      O     -2.945973     -0.745264     -0.075714
54905      H     -0.478826     -1.198618      1.642631
54906      C      1.733569      1.833400      0.149113
54907      H      2.593955      1.813668      0.814252
54908      H      1.097898      2.676794      0.434132
54909      H      2.066663      2.009150     -0.872841

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54910	C	2.548834	-0.821940	-0.202286	
54911	O	2.466827	-1.364236	-1.202696	
54912	H	-2.839239	0.193698	0.150296	
54913	H	0.553224	0.274981	-1.800677	
54914	O	-0.846935	1.420098	-1.030616	
54915	O	-1.626671	1.619362	0.138425	
54916	H	-1.021239	2.052628	0.756441	
54917	H	-1.372768	-1.099208	-1.787299	
54918	H	-0.075826	-1.869350	-0.846284	
54919	Rotational constants (GHz):		1.2330500	0.7612700	0.6706800
54920	Vibrational harmonic frequencies (cm-1):				
54921		i327.2187	48.5333		53.3586
54922		107.9542	113.1549		147.4176
54923		169.3473	189.1156		208.4787
54924		234.4560	237.8193		252.1780
54925		256.9276	269.5366		305.3518
54926		333.1357	389.4346		415.1597
54927		480.1279	524.8514		581.2449
54928		601.9094	617.9708		712.6420
54929		826.7698	918.6337		946.3569
54930		951.7134	1015.3434		1039.3619
54931		1049.1600	1057.7911		1108.1654
54932		1146.4012	1202.8579		1297.0098
54933		1330.2113	1354.9544		1377.5411
54934		1397.8914	1412.3699		1422.1552
54935		1459.6601	1462.8535		1469.8102
54936		1477.7326	1489.4453		2074.9131
54937		3045.3388	3065.8556		3095.0808
54938		3119.5722	3149.6927		3163.3547
54939		3651.6162	3707.5156		3782.7673
54940	Zero-point correction (Hartree): 0.153366				
54941	TS.triHPacyl.COelim.pmpmttprm				
54942	-----				
54943	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16177923				
54944	Electronic state : 2-A				
54945	Cartesian coordinates (Angs):				
54946	O	-1.117270	-1.865829	-0.761800	
54947	O	-1.009317	-0.608480	-1.424665	
54948	C	-0.997730	0.424014	-0.529901	
54949	C	0.173627	0.594972	0.414331	
54950	C	0.767179	-0.650051	1.058182	
54951	O	1.386248	-1.534418	0.133138	
54952	O	2.635137	-0.992728	-0.273249	
54953	H	-0.199709	-2.180048	-0.799138	
54954	C	-1.489742	1.667896	-1.198387	
54955	H	-2.484086	1.493039	-1.603389	
54956	H	-0.820665	1.961239	-2.008955	
54957	H	-1.526055	2.486148	-0.480453	
54958	C	-2.572634	-0.031347	0.770787	
54959	O	-2.322659	-0.046032	1.883775	
54960	H	2.389318	-0.512859	-1.078209	
54961	H	-0.154270	1.257485	1.222163	
54962	O	1.161114	1.289371	-0.357072	
54963	O	2.169835	1.762759	0.524363	
54964	H	2.803389	1.028119	0.515995	
54965	H	1.499315	-0.365314	1.813216	
54966	H	-0.016149	-1.237857	1.532774	
54967	Rotational constants (GHz):		1.1939100	0.7459000	0.6560600
54968	Vibrational harmonic frequencies (cm-1):				
54969		i336.7000	58.0830		69.7127
54970		96.2455	119.4677		167.1847
54971		176.2901	184.2577		218.0742
54972		224.6181	242.9856		251.9907
54973		258.9585	305.1853		317.9830
54974		348.8889	425.4873		438.6081
54975		473.5542	528.1014		535.6347
54976		558.7699	570.7343		722.2306
54977		836.6429	879.8203		948.0687
54978		971.3889	1017.5475		1027.3845
54979		1044.8987	1064.1674		1100.8736
54980		1139.5887	1205.0206		1288.9876


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54982      1314.8717      1351.8797      1395.2013
54983      1409.3391      1412.6878      1426.9989
54984      1443.1453      1446.9796      1472.8234
54985      1479.4118      1491.1535      2074.6911
54986      3055.2669      3064.9233      3101.3968
54987      3132.9292      3159.4249      3161.4674
54988      3733.4011      3744.1992      3770.9724
54989      Zero-point correction (Hartree): 0.153687
54990
54991      TS.triHPacyl.COelim.pmpppmpmmd
54992      -----
54993      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16192837
54994      Electronic state : 2-A
54995      Cartesian coordinates (Angs):
54996      O      0.091789      -0.333441      1.750566
54997      O      0.959207      0.606062      1.134353
54998      C      0.891496      0.544796      -0.237006
54999      C      -0.495106      0.626804      -0.872752
55000      C      -1.089374      -0.685387      -1.377290
55001      O      -1.081544      -1.732274      -0.439312
55002      O      -2.150737      -1.523984      0.469333
55003      H      0.630269      -1.140664      1.738320
55004      C      1.955600      1.433080      -0.799033
55005      H      2.915509      1.231979      -0.326491
55006      H      1.691335      2.482170      -0.642897
55007      H      2.044711      1.255194      -1.869712
55008      C      1.724577      -1.322149      -0.661034
55009      O      2.137894      -1.818771      0.282112
55010      H      -1.770927      -0.869315      1.077660
55011      H      -0.403759      1.285443      -1.744167
55012      O      -1.436982      1.199078      0.016069
55013      O      -1.005218      2.519150      0.313610
55014      H      -0.564132      2.393605      1.166007
55015      H      -2.107068      -0.505665      -1.726389
55016      H      -0.474357      -1.042172      -2.203478
55017      Rotational constants (GHz):      1.0342700      0.9838700      0.7093800
55018      Vibrational harmonic frequencies (cm-1):
55019      i327.3724      70.3732      93.3140
55020      114.4886      146.0912      151.2511
55021      180.9422      203.1501      217.8063
55022      235.4192      250.1553      252.5139
55023      264.4715      280.4623      304.5885
55024      359.5598      370.1169      395.7368
55025      434.5444      474.6293      501.2261
55026      526.6195      634.7997      682.3050
55027      830.1724      880.6912      949.8011
55028      986.6337      1033.2685      1045.1133
55029      1056.3841      1065.7439      1144.6464
55030      1167.1376      1198.3555      1284.5825
55031      1320.4726      1339.6074      1387.6831
55032      1404.9073      1414.0201      1422.7107
55033      1428.6411      1458.4856      1460.1521
55034      1478.5118      1489.4070      2057.8180
55035      3033.7794      3052.6058      3084.4543
55036      3127.7452      3139.9473      3157.1980
55037      3732.7976      3755.2595      3782.9578
55038      Zero-point correction (Hartree): 0.153358
55039
55040      TS.triHPacyl.COelim.pmppptppmd
55041      -----
55042      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16266389
55043      Electronic state : 2-A
55044      Cartesian coordinates (Angs):
55045      O      -0.379625      0.007290      1.892499
55046      O      0.508504      0.957061      1.325764
55047      C      0.861702      0.593982      0.049432
55048      C      -0.283824      0.380946      -0.943671
55049      C      -0.668203      -1.061594      -1.265563
55050      O      -0.899331      -1.877830      -0.144254
55051      O      -2.183809      -1.571201      0.374088
55052      H      0.183098      -0.786940      1.932179
55053      C      2.006704      1.441990      -0.403912

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55054	H	2.789478	1.470668	0.351596	
55055	H	1.662038	2.460213	-0.602802	
55056	H	2.418946	1.033953	-1.326439	
55057	C	1.822658	-1.200980	0.428606	
55058	O	2.454833	-1.614489	-0.426292	
55059	H	-2.000538	-0.779785	0.907508	
55060	H	0.032993	0.837032	-1.888797	
55061	O	-1.461341	1.035290	-0.509163	
55062	O	-1.182089	2.425573	-0.433884	
55063	H	-0.991522	2.534372	0.508956	
55064	H	-1.548541	-1.056644	-1.909838	
55065	H	0.162690	-1.532491	-1.791779	
55066	Rotational constants (GHz):		1.0262800	0.9548700	0.6995800
55067	Vibrational harmonic frequencies (cm-1):				
55068	i	326.5571	55.5124		89.8293
55069		129.3258	150.6515		164.2894
55070		176.3355	203.7252		214.4567
55071		228.2104	246.6773		253.7279
55072		261.1716	298.9646		344.2405
55073		383.5368	391.3037		419.7454
55074		461.6523	477.2759		516.0978
55075		533.9550	633.8658		676.7518
55076		825.9652	881.4344		949.9797
55077		985.5478	1032.7622		1046.0597
55078		1054.6579	1066.0650		1143.9087
55079		1167.0486	1202.9681		1280.6970
55080		1320.5625	1337.5662		1386.8207
55081		1404.1985	1413.8083		1426.5128
55082		1447.1938	1463.8990		1466.9245
55083		1476.8980	1489.8538		2077.5250
55084		3035.1459	3050.6595		3084.5492
55085		3123.6995	3138.2297		3156.4017
55086		3685.3597	3715.5622		3782.8575
55087	Zero-point correction (Hartree): 0.153623				
55088	TS.triHPacyl.COelim.pmtmmmmrmd				
55089	-----				
55091	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16114993				
55092	Electronic state : 2-A				
55093	Cartesian coordinates (Angs):				
55094	O	-0.723473	-0.612805	1.850436	
55095	O	-1.419164	-1.062503	0.700251	
55096	C	-1.135051	-0.298376	-0.392094	
55097	C	0.304943	0.064114	-0.696555	
55098	C	0.980763	1.115889	0.178662	
55099	O	2.243833	1.476991	-0.353383	
55100	O	3.202559	0.510635	0.072085	
55101	H	0.085019	-1.148699	1.779185	
55102	C	-1.936393	-0.825962	-1.542630	
55103	H	-2.957832	-1.025319	-1.224369	
55104	H	-1.493719	-1.753283	-1.914089	
55105	H	-1.951671	-0.097700	-2.352220	
55106	C	-2.107389	1.521230	-0.062307	
55107	O	-3.123499	1.370429	0.431952	
55108	H	3.797064	1.057555	0.599588	
55109	H	0.300537	0.471983	-1.710574	
55110	O	1.099580	-1.110990	-0.860422	
55111	O	1.443460	-1.643696	0.411881	
55112	H	2.316325	-1.236914	0.536541	
55113	H	0.388822	2.028685	0.135792	
55114	H	1.087842	0.817829	1.217295	
55115	Rotational constants (GHz):		1.4091400	0.6360900	0.5752700
55116	Vibrational harmonic frequencies (cm-1):				
55117	i	296.4038	37.9233		64.6877
55118		83.5017	105.5639		165.4002
55119		173.6652	191.5365		203.2541
55120		222.3029	228.4087		238.8621
55121		250.2460	279.7533		284.2622
55122		323.2956	367.1013		392.7188
55123		497.7928	504.4165		551.5852
55124		574.5970	582.3128		705.6223
55125		847.7569	908.9951		947.2980

55126	980.1683	1007.2981	1049.7487			
55127	1059.7601	1095.9496	1103.5637			
55128	1129.7380	1206.2843	1303.6723			
55129	1319.8365	1345.8170	1370.6259			
55130	1392.9140	1404.8177	1420.7308			
55131	1449.2091	1473.9568	1477.6769			
55132	1485.1125	1496.0186	2083.4388			
55133	3054.7756	3087.9257	3116.4149			
55134	3127.7433	3159.0006	3174.9514			
55135	3697.7187	3743.4527	3828.2855			
55136	Zero-point correction (Hartree): 0.153502					
55137						
55138	TS.triHPacyl.COelim.pmtmmmmmpd					
55139	-----					
55140	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16228872					
55141	Electronic state : 2-A					
55142	Cartesian coordinates (Angs):					
55143	O	0.795321	-0.646533	-1.842040		
55144	O	1.428456	-1.088967	-0.654006		
55145	C	1.109884	-0.296820	0.407833		
55146	C	-0.331244	0.104475	0.640166		
55147	C	-0.977028	1.110181	-0.307448		
55148	O	-2.222488	1.555842	0.198114		
55149	O	-3.202358	0.555088	-0.075276		
55150	H	-0.001573	-1.201546	-1.825910		
55151	C	1.849372	-0.812480	1.604470		
55152	H	2.880857	-1.033198	1.336729		
55153	H	1.377056	-1.725610	1.974285		
55154	H	1.840305	-0.067558	2.398855		
55155	C	2.116231	1.500060	0.090744		
55156	O	3.145459	1.333276	-0.369714		
55157	H	-3.374539	0.209557	0.810881		
55158	H	-0.349961	0.565898	1.631205		
55159	O	-1.155066	-1.052713	0.836394		
55160	O	-1.444896	-1.648410	-0.421354		
55161	H	-2.266957	-1.185088	-0.655488		
55162	H	-0.358378	2.005175	-0.342114		
55163	H	-1.105517	0.739209	-1.319964		
55164	Rotational constants (GHz):			1.4077800	0.6393600	0.5776000
55165	Vibrational harmonic frequencies (cm-1):					
55166	i301.2115	40.7751	63.6851			
55167	91.6776	103.8502	157.0968			
55168	173.9598	195.6807	204.3379			
55169	218.5517	227.5085	234.7603			
55170	271.6563	286.5375	309.9057			
55171	367.6503	374.7172	397.1785			
55172	494.2645	498.1505	558.1130			
55173	585.0962	617.9679	704.9571			
55174	853.6574	910.8279	943.8253			
55175	980.8017	1004.0674	1050.5576			
55176	1059.9778	1099.7895	1101.6944			
55177	1121.7765	1206.3081	1300.7537			
55178	1319.7366	1342.8878	1371.7044			
55179	1401.9198	1405.3912	1416.8500			
55180	1444.3469	1468.6240	1478.7444			
55181	1482.4260	1495.8902	2084.9144			
55182	3054.9595	3083.3832	3121.4256			
55183	3127.7054	3158.4356	3177.1812			
55184	3720.1366	3730.3056	3804.0569			
55185	Zero-point correction (Hartree): 0.153783					
55186						
55187	TS.triHPacyl.COelim.pmtmtmmmpd					
55188	-----					
55189	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16089299					
55190	Electronic state : 2-A					
55191	Cartesian coordinates (Angs):					
55192	O	0.586726	-1.312177	-1.757336		
55193	O	1.362828	-1.446360	-0.580989		
55194	C	1.217107	-0.374432	0.244245		
55195	C	-0.161079	0.195751	0.505977		
55196	C	-0.891755	0.918968	-0.622277		
55197	O	-2.032811	1.598302	-0.130305		

55198	O	-3.083450	0.647279	0.032699		
55199	H	-0.209973	-1.798419	-1.489938		
55200	C	2.074833	-0.597577	1.451707		
55201	H	3.056734	-0.957825	1.150602		
55202	H	1.615356	-1.341467	2.106896		
55203	H	2.191450	0.332885	2.004754		
55204	C	2.245360	1.231187	-0.666088		
55205	O	2.314918	2.155043	0.002064		
55206	H	-3.138881	0.587349	0.995891		
55207	H	-0.028208	0.930514	1.304940		
55208	O	-1.002330	-0.778908	1.140699		
55209	O	-1.477223	-1.701162	0.169003		
55210	H	-2.307393	-1.271773	-0.098104		
55211	H	-0.256111	1.709019	-1.019357		
55212	H	-1.179045	0.270205	-1.443740		
55213	Rotational constants (GHz):			1.2074500	0.7251800	0.5950000
55214	Vibrational harmonic frequencies (cm-1):					
55215	i295.1896		40.6121			55.7413
55216	93.6219		107.9117			150.8255
55217	171.7230		184.1588			193.0004
55218	206.7667		215.6123			261.2183
55219	271.9279		286.9568			312.7317
55220	361.4580		384.2534			414.2848
55221	479.5432		490.7465			556.6275
55222	567.1437		610.6428			694.3449
55223	850.3047		909.0068			943.8839
55224	980.3079		1002.1076			1048.1085
55225	1061.6409		1095.3046			1101.9266
55226	1120.3126		1207.1307			1302.8767
55227	1323.0060		1348.3540			1373.8203
55228	1404.3212		1406.9176			1417.3214
55229	1443.5060		1468.3957			1474.4076
55230	1482.6087		1497.1856			2063.9723
55231	3055.3796		3080.9753			3120.9978
55232	3128.2090		3159.4752			3176.3488
55233	3694.2911		3730.8787			3804.9126
55234	Zero-point correction (Hartree):			0.153526		
55235						
55236	TS.triHPacyl.COelim.pmtmpmmmpd					
55237	-----					
55238	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16195893					
55239	Electronic state : 2-A					
55240	Cartesian coordinates (Angs):					
55241	O	1.222976	-1.032322	1.583668		
55242	O	1.375960	0.331250	1.205840		
55243	C	0.990359	0.537323	-0.087825		
55244	C	-0.373753	0.121287	-0.586735		
55245	C	-0.996186	-1.133114	0.014368		
55246	O	-2.236713	-1.420414	-0.604229		
55247	O	-3.234540	-0.589191	-0.019074		
55248	H	2.142054	-1.332783	1.549521		
55249	C	1.458419	1.888864	-0.520930		
55250	H	2.519899	2.006107	-0.310020		
55251	H	0.901579	2.664682	0.008194		
55252	H	1.281827	2.011589	-1.588258		
55253	C	2.272077	-0.720946	-1.194445		
55254	O	3.198157	-1.014326	-0.593809		
55255	H	-3.329029	0.097500	-0.693818		
55256	H	-0.278397	-0.031752	-1.665578		
55257	O	-1.284731	1.221286	-0.529904		
55258	O	-1.492766	1.565998	0.831260		
55259	H	-2.232529	0.984373	1.070435		
55260	H	-0.368775	-1.996866	-0.199042		
55261	H	-1.128861	-1.061589	1.091963		
55262	Rotational constants (GHz):			1.4314000	0.6342900	0.5621900
55263	Vibrational harmonic frequencies (cm-1):					
55264	i294.9303		27.5032			68.3689
55265	93.0704		127.4728			145.2260
55266	159.6201		182.5361			201.8594
55267	206.7698		221.2857			242.4037
55268	273.6800		284.6265			309.5192
55269	319.6605		358.8361			397.2110

55270	413.2879	484.4687	546.6090			
55271	576.1332	593.5839	686.6599			
55272	843.9182	908.7190	949.2830			
55273	977.4123	1003.8769	1032.3039			
55274	1053.6116	1102.9413	1108.5034			
55275	1126.8857	1208.5102	1299.3876			
55276	1314.2337	1330.0469	1368.6710			
55277	1405.4497	1409.1850	1414.5020			
55278	1419.6763	1442.3705	1469.9331			
55279	1471.3785	1492.3545	2065.8687			
55280	3061.6447	3077.5345	3107.6079			
55281	3131.9920	3159.6155	3161.9577			
55282	3719.0326	3788.9084	3794.2703			
55283	Zero-point correction (Hartree): 0.152961					
55284						
55285	TS.triHPacyl.COelim.pmtmptmmpd					
55286	-----					
55287	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16213565					
55288	Electronic state : 2-A					
55289	Cartesian coordinates (Angs):					
55290	O	1.094204	-0.616576	2.084433		
55291	O	1.282045	0.616633	1.405682		
55292	C	1.084049	0.474339	0.062252		
55293	C	-0.224858	-0.053160	-0.486188		
55294	C	-1.004695	-1.031845	0.385046		
55295	O	-2.189256	-1.449845	-0.267125		
55296	O	-3.178911	-0.439366	-0.099156		
55297	H	1.956535	-1.036310	1.942355		
55298	C	1.663445	1.650421	-0.654032		
55299	H	2.696495	1.806284	-0.348654		
55300	H	1.084869	2.547513	-0.424845		
55301	H	1.618788	1.484016	-1.729257		
55302	C	2.446212	-1.047106	-0.438440		
55303	O	2.436552	-1.320350	-1.545621		
55304	H	-3.158651	-0.008794	-0.965173		
55305	H	-0.012243	-0.538450	-1.444133		
55306	O	-1.056601	1.032728	-0.902749		
55307	O	-1.400372	1.802797	0.238833		
55308	H	-2.199074	1.346535	0.550636		
55309	H	-0.429495	-1.944574	0.528861		
55310	H	-1.243428	-0.620286	1.364008		
55311	Rotational constants (GHz):			1.2456500	0.6563900	0.6171500
55312	Vibrational harmonic frequencies (cm-1):					
55313	i297.8782			37.8835		60.9959
55314	96.8060			133.1981		160.0804
55315	170.2098			199.6341		203.7332
55316	208.8977			212.9669		254.8224
55317	268.7179			313.4376		323.3984
55318	368.1448			389.3801		409.7250
55319	419.5859			476.3500		552.7576
55320	576.3609			588.2649		677.9951
55321	842.4544			908.9080		951.1843
55322	975.5086			1003.6248		1035.2837
55323	1053.5442			1104.0613		1107.5525
55324	1126.7545			1210.3045		1301.9418
55325	1313.5611			1330.7878		1377.4720
55326	1405.3521			1410.3025		1418.3189
55327	1428.3382			1445.7835		1469.5859
55328	1470.8893			1492.2498		2081.4209
55329	3061.5859			3068.4987		3107.1047
55330	3131.6128			3159.5358		3161.5916
55331	3711.6448			3760.6796		3794.7878
55332	Zero-point correction (Hartree): 0.153379					
55333						
55334	TS.triHPacyl.COelim.ppmmmmpd					
55335	-----					
55336	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16086248					
55337	Electronic state : 2-A					
55338	Cartesian coordinates (Angs):					
55339	O	-0.101412	-2.153687	-0.780904		
55340	O	0.106291	-1.605994	0.508026		
55341	C	0.445297	-0.278417	0.478116		

55342	C	-0.257747	0.579777	-0.558267	
55343	C	-1.550662	1.189392	-0.016615	
55344	O	-2.374048	0.199800	0.572538	
55345	O	-2.681686	-0.752881	-0.444437	
55346	H	-1.071033	-2.147927	-0.820881	
55347	C	0.550933	0.162171	1.907896	
55348	H	1.214339	-0.512790	2.447273	
55349	H	-0.431824	0.125181	2.383352	
55350	H	0.937644	1.174613	1.969831	
55351	C	2.429696	-0.206204	-0.114887	
55352	O	2.856211	-1.232897	-0.367472	
55353	H	-3.642799	-0.686004	-0.488451	
55354	H	-0.493793	-0.047545	-1.413873	
55355	O	0.546553	1.583411	-1.141610	
55356	O	1.057071	2.435500	-0.127187	
55357	H	1.929480	2.033284	0.016146	
55358	H	-1.341461	1.884685	0.796083	
55359	H	-2.077489	1.710168	-0.818571	
55360	Rotational constants (GHz):		1.1482500	0.8312500	0.6184700
55361	Vibrational harmonic frequencies (cm-1):				
55362	i305.3364		49.2758		86.0530
55363	98.2116		117.3915		160.3357
55364	168.4681		177.7018		190.2118
55365	196.4650		213.0150		233.0568
55366	262.6754		279.1870		292.0770
55367	337.2538		390.1687		413.4771
55368	471.2453		494.3754		514.9664
55369	538.3250		601.6225		666.4978
55370	795.4578		941.8257		955.7452
55371	980.2209		1006.7316		1055.6467
55372	1066.2027		1092.3619		1127.1295
55373	1139.6914		1226.0656		1274.1406
55374	1290.8323		1343.5276		1367.9166
55375	1396.4114		1403.1187		1423.4379
55376	1439.9452		1458.7535		1477.8012
55377	1484.8412		1504.7442		2085.3212
55378	3062.7651		3073.1215		3129.7819
55379	3140.2188		3157.5602		3184.6744
55380	3712.6639		3747.7479		3837.2108
55381	Zero-point correction (Hartree):		0.153402		
55382	TS.triHPacyl.COelim.pmmmpmmd				
55383	-----				
55384	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16330155				
55385	Electronic state : 2-A				
55386	Cartesian coordinates (Angs):				
55387	O	-0.128671	-1.714058	-1.309269	
55388	O	0.062292	-1.633936	0.095513	
55389	C	0.443762	-0.380431	0.469459	
55390	C	-0.288691	0.798192	-0.136386	
55391	C	-1.660305	1.028121	0.508506	
55392	O	-2.428005	-0.153115	0.595490	
55393	O	-2.677482	-0.583871	-0.742083	
55394	H	-1.094776	-1.629104	-1.366258	
55395	C	0.707934	-0.368886	1.940067	
55396	H	1.429724	-1.142079	2.197873	
55397	H	-0.214630	-0.565153	2.493344	
55398	H	1.099039	0.604623	2.231205	
55399	C	2.384290	-0.222964	-0.276828	
55400	O	2.967569	-1.189668	-0.116841	
55401	H	-3.640476	-0.636159	-0.752224	
55402	H	-0.398476	0.666484	-1.209651	
55403	O	0.419511	1.998950	0.113369	
55404	O	1.170313	2.357651	-1.033594	
55405	H	1.945214	1.777336	-0.948743	
55406	H	-1.536137	1.340504	1.546176	
55407	H	-2.195638	1.803741	-0.041297	
55408	Rotational constants (GHz):		1.1385100	0.7781800	0.6135700
55409	Vibrational harmonic frequencies (cm-1):				
55410	i287.8839		43.9171		62.2958
55411	105.5396		121.9979		132.1246
55412	141.8497		190.5885		197.5445

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55414      198.0802      214.8351      232.4151
55415      258.9637      267.9727      282.5271
55416      359.4565      373.9001      440.2565
55417      474.6163      495.5688      500.0949
55418      520.2423      592.8114      650.0105
55419      787.5923      939.3550      954.1417
55420      1002.0312     1020.2120     1053.2757
55421      1059.1092     1100.2612     1119.8693
55422      1163.6251     1240.6446     1282.3002
55423      1301.1376     1337.8602     1368.1698
55424      1390.2337     1403.0584     1412.4973
55425      1462.4808     1467.8114     1477.1059
55426      1480.7877     1502.5992     2084.7039
55427      3048.5593     3075.8337     3123.6334
55428      3132.0292     3149.4193     3159.7841
55429      3702.0579     3719.8077     3837.8543
55430      Zero-point correction (Hartree): 0.153133
55431
55432      TS.triHPacyl.COelim.ppmmmmtmmd
55433      -----
55434      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16113103
55435      Electronic state : 2-A
55436      Cartesian coordinates (Angs):
55437      O      0.179515      -2.033067      -0.719816
55438      O      0.721097      -1.556691      0.504815
55439      C      0.856182      -0.197362      0.474031
55440      C      -0.342868      0.575339      -0.014556
55441      C      -1.616278      0.296333      0.786425
55442      O      -2.176219      -0.973117      0.488998
55443      O      -2.669656      -0.920500      -0.848314
55444      H      -0.758316      -2.129414      -0.489074
55445      C      1.587746      0.255784      1.693178
55446      H      2.509130      -0.315794      1.793529
55447      H      0.988514      0.101499      2.595581
55448      H      1.824940      1.313890      1.611729
55449      C      2.229563      0.160884      -1.077037
55450      O      3.252727      -0.299770      -0.876256
55451      H      -3.623589      -0.957387      -0.704753
55452      H      -0.517152      0.350926      -1.067752
55453      O      0.003940      1.942416      0.131515
55454      O      -0.887489      2.702224      -0.668285
55455      H      -0.351339      2.861399      -1.456368
55456      H      -1.405572      0.252728      1.855751
55457      H      -2.343997      1.084317      0.587859
55458      Rotational constants (GHz):      1.0947700      0.7537700      0.5742100
55459      Vibrational harmonic frequencies (cm-1):
55460      i296.9009      29.8526      50.3707
55461      76.5278      95.5458      129.5049
55462      149.5464      158.3417      172.1875
55463      203.8380      215.8680      222.0364
55464      237.7454      254.0056      272.8874
55465      289.8539      336.9708      374.7484
55466      434.5103      467.3456      495.1644
55467      542.7703      577.6753      614.5006
55468      802.7586      934.6315      955.8286
55469      1009.8318      1030.1499      1050.6703
55470      1063.7373      1086.3481      1124.5616
55471      1143.0005      1250.7898      1285.1948
55472      1308.1775      1340.4071      1382.9783
55473      1389.7888      1408.3085      1410.3581
55474      1424.4748      1428.7462      1472.6816
55475      1479.3677      1493.7910      2084.2112
55476      3043.0737      3077.7226      3101.4531
55477      3123.3589      3137.2264      3169.0321
55478      3747.1220      3803.3914      3822.9193
55479      Zero-point correction (Hartree): 0.152154
55480
55481      TS.triHPacyl.COelim.ppmmmptmmd
55482      -----
55483      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16200242
55484      Electronic state : 2-A
55485      Cartesian coordinates (Angs):

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55486	O	-0.577791	-1.873643	-1.056339		
55487	O	-0.042143	-1.920819	0.258617		
55488	C	0.663481	-0.784659	0.526524		
55489	C	-0.014384	0.517359	0.175535		
55490	C	-1.357520	0.726328	0.877356		
55491	O	-2.374656	-0.119582	0.367539		
55492	O	-2.655474	0.304897	-0.965456		
55493	H	-1.492064	-1.597462	-0.884600		
55494	C	1.361976	-0.928157	1.836398		
55495	H	1.943362	-1.848117	1.833142		
55496	H	0.647292	-0.974500	2.663304		
55497	H	2.026014	-0.082065	1.996757		
55498	C	2.247114	-0.770653	-0.874165		
55499	O	2.243057	0.123718	-1.585325		
55500	H	-3.547892	0.661005	-0.872418		
55501	H	-0.162896	0.574973	-0.902954		
55502	O	0.879433	1.539629	0.585467		
55503	O	0.633387	2.684093	-0.213121		
55504	H	1.277863	2.560968	-0.924972		
55505	H	-1.293304	0.463998	1.934048		
55506	H	-1.648879	1.773549	0.776741		
55507	Rotational constants (GHz):			1.0336300	0.8229100	0.6562200
55508	Vibrational harmonic frequencies (cm-1):					
55509	i292.9012		30.1407			60.1001
55510	78.6274		93.8942			134.5900
55511	148.0822		167.7852			171.7090
55512	203.9672		210.4176			230.6765
55513	250.3463		277.9524			309.7154
55514	328.0705		348.6620			358.1569
55515	433.0923		484.0125			497.8685
55516	538.8030		572.7646			614.7325
55517	801.1463		934.9254			954.7789
55518	1012.8801		1031.4549			1051.2704
55519	1062.7585		1087.4480			1127.2943
55520	1141.8795		1253.4547			1285.3560
55521	1312.2597		1343.6880			1381.8950
55522	1390.1705		1407.7154			1413.0947
55523	1422.1135		1431.7204			1472.2651
55524	1479.3388		1493.7420			2060.9926
55525	3046.0532		3073.3861			3110.1079
55526	3127.7226		3136.0815			3169.2503
55527	3765.3514		3778.3518			3824.7604
55528	Zero-point correction (Hartree):			0.152475		
55529	-----					
55530	TS.triHPacyl.COelim.ppmmtmpmd					
55531	-----					
55532	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.16050309		
55533	Electronic state : 2-A					
55534	Cartesian coordinates (Angs):					
55535	O	0.933029	2.074259	-0.903736		
55536	O	0.480151	1.716660	0.389625		
55537	C	-0.300076	0.591127	0.385047		
55538	C	0.132090	-0.530798	-0.536072		
55539	C	1.154745	-1.463825	0.115116		
55540	O	2.226761	-0.737864	0.684240		
55541	O	2.870274	-0.034295	-0.377478		
55542	H	1.841902	1.735721	-0.872399		
55543	C	-0.696807	0.333298	1.804779		
55544	H	-1.074146	1.253851	2.247754		
55545	H	0.170874	0.008292	2.385321		
55546	H	-1.463691	-0.432794	1.861566		
55547	C	-2.133529	1.187732	-0.518343		
55548	O	-3.039154	0.612085	-0.119803		
55549	H	3.763730	-0.394884	-0.335164		
55550	H	0.569858	-0.081807	-1.424595		
55551	O	-0.927947	-1.288607	-1.086588		
55552	O	-1.609685	-1.982821	-0.047922		
55553	H	-2.443296	-1.491275	-0.012316		
55554	H	0.712023	-1.991390	0.959250		
55555	H	1.516789	-2.186245	-0.619280		
55556	Rotational constants (GHz):			1.2697000	0.7773700	0.6108500
55557	Vibrational harmonic frequencies (cm-1):					

55558	i285.2543	63.3768	94.7985	
55559	103.1581	117.2047	144.8914	
55560	155.9196	167.2436	176.3566	
55561	180.5709	204.4258	218.8433	
55562	233.9570	290.8616	291.4703	
55563	327.1909	361.7170	399.2772	
55564	435.0377	481.8975	493.4569	
55565	540.2963	585.9217	661.6196	
55566	785.2737	941.0580	954.8756	
55567	975.8359	1004.1673	1048.3552	
55568	1063.1704	1094.7566	1123.2293	
55569	1140.1317	1229.8678	1275.4594	
55570	1296.3041	1342.4416	1366.6554	
55571	1394.6609	1402.8190	1418.3022	
55572	1437.6086	1459.2570	1471.6705	
55573	1482.5905	1502.2378	2044.4816	
55574	3054.1566	3070.3100	3128.2909	
55575	3139.9430	3154.6621	3185.3797	
55576	3749.1716	3772.1057	3838.3630	
55577	Zero-point correction (Hartree): 0.152813			
55578				
55579	TS.triHPacyl.COelim.ppmmtpppd			
55580	-----			
55581	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16174452			
55582	Electronic state : 2-A			
55583	Cartesian coordinates (Angs):			
55584	O	-0.281588	-1.723367	-1.489380
55585	O	-0.356367	-1.672982	-0.069953
55586	C	0.249240	-0.528496	0.403385
55587	C	-0.216198	0.769447	-0.222326
55588	C	-1.496869	1.291023	0.449239
55589	O	-2.446640	0.277939	0.659689
55590	O	-2.862730	-0.184541	-0.618392
55591	H	0.675949	-1.831004	-1.625479
55592	C	0.377578	-0.595170	1.888394
55593	H	0.900651	-1.501292	2.187492
55594	H	-0.610472	-0.592899	2.354747
55595	H	0.942638	0.269566	2.234055
55596	C	2.178350	-0.888429	-0.231369
55597	O	3.002871	-0.550708	0.479024
55598	H	-2.388534	-1.026848	-0.686201
55599	H	-0.385972	0.627645	-1.286902
55600	O	0.719182	1.813829	-0.017943
55601	O	1.721931	1.726857	-1.022432
55602	H	1.520948	2.502317	-1.561277
55603	H	-1.263439	1.667135	1.446462
55604	H	-1.917659	2.098915	-0.151740
55605	Rotational constants (GHz): 1.2427100 0.7485600 0.6337000			
55606	Vibrational harmonic frequencies (cm-1):			
55607	i323.4487	47.9022	75.0836	
55608	109.3593	132.1407	157.6905	
55609	164.1097	185.6612	201.4912	
55610	209.6919	228.3916	245.2292	
55611	254.4971	270.9785	309.0606	
55612	353.8021	366.8134	407.6871	
55613	429.8120	444.0951	481.5795	
55614	507.3291	597.2161	654.4033	
55615	783.0893	939.8880	957.0332	
55616	1002.3467	1014.3443	1038.1657	
55617	1051.5711	1096.4924	1131.6549	
55618	1166.1020	1223.9865	1274.5638	
55619	1297.1315	1335.1245	1377.8299	
55620	1401.2158	1405.1426	1419.3300	
55621	1422.8072	1437.0093	1473.8961	
55622	1482.3783	1501.3411	2087.5815	
55623	3057.1325	3072.0774	3125.8682	
55624	3131.3087	3143.0144	3158.9607	
55625	3693.1860	3770.7471	3818.8906	
55626	Zero-point correction (Hartree): 0.152923			
55627				
55628	TS.triHPacyl.COelim.ppmmpmpmpd			
55629	-----			

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55630 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16334862
55631 Electronic state : 2-A
55632 Cartesian coordinates (Angs):
55633 O 0.201306 -1.740400 -1.229082
55634 O 0.092998 -1.576972 0.182431
55635 C 0.348088 -0.279591 0.542993
55636 C -0.349656 0.809961 -0.242197
55637 C -1.791761 1.013561 0.252472
55638 O -2.475878 -0.195157 0.464803
55639 O -2.650482 -0.808784 -0.806050
55640 H 1.051871 -2.197531 -1.296812
55641 C 0.376922 -0.178910 2.031592
55642 H 1.091355 -0.884957 2.452198
55643 H -0.611009 -0.402077 2.442884
55644 H 0.660737 0.833839 2.312820
55645 C 2.422609 -0.125131 0.104781
55646 O 2.854837 -1.165294 -0.083206
55647 H -1.999819 -1.524853 -0.775885
55648 H -0.343375 0.580601 -1.304602
55649 O 0.263375 2.065731 -0.021159
55650 O 1.236140 2.303047 -1.024165
55651 H 2.037483 1.951608 -0.609202
55652 H -1.776041 1.500423 1.228795
55653 H -2.326796 1.646240 -0.456624
55654 Rotational constants (GHz): 1.1295200 0.7966600 0.6203700
55655 Vibrational harmonic frequencies (cm-1):
55656 i287.8299 45.4365 67.1060
55657 90.4147 131.7209 133.3507
55658 160.6521 187.2508 202.7986
55659 223.3570 234.6281 252.3446
55660 261.2238 273.8419 302.9837
55661 345.7164 363.1983 403.9844
55662 424.6005 448.5851 480.1135
55663 508.6890 598.5689 658.0038
55664 787.1464 940.0872 956.5033
55665 1000.6419 1017.0769 1035.7318
55666 1052.2092 1098.1515 1130.9337
55667 1165.9393 1223.3409 1274.7747
55668 1297.6267 1327.1983 1372.6587
55669 1396.3279 1406.4610 1412.6052
55670 1418.7527 1437.6552 1474.5074
55671 1481.1263 1500.5482 2068.9965
55672 3051.9957 3078.2225 3125.0141
55673 3131.4642 3149.8577 3158.3589
55674 3762.1062 3787.7533 3791.0944
55675 Zero-point correction (Hartree): 0.152891
55676
55677 TS.triHPacyl.COelim.ppmppmmpd
55678 -----
55679 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15909768
55680 Electronic state : 2-A
55681 Cartesian coordinates (Angs):
55682 O 0.153828 -2.150345 -0.007894
55683 O 0.555578 -1.262281 1.021857
55684 C 0.694051 0.026905 0.563184
55685 C -0.313331 0.503668 -0.460306
55686 C -1.737151 0.648416 0.095293
55687 O -2.283159 -0.579188 0.503940
55688 O -2.512636 -1.363197 -0.659370
55689 H 1.006133 -2.432282 -0.372514
55690 C 1.108704 0.896248 1.701606
55691 H 1.861903 0.380042 2.295076
55692 H 0.261048 1.135366 2.348520
55693 H 1.527502 1.821307 1.315768
55694 C 2.497770 -0.105585 -0.575377
55695 O 2.634759 -1.162614 -0.993638
55696 H -1.790929 -2.005216 -0.587448
55697 H -0.346951 -0.203764 -1.288710
55698 O 0.112598 1.696957 -1.088872
55699 O -0.070522 2.788498 -0.184034
55700 H -0.630820 3.368591 -0.713146
55701 H -1.747464 1.264668 0.992354

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55702      H      -2.364245      1.110753      -0.672206
55703 Rotational constants (GHz):      1.0146300      0.8744800      0.6110900
55704 Vibrational harmonic frequencies (cm-1):
55705      i285.9414      19.0279      45.7944
55706      113.5759      124.3301      158.5236
55707      167.6097      193.3509      198.5052
55708      208.8793      244.8917      246.4730
55709      249.6914      283.5637      291.7515
55710      303.7382      357.9286      371.7555
55711      429.7825      451.9310      496.8948
55712      541.4056      577.8986      665.1928
55713      784.1216      940.8802      958.3675
55714      972.0201      1012.1551      1049.3481
55715      1053.0197      1110.4748      1129.2557
55716      1145.8649      1229.4796      1281.7740
55717      1309.1280      1331.5386      1372.3171
55718      1397.1803      1412.4693      1414.5239
55719      1420.0566      1452.6811      1476.9600
55720      1481.8249      1493.1555      2040.5488
55721      3054.8874      3057.3734      3120.9448
55722      3128.9692      3149.5138      3178.1834
55723      3767.8275      3771.9839      3831.5032
55724 Zero-point correction (Hartree): 0.152803
55725
55726 TS.triHPacyl.COelim.ppmppmpped
55727 -----
55728 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16355625
55729 Electronic state : 2-A
55730 Cartesian coordinates (Angs):
55731      O      0.424558      -2.095967      -0.865338
55732      O      0.277337      -1.589617      0.454010
55733      C      0.380212      -0.218118      0.493325
55734      C      -0.365199      0.536465      -0.591001
55735      C      -1.743999      0.993097      -0.108666
55736      O      -2.445721      -0.060652      0.515016
55737      O      -2.662909      -1.069254      -0.465880
55738      H      1.365181      -2.326349      -0.876678
55739      C      0.315394      0.197833      1.928654
55740      H      1.064136      -0.342022      2.507075
55741      H      -0.670402      -0.028919      2.340584
55742      H      0.493043      1.266246      2.013284
55743      C      2.427813      0.132045      0.044384
55744      O      2.954227      -0.847904      -0.215169
55745      H      -2.039601      -1.755399      -0.187069
55746      H      -0.491509      -0.129013      -1.441834
55747      O      0.357051      1.616792      -1.146355
55748      O      0.667090      2.549287      -0.119654
55749      H      1.580922      2.296535      0.083748
55750      H      -1.650212      1.759210      0.660550
55751      H      -2.309959      1.390296      -0.952879
55752 Rotational constants (GHz):      1.1474000      0.8292900      0.6192700
55753 Vibrational harmonic frequencies (cm-1):
55754      i289.7674      55.8080      82.5366
55755      94.0433      154.7695      157.0505
55756      165.9927      184.1280      188.7508
55757      209.1067      237.7225      255.5780
55758      269.6666      284.7341      326.8673
55759      342.4427      377.9680      387.4531
55760      411.4011      457.5707      487.9597
55761      536.0882      612.1656      664.7475
55762      795.4037      945.4144      954.9112
55763      976.9245      1010.3363      1045.6111
55764      1053.2838      1105.0785      1123.8301
55765      1134.7161      1216.7637      1270.3918
55766      1294.1945      1340.4548      1372.8033
55767      1402.5482      1412.6486      1416.0268
55768      1417.6308      1435.0050      1476.0989
55769      1486.8638      1502.1087      2066.4171
55770      3062.4649      3079.2963      3129.3288
55771      3140.2101      3154.1437      3178.3920
55772      3737.0089      3781.7037      3783.3451
55773 Zero-point correction (Hartree): 0.153197

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55774
55775 TS.triHPacyl.COelim.ppmmpptmpd
55776 -----
55777 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15962485
55778 Electronic state : 2-A
55779 Cartesian coordinates (Angs):
55780 O 0.214016 -1.968436 -0.804149
55781 O 0.591913 -1.629420 0.516988
55782 C 0.693056 -0.271644 0.698441
55783 C -0.257167 0.616686 -0.063294
55784 C -1.688680 0.573007 0.484494
55785 O -2.242899 -0.718862 0.447763
55786 O -2.511067 -1.031468 -0.913897
55787 H 1.066091 -1.999714 -1.264625
55788 C 0.977201 0.007388 2.134243
55789 H 1.838548 -0.571265 2.463430
55790 H 0.121249 -0.260912 2.758652
55791 H 1.194809 1.066077 2.255708
55792 C 2.553553 0.131522 -0.268789
55793 O 2.597895 -0.409276 -1.277380
55794 H -1.777786 -1.631336 -1.114483
55795 H -0.256545 0.353770 -1.121149
55796 O 0.266608 1.929600 0.096741
55797 O -0.431483 2.776220 -0.804813
55798 H 0.260861 2.987912 -1.443313
55799 H -1.685611 0.852131 1.539067
55800 H -2.309259 1.274720 -0.073890
55801 Rotational constants (GHz): 1.0030000 0.8321600 0.6377600
55802 Vibrational harmonic frequencies (cm-1):
55803 1284.5040 17.7376 41.1174
55804 92.6736 109.3694 146.9620
55805 158.5429 168.1145 188.2917
55806 197.9994 217.1983 224.3246
55807 243.5237 262.2388 282.9432
55808 326.1579 330.4935 362.8807
55809 440.0377 453.7334 473.0105
55810 518.9600 577.9142 612.6907
55811 793.9560 943.9416 959.5672
55812 1008.6477 1031.6209 1051.7398
55813 1064.0323 1105.0381 1125.2583
55814 1141.5321 1241.5258 1284.3470
55815 1311.9513 1338.9376 1377.2431
55816 1410.1367 1410.9942 1415.5340
55817 1418.8294 1457.1304 1474.3185
55818 1477.4788 1498.0201 2037.9880
55819 3053.8405 3080.7602 3107.8215
55820 3130.1450 3138.4562 3168.8118
55821 3770.2749 3773.5016 3820.0759
55822 Zero-point correction (Hartree): 0.152342
55823
55824 TS.triHPacyl.COelim.ppmmpptmpd
55825 -----
55826 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16388355
55827 Electronic state : 2-A
55828 Cartesian coordinates (Angs):
55829 O 0.464372 2.218972 -0.960960
55830 O 0.415371 1.718620 0.366988
55831 C -0.237570 0.508431 0.422078
55832 C 0.209900 -0.526240 -0.590785
55833 C 1.304881 -1.433192 -0.021570
55834 O 2.310516 -0.683257 0.622077
55835 O 2.928886 0.138170 -0.361744
55836 H -0.460795 2.478965 -1.102035
55837 C -0.467731 0.159439 1.855479
55838 H -0.946859 0.990983 2.370113
55839 H 0.486340 -0.047292 2.347061
55840 H -1.095469 -0.724617 1.928658
55841 C -2.166342 1.082801 -0.271847
55842 O -3.013948 0.408170 0.087782
55843 H 2.573262 1.011300 -0.140704
55844 H 0.602176 0.001952 -1.457329
55845 O -0.840476 -1.291850 -1.149059

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55846	O	-1.431963	-2.090116	-0.127854	
55847	H	-2.307306	-1.684815	-0.055843	
55848	H	0.902221	-2.081472	0.755847	
55849	H	1.725545	-2.042099	-0.823740	
55850	Rotational constants (GHz):		1.2227100	0.7992500	0.6191600
55851	Vibrational harmonic frequencies (cm-1):				
55852		i277.7947	67.9794		95.8579
55853		113.0816	141.1590		150.4693
55854		153.0553	167.2394		177.1826
55855		210.6459	214.2288		236.9693
55856		276.0342	293.9303		326.6923
55857		341.1268	361.0817		381.4113
55858		394.5204	423.1155		489.7953
55859		535.9838	604.1262		661.4296
55860		786.7308	943.3844		954.1481
55861		974.0022	1007.7363		1042.1995
55862		1049.2954	1106.9913		1121.8882
55863		1137.7570	1219.5821		1270.9200
55864		1297.4792	1340.4990		1372.7955
55865		1399.5285	1410.1321		1418.5116
55866		1431.7986	1432.9710		1471.8398
55867		1486.3543	1500.9491		2071.6662
55868		3057.9967	3077.7340		3129.1565
55869		3138.0920	3151.4551		3175.3432
55870		3730.5815	3777.8553		3792.3384
55871	Zero-point correction (Hartree):		0.152858		
55872					
55873	TS.triHPacyl.COelim.ppmptmpd				
55874	-----				
55875	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.16267083		
55876	Electronic state : 2-A				
55877	Cartesian coordinates (Angs):				
55878	O	-0.361710	-1.776930	-1.411764	
55879	O	-0.412257	-1.675951	0.005108	
55880	C	0.219386	-0.532060	0.430381	
55881	C	-0.191438	0.759847	-0.243046	
55882	C	-1.467105	1.337458	0.393863	
55883	O	-2.445592	0.358283	0.631743	
55884	O	-2.876345	-0.124759	-0.633949	
55885	H	0.577402	-1.982308	-1.555140	
55886	C	0.362803	-0.550668	1.914705	
55887	H	0.863304	-1.460020	2.242622	
55888	H	-0.621084	-0.507180	2.388728	
55889	H	0.948727	0.312413	2.228154	
55890	C	2.174461	-0.988410	-0.204628	
55891	O	3.005186	-0.494039	0.402630	
55892	H	-2.436623	-0.986615	-0.677316	
55893	H	-0.347194	0.597849	-1.306423	
55894	O	0.767844	1.782594	-0.054126	
55895	O	1.695976	1.725551	-1.132951	
55896	H	2.532121	1.633154	-0.658967	
55897	H	-1.233880	1.744080	1.379199	
55898	H	-1.856218	2.133631	-0.242045	
55899	Rotational constants (GHz):		1.2469400	0.7456800	0.6292200
55900	Vibrational harmonic frequencies (cm-1):				
55901		i289.1547	48.6671		74.6851
55902		102.5720	144.4021		146.5802
55903		158.6728	171.7735		191.1883
55904		198.6503	224.0139		240.9425
55905		261.8804	296.0807		333.9309
55906		345.1250	365.7478		376.7857
55907		405.9013	430.0361		479.1854
55908		507.2246	595.3804		653.0675
55909		780.2794	939.9591		956.8926
55910		1001.1613	1015.0422		1038.9198
55911		1051.3724	1101.5783		1129.9011
55912		1160.8943	1228.6687		1274.0044
55913		1297.1057	1330.9323		1375.2822
55914		1399.8265	1412.8346		1416.0377
55915		1418.5275	1428.0057		1471.5517
55916		1481.0961	1499.7541		2070.4447
55917		3054.0957	3076.8382		3126.8726

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55918          3129.8589              3149.4787              3156.7863
55919          3716.7023              3778.6047              3820.9855
55920 Zero-point correction (Hartree): 0.152735
55921
55922 TS.triHPacyl.COelim.ppmptpppd
55923 -----
55924 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16106733
55925 Electronic state : 2-A
55926 Cartesian coordinates (Angs):
55927 O      -0.744097      -1.893789      -0.768326
55928 O      -0.192559      -1.622751      0.509630
55929 C       0.471154      -0.418304      0.495676
55930 C      -0.252706       0.746836     -0.151555
55931 C      -1.582060       1.099643      0.538200
55932 O      -2.528651       0.067387      0.497333
55933 O      -2.944048      -0.084990     -0.852988
55934 H       0.057819      -2.031381     -1.302467
55935 C       1.139249      -0.197182      1.811397
55936 H       1.663134      -1.099877      2.118391
55937 H       0.407708       0.059089      2.581697
55938 H       1.853379       0.618425      1.720291
55939 C       1.981892      -0.967984     -0.756647
55940 O       3.044613      -0.818098     -0.367638
55941 H      -2.454305      -0.884849     -1.098629
55942 H      -0.437038       0.549868     -1.208272
55943 O       0.497558       1.937047     -0.010290
55944 O       1.651768       1.838201     -0.835265
55945 H       1.483823       2.534686     -1.482147
55946 H      -1.417872       1.289298      1.599500
55947 H      -1.978502       2.002643      0.069554
55948 Rotational constants (GHz): 1.2723800      0.7409200      0.6003500
55949 Vibrational harmonic frequencies (cm-1):
55950 i319.7794          31.8423          70.9395
55951 105.1777          131.8438         146.8363
55952 164.3776          183.0684         189.0009
55953 198.3912          209.2736         222.9329
55954 258.2058          284.1941         312.8027
55955 341.0920          370.2226         423.6252
55956 435.2899          483.4831         496.0260
55957 525.6613          585.7866         634.4170
55958 769.1526          940.2938         957.2605
55959 1000.6635         1024.7630        1049.3451
55960 1050.7070         1107.0950        1141.9305
55961 1162.4073         1240.7583        1279.5889
55962 1295.7108         1334.1195        1378.7507
55963 1401.4676         1407.9258        1417.9771
55964 1429.1526         1462.9730        1472.3331
55965 1481.0685         1493.1054        2073.2994
55966 3056.1769         3069.1213        3099.3936
55967 3131.0050         3134.5719        3169.9054
55968 3686.4665         3752.4098        3824.2853
55969 Zero-point correction (Hartree): 0.152864
55970
55971 TS.triHPacyl.COelim.ppmpttmpd
55972 -----
55973 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16082380
55974 Electronic state : 2-A
55975 Cartesian coordinates (Angs):
55976 O      -0.452006      -1.961701      -1.028735
55977 O       0.074678      -1.818218      0.278425
55978 C       0.602303      -0.567356      0.459680
55979 C      -0.191166       0.604960     -0.064832
55980 C      -1.504952       0.839749      0.689099
55981 O      -2.386824      -0.251822      0.604862
55982 O      -2.842197      -0.334128     -0.740170
55983 H       0.356332      -1.969149     -1.568652
55984 C       1.238466      -0.482568      1.805492
55985 H       1.899500      -1.333424      1.960344
55986 H       0.480149      -0.489526      2.592813
55987 H       1.813857       0.437805      1.878083
55988 C       2.193539      -0.652537     -0.888529
55989 O       3.166639      -0.183113     -0.524546

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55990	H	-2.310005	-1.073412	-1.070302	
55991	H	-0.398249	0.474711	-1.127100	
55992	O	0.661814	1.728199	0.113232	
55993	O	0.108009	2.805145	-0.628641	
55994	H	0.767982	2.916910	-1.324180	
55995	H	-1.305786	0.961271	1.754742	
55996	H	-1.973816	1.746419	0.303395	
55997	Rotational constants (GHz):		1.0973300	0.7858300	0.5912900
55998	Vibrational harmonic frequencies (cm-1):				
55999	i281.7247		26.1679		61.3273
56000	91.6601		112.5565		133.7977
56001	151.6247		159.3166		184.6472
56002	190.8428		215.1070		223.8292
56003	239.8556		272.1701		301.1687
56004	327.3601		363.0448		395.3302
56005	442.1880		463.4314		474.6470
56006	522.4419		575.4292		617.3513
56007	792.2584		944.4685		959.3578
56008	1007.8768		1030.3421		1050.2365
56009	1059.6960		1106.2575		1128.7562
56010	1142.3792		1250.1219		1284.0924
56011	1306.9780		1340.4152		1378.3135
56012	1408.4582		1412.6871		1415.6819
56013	1422.9583		1456.2831		1472.9823
56014	1478.3426		1497.5013		2083.1169
56015	3052.1977		3076.2722		3104.0478
56016	3128.3455		3134.5371		3167.2294
56017	3714.6702		3762.2964		3818.2843
56018	Zero-point correction (Hartree): 0.152484				
56019					
56020	TS.triHPacyl.COelim.ppmpttpd				
56021	-----				
56022	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16024731				
56023	Electronic state : 2-A				
56024	Cartesian coordinates (Angs):				
56025	O	-0.421740	-1.960498	-1.035989	
56026	O	0.100882	-1.812807	0.272617	
56027	C	0.613236	-0.554758	0.454831	
56028	C	-0.201272	0.605493	-0.064123	
56029	C	-1.514392	0.818749	0.695567	
56030	O	-2.383227	-0.282984	0.619667	
56031	O	-2.838952	-0.379282	-0.723761	
56032	H	0.384991	-1.923384	-1.578214	
56033	C	1.247752	-0.462591	1.801110	
56034	H	1.923233	-1.302296	1.954091	
56035	H	0.490958	-0.483345	2.589716	
56036	H	1.810823	0.465718	1.872957	
56037	C	2.197868	-0.616043	-0.885304	
56038	O	3.177861	-0.174457	-0.506415	
56039	H	-2.283430	-1.100165	-1.057597	
56040	H	-0.408453	0.473343	-1.125196	
56041	O	0.634309	1.743109	0.098383	
56042	O	0.152707	2.741457	-0.793242	
56043	H	-0.035437	3.467680	-0.186740	
56044	H	-1.313666	0.945358	1.760780	
56045	H	-2.002880	1.715677	0.307638	
56046	Rotational constants (GHz):		1.1004400	0.7834300	0.5927900
56047	Vibrational harmonic frequencies (cm-1):				
56048	i293.4088		30.5481		64.7412
56049	91.3402		108.4784		134.4298
56050	156.0759		164.2949		186.0255
56051	191.8747		208.2275		218.2225
56052	238.4666		272.2835		301.6202
56053	328.6919		364.3865		408.2053
56054	441.6126		468.1856		479.0300
56055	522.1015		576.3461		618.5811
56056	792.1602		944.0239		959.7918
56057	1008.8993		1031.3381		1050.7431
56058	1061.6104		1106.7375		1128.0896
56059	1145.6953		1250.1280		1286.3082
56060	1308.9478		1341.4407		1379.2102
56061	1404.8761		1409.7711		1420.6387

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56062      1425.2331      1459.6116      1473.1983
56063      1477.7333      1497.1580      2086.3678
56064      3051.2883      3062.3828      3113.1058
56065      3126.7226      3128.9774      3165.2652
56066      3702.4560      3754.4185      3833.3799
56067 Zero-point correction (Hartree): 0.152549
56068
56069 TS.triHPacyl.COelim.pmpmmpmmd
56070 -----
56071 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16185626
56072 Electronic state : 2-A
56073 Cartesian coordinates (Angs):
56074 O      -0.369831      -1.517986      -1.511838
56075 O      -0.287048      -1.533926      -0.094595
56076 C       0.321004      -0.400237      0.387522
56077 C      -0.044434      0.908027      -0.278761
56078 C      -1.519465      1.287988      -0.086082
56079 O      -2.388985      0.255846      -0.530675
56080 O      -2.813696      -0.512550      0.586642
56081 H      -1.233816      -1.090792      -1.647829
56082 C       0.374874      -0.467106      1.878647
56083 H       0.794369      -1.421139      2.194757
56084 H      -0.625733      -0.366240      2.309392
56085 H       0.994352      0.344805      2.253415
56086 C       2.345504      -0.644873      -0.075681
56087 O       2.643410      -1.743839      -0.094861
56088 H      -2.203318      -1.265957      0.560702
56089 H       0.175419      0.858974      -1.343836
56090 O       0.703225      1.962736      0.293809
56091 O       1.796961      2.285784      -0.548837
56092 H       2.433605      1.586184      -0.332309
56093 H      -1.736322      1.521482      0.955175
56094 H      -1.735734      2.161362      -0.700501
56095 Rotational constants (GHz):      1.1275100      0.8024700      0.6028900
56096 Vibrational harmonic frequencies (cm-1):
56097 i301.0808      50.3924      83.0264
56098      104.6504      111.8803      136.0064
56099      173.8061      194.6686      205.5355
56100      215.4512      220.7454      256.0372
56101      276.6505      289.7290      338.5476
56102      379.4106      435.8345      454.2651
56103      463.6999      481.3110      530.2710
56104      554.1521      589.5857      627.4119
56105      778.7294      931.2733      962.2304
56106      1012.6661      1024.8139      1055.6104
56107      1060.8711      1107.3508      1116.6639
56108      1151.3538      1231.1424      1274.7242
56109      1310.2452      1341.4595      1371.3497
56110      1398.1703      1410.8593      1445.2475
56111      1457.3634      1469.6769      1478.7318
56112      1482.9829      1501.5544      2094.7346
56113      3046.7539      3093.1714      3118.2297
56114      3123.4499      3153.1607      3164.2047
56115      3704.1991      3730.7193      3746.1402
56116 Zero-point correction (Hartree): 0.153828
56117
56118 TS.triHPacyl.COelim.pmpmptmmd
56119 -----
56120 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16092818
56121 Electronic state : 2-A
56122 Cartesian coordinates (Angs):
56123 O       0.130775      2.199389      -1.244138
56124 O       0.277132      1.808134      0.111787
56125 C      -0.238299      0.549895      0.328090
56126 C       0.192424      -0.523260      -0.654482
56127 C       1.413366      -1.338069      -0.208532
56128 O       2.612905      -0.611364      -0.360715
56129 O       2.739591      0.277776      0.741971
56130 H      -0.826630      2.356257      -1.293062
56131 C      -0.301809      0.302953      1.799988
56132 H      -0.829448      1.119412      2.291009
56133 H       0.705819      0.239180      2.215976

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56134	H	-0.817292	-0.633280	1.997794	
56135	C	-2.258982	0.881409	-0.169382	
56136	O	-2.999418	0.183754	0.350045	
56137	H	2.465055	1.123399	0.359755	
56138	H	0.449841	-0.033085	-1.593116	
56139	O	-0.866727	-1.385804	-1.033906	
56140	O	-1.231370	-2.180176	0.091160	
56141	H	-2.122593	-1.851173	0.274726	
56142	H	1.321658	-1.707512	0.812397	
56143	H	1.510289	-2.184453	-0.889206	
56144	Rotational constants (GHz):		1.1918000	0.7932400	0.6173800
56145	Vibrational harmonic frequencies (cm-1):				
56146	i294.4304		62.2868		88.0664
56147	116.2769		144.1086		150.5262
56148	164.5943		168.1540		174.7287
56149	207.5975		221.3845		243.0130
56150	281.7685		299.1805		334.5061
56151	359.8379		367.7530		372.3858
56152	381.0514		430.4365		497.0485
56153	525.1420		569.8607		658.0037
56154	819.9640		941.3177		955.6658
56155	963.1742		1021.6448		1046.4969
56156	1053.2987		1086.8844		1122.0981
56157	1130.4289		1221.7805		1275.8151
56158	1299.8537		1327.8417		1386.8883
56159	1396.7230		1407.3891		1425.0319
56160	1431.5937		1438.6567		1470.8784
56161	1478.8127		1504.3437		2065.3856
56162	3064.2282		3086.8169		3125.4459
56163	3132.3792		3144.9783		3172.8937
56164	3727.9127		3783.7473		3787.9590
56165	Zero-point correction (Hartree): 0.152902				
56166	TS.triHPacyl.COelim.pppppmpmd				
56167	-----				
56168	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16201046				
56169	Electronic state : 2-A				
56170	Cartesian coordinates (Angs):				
56171	O	2.279769	-1.320909	-0.995546	
56172	O	1.696059	-1.306623	0.297936	
56173	C	0.707675	-0.362153	0.403264	
56174	C	-0.271085	-0.303255	-0.756603	
56175	C	-1.523140	-1.156024	-0.529306	
56176	O	-2.355027	-0.749388	0.532352	
56177	O	-3.293064	0.194220	0.042190	
56178	H	3.067421	-0.776918	-0.849909	
56179	C	0.250722	-0.343664	1.827786	
56180	H	1.112983	-0.255010	2.487684	
56181	H	-0.280943	-1.266356	2.071589	
56182	H	-0.434600	0.482134	1.992506	
56183	C	1.792409	1.450683	0.298892	
56184	O	2.908836	1.247533	0.167330	
56185	H	-2.799243	1.025810	0.120258	
56186	H	0.233373	-0.724031	-1.626672	
56187	O	-0.551066	1.018068	-1.194480	
56188	O	-1.069596	1.787293	-0.120373	
56189	H	-0.262739	2.198457	0.230470	
56190	H	-2.106974	-1.191164	-1.450051	
56191	H	-1.196034	-2.167989	-0.275360	
56192	Rotational constants (GHz):		1.5008800	0.6584400	0.5831300
56193	Vibrational harmonic frequencies (cm-1):				
56194	i285.1659		56.3504		78.8860
56195	95.6779		160.8316		166.6129
56196	192.2644		213.3304		231.1577
56197	250.2791		259.7350		260.6022
56198	265.1723		291.8848		328.5399
56199	335.8604		371.1828		435.2433
56200	487.3452		507.6457		550.2301
56201	558.1157		573.1855		726.6574
56202	832.7301		911.4639		958.2410
56203	959.7015		1003.2225		1033.4623
56204	1052.0898		1061.7705		1125.6194

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56206      1155.3831      1215.5125      1283.0113
56207      1320.2640      1341.1471      1394.2799
56208      1402.9691      1415.9324      1421.3615
56209      1427.9417      1457.4333      1459.3989
56210      1476.6129      1491.6462      2067.1538
56211      3060.2101      3061.5329      3117.0360
56212      3121.0535      3127.0090      3184.8286
56213      3707.1085      3733.8727      3783.1903
56214      Zero-point correction (Hartree): 0.153915
56215
56216      TS.triHPacyl.COelim.pppppppmmd
56217      -----
56218      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16116944
56219      Electronic state : 2-A
56220      Cartesian coordinates (Angs):
56221      O      1.582529      -1.665243      -1.102169
56222      O      1.201426      -1.505597      0.257341
56223      C      0.601638      -0.293363      0.450396
56224      C      -0.347803      0.166089      -0.641367
56225      C      -1.482184      -0.840128      -0.862052
56226      O      -2.290691      -1.013295      0.280234
56227      O      -3.284422      0.000846      0.298466
56228      H      2.527828      -1.460640      -1.054696
56229      C      0.216730      -0.153598      1.885889
56230      H      1.072672      -0.369530      2.524039
56231      H      -0.595089      -0.840781      2.131268
56232      H      -0.122108      0.862855      2.074613
56233      C      2.257435      1.029595      0.351147
56234      O      3.208880      0.449917      0.095837
56235      H      -2.785616      0.793517      0.547336
56236      H      0.180027      0.292360      -1.586456
56237      O      -0.948353      1.397994      -0.279854
56238      O      -0.115815      2.474869      -0.673353
56239      H      0.561876      2.494343      0.019969
56240      H      -2.098399      -0.522396      -1.703555
56241      H      -1.044520      -1.817215      -1.068623
56242      Rotational constants (GHz):      1.3219600      0.6923100      0.5735100
56243      Vibrational harmonic frequencies (cm-1):
56244      i271.9741      23.8919      43.2891
56245      75.2246      108.4446      148.1843
56246      153.2587      172.4658      185.1854
56247      211.5665      241.5540      242.3159
56248      263.1574      291.5342      314.4266
56249      319.7235      385.2411      393.7524
56250      404.1782      453.7919      482.3141
56251      517.5664      600.6907      706.9530
56252      814.0083      890.9782      948.9026
56253      990.8785      1001.5366      1049.8954
56254      1064.1074      1076.2794      1131.3524
56255      1159.6297      1244.1794      1291.5884
56256      1313.2744      1320.7495      1370.8146
56257      1396.8296      1410.6450      1419.0948
56258      1450.4506      1457.1159      1463.6016
56259      1473.1681      1493.4006      2060.4108
56260      3062.9417      3081.6713      3111.5989
56261      3133.0704      3142.5085      3161.1031
56262      3743.3746      3762.4710      3785.2112
56263      Zero-point correction (Hartree): 0.152673
56264
56265      TS.triHPacyl.COelim.pppppptpmd
56266      -----
56267      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16294967
56268      Electronic state : 2-A
56269      Cartesian coordinates (Angs):
56270      O      1.812471      -1.316609      -1.230860
56271      O      1.500893      -1.314840      0.155065
56272      C      0.797505      -0.189097      0.495381
56273      C      -0.234880      0.269510      -0.509028
56274      C      -1.203344      -0.850776      -0.899269
56275      O      -1.981451      -1.314745      0.185875
56276      O      -3.007282      -0.359234      0.442379
56277      H      2.697267      -0.922166      -1.227143

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56278	C	0.475272	-0.222833	1.951230	
56279	H	1.369239	-0.475504	2.519789	
56280	H	-0.294454	-0.970525	2.158848	
56281	H	0.122691	0.757162	2.263666	
56282	C	2.275124	1.343701	0.385643	
56283	O	3.212095	0.959015	-0.145206	
56284	H	-2.635809	0.130182	1.189936	
56285	H	0.249265	0.629136	-1.420157	
56286	O	-0.901011	1.352758	0.121247	
56287	O	-1.771772	1.939203	-0.828850	
56288	H	-2.586349	1.430766	-0.685977	
56289	H	-1.857150	-0.527402	-1.710510	
56290	H	-0.634310	-1.719062	-1.229390	
56291	Rotational constants (GHz):			1.4077300	0.6554900 0.5798900
56292	Vibrational harmonic frequencies (cm-1):				
56293	i288.9078		31.9079		61.0298
56294	74.3626		127.1543		155.3094
56295	170.4823		192.5621		198.9964
56296	214.7372		225.2109		232.1286
56297	263.0252		275.2587		309.7422
56298	360.3671		375.2746		395.5928
56299	440.6840		479.7648		535.4427
56300	551.5282		579.7969		736.9159
56301	817.2600		883.9926		952.0641
56302	967.5992		1017.4065		1048.9744
56303	1054.8143		1075.2306		1113.0273
56304	1165.3173		1252.3600		1292.9677
56305	1305.2586		1343.9438		1374.4412
56306	1399.9402		1406.3319		1414.7514
56307	1419.8512		1452.8285		1477.7740
56308	1478.1400		1496.1390		2052.6248
56309	3053.0464		3071.2471		3085.4201
56310	3127.6114		3148.4086		3166.6091
56311	3729.1663		3772.7957		3787.2691
56312	Zero-point correction (Hartree): 0.153074				
56313	-----				
56314	TS.triHPacyl.COelim.pppppptppd				
56315	-----				
56316	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16134667				
56317	Electronic state : 2-A				
56318	Cartesian coordinates (Angs):				
56319	O	1.781427	-1.380134	-1.196364	
56320	O	1.485265	-1.322678	0.192580	
56321	C	0.817800	-0.165453	0.502617	
56322	C	-0.219893	0.286469	-0.499695	
56323	C	-1.203949	-0.832237	-0.853942	
56324	O	-1.984691	-1.255462	0.247866	
56325	O	-3.040762	-0.313741	0.429873	
56326	H	2.672576	-1.001165	-1.215489	
56327	C	0.520170	-0.131931	1.962767	
56328	H	1.410828	-0.408672	2.525305	
56329	H	-0.288152	-0.825033	2.205895	
56330	H	0.213567	0.872716	2.241754	
56331	C	2.344234	1.321797	0.306348	
56332	O	3.269874	0.878431	-0.198585	
56333	H	-3.813039	-0.873098	0.282238	
56334	H	0.258797	0.605234	-1.430163	
56335	O	-0.848426	1.393962	0.111849	
56336	O	-1.776688	1.934576	-0.810517	
56337	H	-2.594379	1.515299	-0.501887	
56338	H	-1.854856	-0.521176	-1.671527	
56339	H	-0.643509	-1.715610	-1.158319	
56340	Rotational constants (GHz):			1.4279500	0.6437200 0.5688500
56341	Vibrational harmonic frequencies (cm-1):				
56342	i285.4479		28.5290		59.1467
56343	67.7956		124.3357		159.6439
56344	171.1021		178.2342		180.4033
56345	205.2889		221.2550		231.6262
56346	259.7769		272.2694		295.4780
56347	303.7745		356.3252		375.6693
56348	439.1429		480.7237		490.0687
56349	545.5899		579.2025		734.9450

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56350      810.5347      880.0741      951.2265
56351      971.4512      1016.4648     1048.9056
56352     1052.9135     1076.6972     1109.7351
56353     1173.5415     1250.3792     1296.6542
56354     1305.8998     1347.5530     1375.6996
56355     1392.0335     1407.8536     1414.9554
56356     1417.2565     1451.2551     1471.5456
56357     1474.3706     1490.3599     2050.2729
56358     3059.4981     3060.6582     3087.1010
56359     3131.7302     3148.0796     3172.2259
56360     3752.9061     3773.0294     3825.3457
56361 Zero-point correction (Hartree): 0.152657
56362
56363 TS.triHPacyl.COelim.pppptmpmd
56364 -----
56365 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16111838
56366 Electronic state : 2-A
56367 Cartesian coordinates (Angs):
56368 O      2.332782     -1.611271     -0.852633
56369 O      1.730553     -1.433507      0.418547
56370 C      0.826434     -0.401650      0.407555
56371 C     -0.168134     -0.428276     -0.736607
56372 C     -1.412623     -1.265055     -0.424013
56373 O     -2.228231     -0.777829      0.616955
56374 O     -3.213356      0.079103      0.064103
56375 H      2.941082     -0.855106     -0.879916
56376 C      0.419732     -0.124054      1.817984
56377 H      1.306689      0.009117      2.436092
56378 H     -0.160406     -0.959735      2.217441
56379 H     -0.207174      0.760820      1.866785
56380 C      2.132170      1.218908     -0.072814
56381 O      1.760253      2.246175      0.261350
56382 H     -2.750883      0.931407      0.044115
56383 H      0.325782     -0.918184     -1.576421
56384 O     -0.451102      0.852204     -1.282659
56385 O     -1.035636      1.688896     -0.292521
56386 H     -0.319241      2.310846     -0.102190
56387 H     -2.012865     -1.378293     -1.327572
56388 H     -1.070574     -2.250275     -0.096093
56389 Rotational constants (GHz): 1.2664900      0.7417000      0.6001500
56390 Vibrational harmonic frequencies (cm-1):
56391 i267.7887      63.9395      75.7256
56392 110.4447      145.3012      150.0876
56393 168.4645      178.4384      201.9155
56394 215.5792      233.6986      258.7567
56395 270.6726      294.5080      323.0184
56396 361.3194      371.9491      389.0125
56397 437.3133      503.5588      519.9440
56398 543.9574      573.3993      720.5176
56399 829.9946      904.3223      954.6898
56400 955.8393     1002.6385     1029.5879
56401 1047.7689     1061.8436     1125.7923
56402 1155.7419     1218.9542     1285.3693
56403 1322.4349     1339.7604     1386.7195
56404 1403.7902     1410.3232     1421.5138
56405 1437.7930     1457.0327     1459.8430
56406 1467.7354     1486.6097     2062.8290
56407 3057.7156     3064.1720     3117.1369
56408 3122.7133     3126.4735     3185.7586
56409 3737.0077     3740.3138     3783.9180
56410 Zero-point correction (Hartree): 0.153265
56411
56412 TS.triHPacyl.COelim.pppptmpmd
56413 -----
56414 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16091731
56415 Electronic state : 2-A
56416 Cartesian coordinates (Angs):
56417 O     -1.061147      2.262817     -0.905037
56418 O     -0.819026      1.785040      0.408826
56419 C     -0.595674      0.434080      0.378139
56420 C      0.324877     -0.052806     -0.727283
56421 C      1.644351      0.724020     -0.747711

```

56422	O	2.354155	0.631327	0.467077
56423	O	3.122396	-0.563096	0.460416
56424	H	-1.966967	1.946377	-1.058136
56425	C	-0.418598	-0.081071	1.767499
56426	H	-1.185255	0.336394	2.417547
56427	H	0.566843	0.193903	2.149025
56428	H	-0.503894	-1.166779	1.784457
56429	C	-2.515171	-0.178790	-0.138238
56430	O	-2.900208	-1.098972	0.420021
56431	H	2.456273	-1.255127	0.586824
56432	H	-0.149807	0.057216	-1.703385
56433	O	0.662800	-1.416444	-0.533302
56434	O	-0.443350	-2.213761	-0.923192
56435	H	-0.867587	-2.430541	-0.081098
56436	H	2.269113	0.369487	-1.568031
56437	H	1.417611	1.781181	-0.880127
56438	Rotational constants (GHz): 1.2122400 0.7527800 0.5920900			
56439	Vibrational harmonic frequencies (cm-1):			
56440	i286.4454	49.6336	60.6645	
56441	91.6364	129.7325	147.3107	
56442	156.4605	164.4061	169.3259	
56443	204.8456	228.5625	244.3729	
56444	271.0339	300.6035	321.2763	
56445	339.8878	373.4747	384.4142	
56446	388.8832	440.4186	495.5886	
56447	512.0922	604.6809	701.5556	
56448	815.9074	887.5042	949.4123	
56449	988.3778	1002.2095	1049.7379	
56450	1057.3814	1071.2174	1131.7929	
56451	1162.4134	1253.8270	1290.6593	
56452	1307.2060	1327.1337	1374.5555	
56453	1396.4667	1403.8909	1418.2461	
56454	1433.2701	1451.0725	1463.6338	
56455	1467.2069	1494.1406	2062.1187	
56456	3062.7131	3086.2144	3097.9706	
56457	3133.5321	3152.6676	3156.9726	
56458	3726.4330	3762.7919	3787.7983	
56459	Zero-point correction (Hartree): 0.152654			
56460				
56461	TS.triHPacyl.COelim.ppppptppmd			
56462	-----			
56463	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16148243			
56464	Electronic state : 2-A			
56465	Cartesian coordinates (Angs):			
56466	O	-1.001851	2.275090	-0.843786
56467	O	-0.786988	1.731005	0.450479
56468	C	-0.593146	0.374373	0.358343
56469	C	0.338264	-0.065256	-0.757203
56470	C	1.644136	0.733678	-0.762006
56471	O	2.325741	0.682080	0.469976
56472	O	3.082524	-0.518454	0.525046
56473	H	-1.898799	1.956746	-1.039243
56474	C	-0.445406	-0.220372	1.717696
56475	H	-1.218539	0.171625	2.375813
56476	H	0.534262	0.025539	2.133711
56477	H	-0.550914	-1.301713	1.655522
56478	C	-2.494507	-0.153084	-0.229720
56479	O	-3.025617	-0.926549	0.419252
56480	H	2.409380	-1.190969	0.707160
56481	H	-0.144734	0.059245	-1.729894
56482	O	0.713945	-1.423436	-0.590119
56483	O	-0.461216	-2.218755	-0.690427
56484	H	-0.295469	-2.704715	-1.508127
56485	H	2.296218	0.377491	-1.560743
56486	H	1.400250	1.782873	-0.920220
56487	Rotational constants (GHz): 1.2406100 0.7546400 0.5941000			
56488	Vibrational harmonic frequencies (cm-1):			
56489	i303.2303	58.0093	69.3689	
56490	90.2995	133.5760	163.2732	
56491	171.3837	172.3824	186.3451	
56492	204.7910	212.9684	230.7040	
56493	250.4334	288.6059	298.8353	

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56494      333.0410      368.2676      383.3624
56495      393.0065      439.1415      496.5730
56496      516.9330      604.2512      703.5041
56497      818.2363      886.1532      951.3950
56498      986.4676      1001.7281     1046.5455
56499      1054.6421     1068.3737     1133.8552
56500      1162.5330     1251.6410     1291.3980
56501      1303.8420     1335.2464     1372.3902
56502      1397.5841     1406.1376     1410.1363
56503      1435.3517     1448.3960     1465.7668
56504      1475.4135     1494.9989     2078.3816
56505      3060.2077     3067.7720     3085.8078
56506      3136.4398     3155.4326     3165.2185
56507      3722.2891     3764.8281     3821.6533
56508 Zero-point correction (Hartree): 0.152695
56509
56510 TS.triHPacyl.COelim.ppppptommd
56511 -----
56512 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16138810
56513 Electronic state : 2-A
56514 Cartesian coordinates (Angs):
56515 O      1.616334      -1.793700      -1.242131
56516 O      1.347045      -1.636038      0.142701
56517 C      0.847167      -0.387197      0.385562
56518 C      -0.204280      0.095218      -0.589940
56519 C      -1.354286      -0.900516      -0.746735
56520 O      -2.015562      -1.131155      0.478300
56521 O      -3.000468      -0.122932      0.659027
56522 H      2.439876      -1.287440      -1.331924
56523 C      0.683341      -0.170375      1.851199
56524 H      1.573852      -0.515590      2.374020
56525 H      -0.184653      -0.720344      2.221959
56526 H      0.539800      0.889440      2.051493
56527 C      2.496951      0.821067      -0.141250
56528 O      2.525627      1.833626      0.381340
56529 H      -2.471409      0.646005      0.916696
56530 H      0.241620      0.275394      -1.571131
56531 O      -0.655475      1.333975      -0.049923
56532 O      -1.445828      1.968617      -1.047088
56533 H      -0.909672      2.747295      -1.243700
56534 H      -2.067175      -0.540360      -1.488595
56535 H      -0.948989      -1.862731      -1.059642
56536 Rotational constants (GHz): 1.1786000      0.7332000      0.5951200
56537 Vibrational harmonic frequencies (cm-1):
56538 i272.1057      39.5603      52.2406
56539 64.6185      110.4499      129.2988
56540 148.3668      170.4003      182.9716
56541 205.4197      217.6236      226.9010
56542 260.6792      276.7084      295.2438
56543 325.4378      348.4843      387.0143
56544 424.6497      444.9857      480.6058
56545 528.2734      583.5006      723.0657
56546 825.3811      883.3407      954.4910
56547 974.2133      1013.6628     1044.4076
56548 1050.8015     1076.3432     1118.3279
56549 1151.6673     1262.6845     1292.8974
56550 1304.2118     1338.0115     1379.4570
56551 1396.7457     1405.6155     1413.2301
56552 1428.4884     1435.0943     1468.5424
56553 1473.6235     1493.4312     2083.7979
56554 3058.6952     3071.3792     3088.7077
56555 3131.9607     3145.9177     3162.4588
56556 3736.6708     3775.6656     3819.2289
56557 Zero-point correction (Hartree): 0.152377
56558
56559 TS.triHPacyl.COelim.ppppptompm
56560 -----
56561 IRC pathway available
56562 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18848260
56563 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07138868
56564 T1 diagnostic: 0.016670
56565 E(MP2/Aug-CC-pVTZ) (Hartree): -721.03225919

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56566 E(MP3/Aug-CC-pVTZ) (Hartree): -721.05011460
56567 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03754098
56568 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05353104
56569 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51222966
56570 E(UHF/Aug-CC-pVTZ) (Hartree): -718.50527032
56571 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16413562
56572 Electronic state : 2-A
56573 Cartesian coordinates (Angs):
56574 O 1.665816 -1.834600 -1.136204
56575 O 1.424431 -1.555839 0.234145
56576 C 0.877770 -0.308239 0.373955
56577 C -0.211120 0.042165 -0.615521
56578 C -1.326109 -1.004533 -0.646212
56579 O -2.021763 -1.113006 0.579490
56580 O -2.906445 -0.000930 0.690548
56581 H 2.431703 -1.263966 -1.314660
56582 C 0.720803 0.023482 1.819421
56583 H 1.634320 -0.227812 2.355772
56584 H -0.108017 -0.541770 2.253369
56585 H 0.525875 1.088161 1.930128
56586 C 2.469185 0.886890 -0.265177
56587 O 2.591085 1.869570 0.298177
56588 H -2.409418 0.586429 1.277247
56589 H 0.202216 0.122922 -1.623592
56590 O -0.679542 1.317523 -0.203283
56591 O -1.587882 1.785564 -1.183196
56592 H -2.429381 1.432164 -0.852253
56593 H -2.029945 -0.793046 -1.452463
56594 H -0.886122 -1.987939 -0.809758
56595 Rotational constants (GHz): 1.2188100 0.7187300 0.5956400
56596 Vibrational harmonic frequencies (cm-1):
56597 1289.0072 49.2456 58.5135
56598 73.6100 131.3731 155.1519
56599 162.9338 180.9778 189.7163
56600 214.3210 228.1673 237.9354
56601 268.9043 299.4523 328.2252
56602 350.8592 395.5108 407.5271
56603 443.1509 481.6229 530.7548
56604 547.6303 586.6333 734.3018
56605 817.6645 883.3549 953.8300
56606 966.9906 1015.7131 1049.3214
56607 1054.0954 1075.6412 1112.8773
56608 1166.3555 1259.6429 1292.5741
56609 1305.0436 1347.2193 1375.4004
56610 1399.9629 1406.9434 1415.1522
56611 1432.7581 1453.4489 1475.6812
56612 1477.9279 1495.3701 2089.9455
56613 3052.3784 3073.5724 3086.1911
56614 3129.0772 3146.3719 3163.8966
56615 3723.1295 3731.6578 3788.3451
56616 Zero-point correction (Hartree): 0.153262
56617
56618 TS.triHPacyl.COelim.ppppttpd
56619 -----
56620 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16274793
56621 Electronic state : 2-A
56622 Cartesian coordinates (Angs):
56623 O 1.622161 -1.865792 -1.129938
56624 O 1.388830 -1.578489 0.240875
56625 C 0.888691 -0.310443 0.380050
56626 C -0.190423 0.080307 -0.605659
56627 C -1.323490 -0.946189 -0.653087
56628 O -2.027025 -1.057196 0.569463
56629 O -2.940689 0.035556 0.653080
56630 H 2.391718 -1.301162 -1.313071
56631 C 0.749144 0.037040 1.822577
56632 H 1.637081 -0.283376 2.364851
56633 H -0.130568 -0.450602 2.248145
56634 H 0.629864 1.113112 1.926526
56635 C 2.529910 0.815004 -0.277485
56636 O 2.696174 1.795316 0.278460
56637 H -3.783851 -0.432312 0.688643

56638	H	0.223293	0.153346	-1.615559		
56639	O	-0.615979	1.358137	-0.177034		
56640	O	-1.571530	1.837160	-1.105134		
56641	H	-2.393182	1.593753	-0.651828		
56642	H	-2.017719	-0.710960	-1.460327		
56643	H	-0.895169	-1.933650	-0.823932		
56644	Rotational constants (GHz):			1.2389700	0.7054200	0.5835500
56645	Vibrational harmonic frequencies (cm-1):					
56646	i283.0136		48.8726			57.1935
56647	67.2930		137.7889			152.3774
56648	162.6675		173.4711			180.9972
56649	200.1636		223.5359			237.2060
56650	256.5189		271.9287			295.4074
56651	326.4755		352.0094			418.0012
56652	443.8056		486.5596			491.8260
56653	535.3315		586.2709			732.6771
56654	811.5791		879.2295			954.0786
56655	971.4797		1015.2652			1049.0889
56656	1053.2233		1077.5634			1109.5638
56657	1175.0716		1258.3343			1295.7435
56658	1306.7124		1350.3736			1377.0421
56659	1392.0740		1407.8657			1416.8538
56660	1434.6920		1451.4473			1470.9864
56661	1472.9972		1490.8535			2090.4247
56662	3059.4316		3060.5846			3087.3260
56663	3134.3326		3146.8354			3167.7141
56664	3717.6102		3754.0895			3827.5999
56665	Zero-point correction (Hartree): 0.152880					
56666	TS.triHPacyl.COelim.pptmppmmmd					
56667	-----					
56668	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16113688					
56669	Electronic state : 2-A					
56670	Cartesian coordinates (Angs):					
56671	O	1.587167	-1.932362	0.184570		
56672	O	1.575313	-0.800677	1.046946		
56673	C	0.964351	0.265357	0.434265		
56674	C	-0.288951	-0.051875	-0.357864		
56675	C	-1.251996	-0.921981	0.451608		
56676	O	-2.369878	-1.335716	-0.310897		
56677	O	-3.316924	-0.271019	-0.347877		
56678	H	2.462451	-1.848719	-0.221301		
56679	C	1.043180	1.460601	1.321353		
56680	H	2.060028	1.562591	1.699123		
56681	H	0.359139	1.375454	2.168999		
56682	H	0.772698	2.346875	0.754007		
56683	C	2.349720	0.787800	-1.093981		
56684	O	3.233946	0.061979	-1.101981		
56685	H	-4.071492	-0.678389	0.094016		
56686	H	-0.028137	-0.606633	-1.261205		
56687	O	-0.881900	1.119982	-0.875258		
56688	O	-1.538727	1.831199	0.166368		
56689	H	-2.441054	1.491511	0.063234		
56690	H	-0.743278	-1.848528	0.713282		
56691	H	-1.580165	-0.420658	1.362592		
56692	Rotational constants (GHz):			1.4649800	0.6181700	0.5328200
56693	Vibrational harmonic frequencies (cm-1):					
56694	i292.3714		35.7776			62.7496
56695	86.4371		115.3058			167.9822
56696	180.1449		197.5003			211.1397
56697	221.9529		234.7995			251.9307
56698	262.2506		283.2793			295.2064
56699	315.6972		329.4948			369.0337
56700	458.7219		490.7024			526.1486
56701	545.7988		586.1688			669.8545
56702	828.0986		896.1437			953.4740
56703	969.0781		999.5290			1039.3538
56704	1045.4666		1106.2879			1121.4024
56705	1155.5494		1237.5506			1292.0693
56706	1312.0182		1329.2350			1380.0756
56707	1388.8857		1411.4531			1414.3965
56708	1416.2609		1460.9378			1468.1715


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56710      1478.8279          1484.5051          2049.0427
56711      3054.5088          3087.0295          3096.0278
56712      3125.0491          3154.4073          3175.3783
56713      3760.6274          3782.9059          3829.4144
56714      Zero-point correction (Hartree): 0.153096
56715
56716      TS.triHPacyl.COelim.pptmppmpd
56717      -----
56718      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16283566
56719      Electronic state : 2-A
56720      Cartesian coordinates (Angs):
56721      O      1.584888      -1.925964      0.179765
56722      O      1.591525      -0.786927      1.032779
56723      C      0.959845      0.269591      0.426373
56724      C     -0.317685     -0.068507     -0.315506
56725      C     -1.259769     -0.926784      0.528655
56726      O     -2.376756     -1.382989     -0.208451
56727      O     -3.295058     -0.304500     -0.367507
56728      H      2.462601     -1.860528     -0.224021
56729      C      1.072774      1.477843      1.292362
56730      H      2.102632      1.577995      1.633678
56731      H      0.417844      1.408312      2.163854
56732      H      0.788667      2.358512      0.723129
56733      C      2.280540      0.765754     -1.156112
56734      O      3.202531      0.089063     -1.141552
56735      H     -3.154930     -0.066394     -1.294116
56736      H     -0.079345     -0.634187     -1.218751
56737      O     -0.942939      1.092206     -0.834372
56738      O     -1.539187      1.833873      0.221866
56739      H     -2.422488      1.432515      0.255430
56740      H     -0.740054     -1.838392      0.818807
56741      H     -1.589203     -0.403309      1.427143
56742      Rotational constants (GHz): 1.4511700      0.6252300      0.5390000
56743      Vibrational harmonic frequencies (cm-1):
56744      i295.9049          37.5258          57.5284
56745      95.5679          114.3258          163.8016
56746      183.6202          203.1156          205.2153
56747      217.4141          236.2783          262.7825
56748      267.9639          294.3793          317.3164
56749      336.6602          348.2915          378.9830
56750      452.2148          494.4182          545.4371
56751      569.8662          591.3850          670.9128
56752      833.6708          900.9167          952.1231
56753      968.9487          999.0359          1040.1249
56754      1046.1934          1110.5399          1120.0939
56755      1147.7700          1238.4969          1288.0547
56756      1314.0883          1327.0338          1379.6933
56757      1400.4444          1410.1889          1412.7020
56758      1414.2649          1452.4131          1475.2719
56759      1479.1416          1486.5936          2051.4943
56760      3055.6579          3083.2017          3093.4315
56761      3125.4580          3156.1524          3175.5126
56762      3718.3339          3783.5407          3801.9624
56763      Zero-point correction (Hartree): 0.153292
56764
56765      TS.triHPacyl.COelim.pptmppmpd
56766      -----
56767      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16170589
56768      Electronic state : 2-A
56769      Cartesian coordinates (Angs):
56770      O      1.450612      -1.735454      -1.083645
56771      O      1.480558      -1.442799      0.305418
56772      C      0.847962     -0.259905      0.563832
56773      C     -0.427529      0.010681     -0.206514
56774      C     -1.484288     -1.048439      0.122205
56775      O     -2.662429     -0.843160     -0.617813
56776      O     -3.495218      0.057352      0.097186
56777      H      2.342880     -1.469174     -1.349399
56778      C      0.882434      0.009720      2.031843
56779      H      1.904057     -0.056787      2.403152
56780      H      0.274384     -0.717473      2.576229
56781      H      0.490194      1.004891      2.226984

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56782	C	2.261305	1.164094	-0.151138		
56783	O	3.155605	0.622380	-0.610978		
56784	H	-3.072611	0.910792	-0.079338		
56785	H	-0.256484	0.007406	-1.281332		
56786	O	-0.969332	1.270157	0.161210		
56787	O	-0.429695	2.278964	-0.678637		
56788	H	0.411897	2.488659	-0.246404		
56789	H	-1.095700	-2.021493	-0.180953		
56790	H	-1.718715	-1.063254	1.187760		
56791	Rotational constants (GHz):			1.3613100	0.6292500	0.5373800
56792	Vibrational harmonic frequencies (cm-1):					
56793		1269.7763	28.1551		60.9434	
56794		73.9968	99.3826		132.9614	
56795		149.9099	170.7782		176.5335	
56796		204.3726	226.9505		230.2431	
56797		267.3407	290.7289		308.2418	
56798		317.6261	364.6921		401.9132	
56799		413.5008	451.4595		484.6920	
56800		564.1005	582.8903		606.4077	
56801		834.5581	888.9479		961.2955	
56802		978.0059	1034.2815		1045.8569	
56803		1053.5603	1111.1872		1131.1651	
56804		1160.3169	1241.6094		1297.1209	
56805		1301.9019	1331.8828		1374.3277	
56806		1398.2808	1411.8099		1419.5702	
56807		1442.5747	1449.5127		1462.2128	
56808		1474.1219	1493.3309		2065.9628	
56809		3053.1835	3076.4348		3123.3500	
56810		3125.8750	3137.8659		3168.1961	
56811		3754.0302	3770.0165		3783.6322	
56812	Zero-point correction (Hartree): 0.152555					
56813	-----					
56814	TS.triHPacyl.COelim.pptmpptmpd					
56815	-----					
56816	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15982491					
56817	Electronic state : 2-A					
56818	Cartesian coordinates (Angs):					
56819	O	1.572350	-1.693323	-0.960333		
56820	O	1.656528	-1.281848	0.397738		
56821	C	1.003010	-0.094298	0.578301		
56822	C	-0.323438	0.053577	-0.128075		
56823	C	-1.259265	-1.109851	0.205593		
56824	O	-2.460680	-1.076264	-0.528998		
56825	O	-3.387306	-0.242201	0.149386		
56826	H	2.443529	-1.428340	-1.288836		
56827	C	1.149031	0.346924	1.995436		
56828	H	2.192075	0.270647	2.299349		
56829	H	0.548922	-0.275510	2.665097		
56830	H	0.816878	1.377515	2.091036		
56831	C	2.214310	1.302785	-0.499885		
56832	O	3.176391	0.797934	-0.852419		
56833	H	-3.216758	0.622694	-0.252033		
56834	H	-0.181129	0.094147	-1.208832		
56835	O	-0.832230	1.308534	0.311571		
56836	O	-1.707779	1.809581	-0.684892		
56837	H	-1.191709	2.534834	-1.058614		
56838	H	-0.769453	-2.039794	-0.085802		
56839	H	-1.482433	-1.130314	1.273990		
56840	Rotational constants (GHz):			1.4206100	0.6033800	0.5312500
56841	Vibrational harmonic frequencies (cm-1):					
56842		1274.9492	43.0413		55.5138	
56843		58.5697	97.4329		141.6932	
56844		150.6277	162.2417		179.3163	
56845		194.4750	205.2406		217.4565	
56846		226.8801	258.0988		288.1123	
56847		320.5140	322.9594		401.3946	
56848		432.7612	452.2902		488.5213	
56849		522.9079	577.3456		596.1782	
56850		875.9124	893.6635		969.3978	
56851		975.4681	1037.2461		1041.2807	
56852		1052.2705	1109.7010		1128.6029	
56853		1144.0096	1245.2548		1297.5113	

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56854      1307.1768          1337.1552          1380.4891
56855      1398.2040          1406.8807          1413.1763
56856      1416.2339          1449.1484          1458.4443
56857      1477.8562          1489.9058          2064.4001
56858      3047.6956          3073.6293          3095.4489
56859      3123.6074          3137.6605          3170.8220
56860      3765.9460          3790.4648          3817.8052
56861 Zero-point correction (Hartree): 0.152150
56862
56863 TS.triHPacyl.COelim.pptmpptpmd
56864 -----
56865 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16043499
56866 Electronic state : 2-A
56867 Cartesian coordinates (Angs):
56868 O      1.573914      -1.707008      -0.906985
56869 O      1.677191      -1.268675      0.440170
56870 C      1.023687      -0.075185      0.617516
56871 C      -0.285795      0.087924      -0.120292
56872 C      -1.210916      -1.091194      0.192698
56873 O      -2.415157      -1.066782      -0.550197
56874 O      -3.288207      -0.125703      0.076108
56875 H      2.365435      -1.309830      -1.299980
56876 C      1.126757      0.347123      2.043531
56877 H      2.159762      0.267779      2.379067
56878 H      0.505838      -0.280170      2.689360
56879 H      0.796186      1.378617      2.132592
56880 C      2.309158      1.325788      -0.374168
56881 O      3.021400      0.777437      -1.080879
56882 H      -4.108657      -0.630529      0.113227
56883 H      -0.124862      0.136545      -1.197930
56884 O      -0.819752      1.324612      0.313531
56885 O      -1.591842      1.882017      -0.735151
56886 H      -2.464233      1.490656      -0.568249
56887 H      -0.726054      -2.017223      -0.115653
56888 H      -1.441129      -1.129775      1.259075
56889 Rotational constants (GHz):      1.3900600      0.6125500      0.5436800
56890 Vibrational harmonic frequencies (cm-1):
56891      1280.8261          30.9742          56.4099
56892      72.9018          111.7830          119.8856
56893      164.4219          172.2252          173.7217
56894      191.5043          196.1906          223.5472
56895      234.8836          260.9732          286.4689
56896      326.3774          370.7784          399.2902
56897      428.3831          453.1299          512.8155
56898      541.0112          579.1528          588.6738
56899      874.4022          894.4418          966.1002
56900      971.3032          1037.7157          1044.1037
56901      1054.7744          1101.9803          1109.9532
56902      1158.1149          1243.0780          1299.7248
56903      1306.8744          1333.3964          1376.5469
56904      1390.9107          1410.9380          1418.0510
56905      1420.0624          1456.3215          1473.7942
56906      1477.9854          1489.4393          2053.3779
56907      3046.9938          3075.9371          3098.9194
56908      3124.4053          3146.6056          3173.3926
56909      3727.2424          3772.2234          3846.0223
56910 Zero-point correction (Hartree): 0.152343
56911
56912 TS.triHPacyl.COelim.pptmptmmd
56913 -----
56914 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16242957
56915 Electronic state : 2-A
56916 Cartesian coordinates (Angs):
56917 O      -1.338862          2.291887          -0.303629
56918 O      -1.454816          1.409170          0.803276
56919 C      -1.030368          0.152666          0.449190
56920 C      0.255592          0.093632          -0.352692
56921 C      1.356903          0.922932          0.307540
56922 O      2.525309          0.992178          -0.487022
56923 O      3.271645          -0.208659          -0.305083
56924 H      -2.060514          1.976211          -0.872733
56925 C      -1.298481          -0.808418          1.556146

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56926	H	-2.305962	-0.648605	1.937356		
56927	H	-0.585504	-0.680352	2.373843		
56928	H	-1.205203	-1.826003	1.184746		
56929	C	-2.461619	-0.342316	-0.985490		
56930	O	-2.750510	-1.444034	-1.022489		
56931	H	4.088855	0.136369	0.074099		
56932	H	0.089371	0.508068	-1.349224		
56933	O	0.629017	-1.239263	-0.631782		
56934	O	1.159456	-1.850027	0.537278		
56935	H	2.106343	-1.694426	0.397296		
56936	H	1.011928	1.953677	0.377285		
56937	H	1.598615	0.554067	1.304780		
56938	Rotational constants (GHz):			1.3087500	0.6692600	0.5434300
56939	Vibrational harmonic frequencies (cm-1):					
56940	i289.3113		48.6595			59.1180
56941	83.5216		136.7024			152.8685
56942	172.9369		193.1762			208.6079
56943	223.9402		235.0215			246.9472
56944	250.4986		285.9961			304.6561
56945	317.7870		336.5617			419.5868
56946	459.6388		482.1319			520.1277
56947	547.4944		583.5473			669.0757
56948	827.2043		895.4464			954.3560
56949	969.5390		1000.8933			1041.2247
56950	1046.4303		1107.0139			1123.0521
56951	1157.9781		1246.2283			1295.7425
56952	1308.3146		1328.6057			1383.3020
56953	1389.5232		1412.8048			1416.5887
56954	1435.5336		1457.8839			1466.4200
56955	1475.5249		1484.2764			2087.0704
56956	3056.8343		3085.7555			3094.6333
56957	3129.4007		3153.1561			3171.3512
56958	3721.2004		3744.1609			3830.7342
56959	Zero-point correction (Hartree):			0.153177		
56960						
56961	TS.triHPacyl.COelim.pptmptmmpd					
56962	-----					
56963	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16395975					
56964	Electronic state : 2-A					
56965	Cartesian coordinates (Angs):					
56966	O	-1.333806	2.281972	-0.337002		
56967	O	-1.481094	1.407754	0.772636		
56968	C	-1.033482	0.152352	0.445810		
56969	C	0.278697	0.106303	-0.312356		
56970	C	1.359120	0.944250	0.369284		
56971	O	2.534012	1.045147	-0.410283		
56972	O	3.249388	-0.184824	-0.321857		
56973	H	-2.048928	1.972287	-0.917057		
56974	C	-1.332548	-0.799546	1.553056		
56975	H	-2.352402	-0.638413	1.899206		
56976	H	-0.647133	-0.660210	2.391965		
56977	H	-1.225388	-1.820779	1.196040		
56978	C	-2.403914	-0.373882	-1.032322		
56979	O	-2.666577	-1.481922	-1.078732		
56980	H	3.085781	-0.566610	-1.194884		
56981	H	0.135105	0.512289	-1.316277		
56982	O	0.684708	-1.226217	-0.573557		
56983	O	1.156992	-1.832542	0.622110		
56984	H	2.096196	-1.586727	0.596085		
56985	H	1.002469	1.969649	0.453211		
56986	H	1.598082	0.566697	1.364357		
56987	Rotational constants (GHz):			1.2903100	0.6798000	0.5518400
56988	Vibrational harmonic frequencies (cm-1):					
56989	i292.0201		46.1780			58.5277
56990	96.3691		135.1523			151.2832
56991	179.7689		197.2974			209.1440
56992	227.9348		239.3350			259.0236
56993	280.7492		304.6796			327.3012
56994	337.0470		390.3784			411.2888
56995	451.4023		486.0029			550.4650
56996	576.2951		591.4217			669.6563
56997	832.5587		899.6415			952.7538

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56998          969.4652                1000.1030                1042.7336
56999          1047.2211                1110.4857                1122.0690
57000          1149.6811                1247.0428                1291.2368
57001          1309.5768                1325.3903                1381.6868
57002          1398.3650                1409.2899                1415.1867
57003          1434.2415                1456.9261                1473.6352
57004          1478.2275                1485.4019                2085.9525
57005          3057.8928                3081.6579                3092.2494
57006          3130.5931                3154.4721                3172.0585
57007          3715.7738                3727.2940                3800.1021
57008 Zero-point correction (Hartree): 0.153612
57009
57010 TS.triHPacyl.COelim.pptmptmpd
57011 -----
57012 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16122023
57013 Electronic state : 2-A
57014 Cartesian coordinates (Angs):
57015 O      -1.033605      2.201687      -0.989807
57016 O      -1.213677      1.757931      0.345039
57017 C      -0.871524      0.435496      0.446148
57018 C       0.409393      0.029201     -0.254191
57019 C      1.575369      0.914568      0.196516
57020 O       2.765683      0.578417     -0.473303
57021 O       3.410543     -0.465238      0.241036
57022 H      -1.797006      1.793445     -1.431181
57023 C      -1.120853     -0.049412      1.835043
57024 H      -2.078495      0.324129      2.192246
57025 H      -0.335862      0.290100      2.515409
57026 H      -1.135293     -1.137563      1.857442
57027 C      -2.442187     -0.381508     -0.662211
57028 O      -2.877877     -1.350296     -0.241311
57029 H       2.903564     -1.243757     -0.031903
57030 H       0.315863      0.103009     -1.337249
57031 O       0.761474     -1.305166      0.077146
57032 O      -0.009195     -2.180571     -0.734493
57033 H      -0.677002     -2.510097     -0.117597
57034 H       1.346046      1.942053     -0.084414
57035 H       1.730229      0.854507      1.274978
57036 Rotational constants (GHz):      1.2613900      0.6807500      0.5371600
57037 Vibrational harmonic frequencies (cm-1):
57038 i280.1260                49.4130                68.3609
57039 76.2533                 127.8372                143.2701
57040 144.4468                149.7320                174.7333
57041 187.3289                217.9365                239.0723
57042 265.1281                296.1916                306.3321
57043 330.6062                374.9481                403.0682
57044 408.0165                438.2406                489.5229
57045 555.7336                586.9530                603.9950
57046 829.8230                890.5369                961.5516
57047 980.3367                1032.3593               1045.4222
57048 1052.1681               1108.9090               1131.2990
57049 1162.3090               1253.7843               1292.7323
57050 1304.3811               1331.0574               1379.1669
57051 1397.4931               1405.3988               1419.9316
57052 1433.5196               1447.8898               1461.6020
57053 1468.2446               1488.1025               2064.7220
57054 3055.5296               3081.3630               3110.6888
57055 3128.7044               3146.7586               3162.3380
57056 3723.2645               3772.9764               3795.9008
57057 Zero-point correction (Hartree): 0.152540
57058
57059 TS.triHPacyl.COelim.pptmptmpd
57060 -----
57061 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16055241
57062 Electronic state : 2-A
57063 Cartesian coordinates (Angs):
57064 O       1.631437      -1.586745      -1.347488
57065 O       1.749468      -1.501036      0.067592
57066 C       1.143485      -0.361136      0.516452
57067 C      -0.216478      -0.056839     -0.065591
57068 C      -1.191084     -1.219352      0.117369
57069 O      -2.389002     -1.035912     -0.600620

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57070	O	-3.255172	-0.209421	0.161974	
57071	H	2.536007	-1.381668	-1.620473	
57072	C	1.383298	-0.212988	1.980721	
57073	H	2.450715	-0.276202	2.185351	
57074	H	0.876826	-1.004592	2.540393	
57075	H	1.002589	0.746872	2.321002	
57076	C	2.301132	1.197320	-0.362457	
57077	O	1.684630	2.063558	-0.778995	
57078	H	-3.013263	0.678997	-0.139844	
57079	H	-0.130353	0.155629	-1.131773	
57080	O	-0.648248	1.126131	0.601863	
57081	O	-1.436842	1.893705	-0.288214	
57082	H	-0.781055	2.492200	-0.673521	
57083	H	-0.741536	-2.119789	-0.304058	
57084	H	-1.412229	-1.375711	1.175066	
57085	Rotational constants (GHz):		1.2019300	0.7111200	0.5757100
57086	Vibrational harmonic frequencies (cm-1):				
57087	i277.4554		45.6594		57.6662
57088	67.5904		99.2503		115.0406
57089	156.2616		165.0137		182.5555
57090	188.9014		205.8022		214.0454
57091	239.5214		275.7915		306.0596
57092	317.2548		336.8214		401.9687
57093	430.0279		470.6387		495.8367
57094	530.6404		572.4998		579.0801
57095	876.1098		896.9010		967.4255
57096	973.6888		1038.5893		1040.9827
57097	1051.2211		1112.5299		1127.7804
57098	1142.8886		1243.0399		1301.8086
57099	1305.6822		1334.7366		1377.8241
57100	1404.7429		1405.6436		1411.1203
57101	1417.4771		1450.1302		1457.4164
57102	1478.4641		1490.0984		2065.5164
57103	3047.3586		3071.0307		3100.8263
57104	3125.7913		3133.4458		3170.2805
57105	3764.1965		3783.1849		3804.3849
57106	Zero-point correction (Hartree): 0.152241				
57107					
57108	TS.triHPacyl.COelim.pptmptpmd				
57109	-----				
57110	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16179497				
57111	Electronic state : 2-A				
57112	Cartesian coordinates (Angs):				
57113	O	1.356232	-1.997382	-1.097822	
57114	O	1.544837	-1.604387	0.253009	
57115	C	1.077831	-0.329970	0.441670	
57116	C	-0.263322	-0.014218	-0.182783	
57117	C	-1.297506	-1.052341	0.256237	
57118	O	-2.552758	-0.891226	-0.376565	
57119	O	-3.232857	0.176293	0.285122	
57120	H	2.012864	-1.442293	-1.551016	
57121	C	1.372063	0.128385	1.829385	
57122	H	2.403210	-0.108020	2.086212	
57123	H	0.714263	-0.360092	2.553809	
57124	H	1.219065	1.203168	1.893928	
57125	C	2.406949	0.755987	-0.763399	
57126	O	2.699677	1.777914	-0.355313	
57127	H	-4.104300	-0.213632	0.419083	
57128	H	-0.196340	-0.019568	-1.271475	
57129	O	-0.583241	1.297700	0.242448	
57130	O	-1.376994	1.920702	-0.751784	
57131	H	-2.271828	1.652690	-0.487920	
57132	H	-0.962020	-2.039581	-0.061738	
57133	H	-1.430173	-1.036627	1.339695	
57134	Rotational constants (GHz):		1.2783600	0.6625400	0.5355700
57135	Vibrational harmonic frequencies (cm-1):				
57136	i283.3226		49.1675		56.1263
57137	62.0922		136.6913		141.0282
57138	146.0867		164.2285		168.4039
57139	182.5345		193.9099		227.7747
57140	237.6557		272.9174		304.2012
57141	320.1965		385.8569		400.4972

57142	428.8324	459.9660	511.7779			
57143	548.8514	572.9702	590.4520			
57144	872.4616	893.7427	966.1350			
57145	970.8101	1037.7210	1042.9786			
57146	1053.6844	1102.7747	1110.6121			
57147	1159.3788	1250.7455	1298.5339			
57148	1307.2887	1332.3989	1378.5923			
57149	1391.2427	1409.5075	1420.1047			
57150	1434.6716	1455.3756	1475.0198			
57151	1477.7374	1489.1119	2093.9836			
57152	3047.5837	3075.3874	3096.8281			
57153	3126.3575	3144.9573	3170.1253			
57154	3718.9637	3728.4224	3845.0810			
57155	Zero-point correction (Hartree): 0.152502					
57156						
57157	TS.triHPacyl.COelim.pptpppmmd					
57158	-----					
57159	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16218134					
57160	Electronic state : 2-A					
57161	Cartesian coordinates (Angs):					
57162	O	-1.422167	-1.897693	-0.526271		
57163	O	-1.539134	-0.625151	-1.152660		
57164	C	-0.962034	0.343576	-0.371951		
57165	C	0.362596	-0.034841	0.251846		
57166	C	1.314558	-0.675558	-0.770002		
57167	O	2.658493	-0.564484	-0.342633		
57168	O	2.791056	-1.276942	0.878169		
57169	H	-2.289461	-1.977145	-0.103000		
57170	C	-1.175231	1.681428	-0.992647		
57171	H	-2.222650	1.783930	-1.274414		
57172	H	-0.556839	1.812055	-1.883874		
57173	H	-0.910787	2.456594	-0.278421		
57174	C	-2.260331	0.441899	1.313579		
57175	O	-3.137575	-0.280119	1.186525		
57176	H	2.653694	-0.575644	1.531685		
57177	H	0.197363	-0.740119	1.067434		
57178	O	0.977835	1.057712	0.909993		
57179	O	1.511354	1.957951	-0.054463		
57180	H	2.399155	1.590941	-0.183338		
57181	H	1.040319	-1.717440	-0.929958		
57182	H	1.292969	-0.142390	-1.720344		
57183	Rotational constants (GHz):			1.3587400	0.6432700	0.5630300
57184	Vibrational harmonic frequencies (cm-1):					
57185	i284.6567		42.7362			54.7063
57186	82.1398		106.9329			154.8879
57187	173.3279		200.7939			206.0038
57188	218.9626		235.1773			251.8657
57189	267.8178		294.8230			311.1616
57190	350.2018		369.2156			404.7295
57191	451.8047		483.4341			496.2616
57192	553.8126		593.6962			715.9283
57193	810.4672		919.7910			953.4395
57194	970.5630		988.7147			1038.1084
57195	1046.4318		1100.2322			1127.6341
57196	1151.2791		1244.6065			1287.3688
57197	1317.4532		1324.3976			1380.5546
57198	1393.9064		1413.4801			1415.8386
57199	1421.2254		1435.5250			1471.6551
57200	1482.2643		1488.6384			2055.9776
57201	3054.8205		3094.5045			3099.8594
57202	3124.6483		3151.1798			3171.9777
57203	3757.5095		3773.2993			3786.1259
57204	Zero-point correction (Hartree): 0.153261					
57205						
57206	TS.triHPacyl.COelim.pptppptmd					
57207	-----					
57208	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16190619					
57209	Electronic state : 2-A					
57210	Cartesian coordinates (Angs):					
57211	O	-1.300324	1.939917	-0.369611		
57212	O	-1.612726	1.102582	0.734705		
57213	C	-1.060299	-0.139890	0.568816		

57214	C	0.340297	-0.165129	0.003989			
57215	C	1.265005	0.750807	0.810220			
57216	O	2.622896	0.576382	0.455457			
57217	O	2.794471	1.064585	-0.866256			
57218	H	-2.089731	1.829441	-0.919921			
57219	C	-1.403327	-1.004840	1.734063			
57220	H	-2.466420	-0.919260	1.953800			
57221	H	-0.843192	-0.711398	2.626340			
57222	H	-1.165806	-2.038563	1.496227			
57223	C	-2.236555	-0.987910	-1.002625			
57224	O	-2.934248	-0.199025	-1.446444			
57225	H	2.623717	0.270988	-1.396792			
57226	H	0.332131	0.138399	-1.043840			
57227	O	0.758367	-1.518588	0.086124			
57228	O	1.843872	-1.706061	-0.811725			
57229	H	2.599238	-1.636627	-0.210289			
57230	H	0.969237	1.792522	0.683424			
57231	H	1.231630	0.477928	1.866262			
57232	Rotational constants (GHz):				1.3147900	0.6300700	0.5706000
57233	Vibrational harmonic frequencies (cm-1):						
57234		i281.0099		33.1243			58.4938
57235		92.4925		108.7092			165.1693
57236		168.4956		173.1098			183.9201
57237		204.1099		223.3423			232.6434
57238		253.7998		284.4783			298.9012
57239		351.3826		392.7406			412.7561
57240		445.1886		467.9614			521.7760
57241		535.1764		578.9587			605.8111
57242		882.6197		902.7866			956.3884
57243		973.9645		1032.9277			1044.4409
57244		1054.4355		1100.3610			1136.4611
57245		1145.2104		1252.6922			1299.5654
57246		1307.7880		1341.8719			1374.2885
57247		1406.7912		1413.3463			1419.1863
57248		1424.7166		1443.1305			1468.1958
57249		1479.0037		1489.6193			2058.3756
57250		3048.8040		3081.1820			3094.1012
57251		3126.5531		3142.0035			3171.7776
57252		3746.6243		3780.1313			3784.1653
57253	Zero-point correction (Hartree):				0.153038		
57254							
57255	TS.triHPacyl.COelim.pptpmtmmmd						
57256	-----						
57257	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.16311808		
57258	Electronic state : 2-A						
57259	Cartesian coordinates (Angs):						
57260	O	-1.087777	2.346537	-0.141342			
57261	O	-1.378668	1.396917	0.874407			
57262	C	-1.029524	0.139810	0.451828			
57263	C	0.319279	0.045229	-0.226880			
57264	C	1.416340	0.751218	0.583591			
57265	O	2.694698	0.258381	0.231883			
57266	O	2.917252	0.554928	-1.138549			
57267	H	-1.806620	2.174499	-0.771384			
57268	C	-1.469515	-0.879339	1.445389			
57269	H	-2.497391	-0.674148	1.740770			
57270	H	-0.836495	-0.865418	2.335664			
57271	H	-1.407899	-1.870672	1.002803			
57272	C	-2.359694	-0.123571	-1.146828			
57273	O	-2.677402	-1.201842	-1.332891			
57274	H	2.635202	-0.266352	-1.566784			
57275	H	0.266247	0.504789	-1.215240			
57276	O	0.678949	-1.291472	-0.527475			
57277	O	1.064259	-1.963515	0.665988			
57278	H	2.011323	-1.759066	0.699477			
57279	H	1.354551	1.827645	0.428919			
57280	H	1.329288	0.529169	1.646995			
57281	Rotational constants (GHz):				1.2348100	0.6840800	0.5810500
57282	Vibrational harmonic frequencies (cm-1):						
57283		i282.1559		44.0703			58.1485
57284		82.8940		121.0076			146.9191
57285		165.1227		193.3368			205.7912


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57286      236.6424      240.4386      252.8542
57287      276.2433      297.8889      333.7951
57288      353.1685      395.5109      414.3554
57289      449.7615      485.0501      496.0767
57290      562.2071      578.0383      716.9044
57291      809.1941      919.9413      952.9664
57292      971.1669      990.4968      1038.9915
57293      1046.9589      1100.9179      1128.4542
57294      1152.7965      1254.6060      1289.5963
57295      1313.5969      1325.6189      1384.5908
57296      1394.8315      1413.2206      1420.8572
57297      1433.5758      1439.5819      1477.0566
57298      1481.5399      1487.2650      2088.0769
57299      3057.3129      3093.3667      3098.0844
57300      3129.0927      3152.5902      3170.0365
57301      3733.1686      3756.2203      3775.9538
57302      Zero-point correction (Hartree): 0.153521
57303
57304      TS.triHPacyl.COelim.pptpptompd
57305      -----
57306      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16176746
57307      Electronic state : 2-A
57308      Cartesian coordinates (Angs):
57309      O      -0.920554      2.385696      -0.016719
57310      O      -1.278552      1.406613      0.948736
57311      C      -1.018444      0.151814      0.458819
57312      C      0.319022      -0.018407      -0.230726
57313      C      1.449714      0.530141      0.644122
57314      O      2.715442      0.091758      0.193536
57315      O      2.920274      0.629981      -1.106312
57316      H      -1.625552      2.267013      -0.674762
57317      C      -1.524455      -0.887435      1.398431
57318      H      -2.535626      -0.633943      1.713015
57319      H      -0.888564      -0.965478      2.283797
57320      H      -1.528350      -1.854219      0.900239
57321      C      -2.371570      0.077639      -1.145850
57322      O      -2.799889      -0.955399      -1.362995
57323      H      3.587758      1.305406      -0.932936
57324      H      0.325762      0.512591      -1.183222
57325      O      0.534107      -1.360137      -0.617341
57326      O      0.937112      -2.125562      0.511868
57327      H      1.899817      -2.096675      0.412667
57328      H      1.393850      1.618879      0.667123
57329      H      1.381777      0.140310      1.659117
57330      Rotational constants (GHz):      1.2186800      0.6812800      0.5719800
57331      Vibrational harmonic frequencies (cm-1):
57332      i278.7945      47.6038      61.6943
57333      70.6127      120.4168      143.7426
57334      161.3855      170.9808      197.5238
57335      232.4601      235.5973      241.8897
57336      253.9618      269.9449      289.1591
57337      325.0493      365.1922      411.6750
57338      424.7484      460.3392      484.4582
57339      560.9149      576.0001      704.7632
57340      815.0122      909.9644      951.5739
57341      968.2453      991.8158      1039.6737
57342      1046.3253      1102.0977      1138.3306
57343      1156.2685      1250.5687      1294.5514
57344      1309.2010      1324.6074      1380.7637
57345      1393.1645      1411.6699      1413.2309
57346      1425.2268      1434.7456      1477.6027
57347      1478.7222      1486.8915      2090.0730
57348      3054.0116      3090.8714      3104.5104
57349      3127.5592      3148.7974      3169.9273
57350      3723.3533      3777.9000      3821.1896
57351      Zero-point correction (Hartree): 0.152907
57352
57353      TS.triHPacyl.COelim.pptpptommd
57354      -----
57355      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16090197
57356      Electronic state : 2-A
57357      Cartesian coordinates (Angs):

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57358	O	1.263945	-1.717093	-1.402543		
57359	O	1.633580	-1.570807	-0.037371		
57360	C	1.169779	-0.379484	0.444890		
57361	C	-0.257355	-0.033662	0.098948		
57362	C	-1.227864	-1.147892	0.498241		
57363	O	-2.567588	-0.726988	0.418328		
57364	O	-2.847559	-0.408929	-0.937666		
57365	H	2.092061	-1.483493	-1.844697		
57366	C	1.679053	-0.164055	1.829374		
57367	H	2.760597	-0.288046	1.845198		
57368	H	1.240655	-0.885398	2.525277		
57369	H	1.420321	0.837313	2.164823		
57370	C	2.217560	1.079696	-0.719261		
57371	O	1.612227	2.026528	-0.920314		
57372	H	-2.749443	0.555153	-0.920853		
57373	H	-0.348122	0.149258	-0.970779		
57374	O	-0.553501	1.168929	0.796490		
57375	O	-1.412898	1.961140	-0.005130		
57376	H	-0.780954	2.560752	-0.427279		
57377	H	-1.051645	-2.025092	-0.128285		
57378	H	-1.096154	-1.410315	1.549096		
57379	Rotational constants (GHz):			1.1446600	0.7404300	0.6073900
57380	Vibrational harmonic frequencies (cm-1):					
57381		1269.3495	37.2320			63.5312
57382		81.7641	92.9456			121.7528
57383		141.8915	157.7435			182.3463
57384		186.8989	209.1125			216.1865
57385		257.2581	270.1435			280.3398
57386		317.3618	382.4433			404.7545
57387		437.0242	465.5281			490.1024
57388		554.0459	568.5690			602.8705
57389		875.7612	906.0385			959.3597
57390		972.3687	1034.1016			1037.9099
57391		1048.7539	1108.4350			1137.3355
57392		1146.0849	1251.9550			1296.1060
57393		1311.2169	1337.8681			1379.5070
57394		1401.4808	1407.9634			1410.7222
57395		1418.9424	1449.8427			1471.3055
57396		1477.1579	1490.6225			2067.3397
57397		3045.1551	3069.9748			3113.5274
57398		3124.4009	3132.0003			3170.0293
57399		3759.9280	3778.6787			3795.6391
57400	Zero-point correction (Hartree):			0.152431		
57401	TS.triHPacyl.COelim.pptpptomd					
57402	-----					
57403	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16297489					
57404	Electronic state : 2-A					
57405	Cartesian coordinates (Angs):					
57406	O	-0.976175	2.120300	-0.969535		
57407	O	-1.421106	1.641495	0.289828		
57408	C	-1.101962	0.317659	0.428575		
57409	C	0.295783	-0.064981	0.000503		
57410	C	1.335033	0.820538	0.690433		
57411	O	2.651894	0.345008	0.489897		
57412	O	2.970168	0.507013	-0.883847		
57413	H	-1.622388	1.710709	-1.568192		
57414	C	-1.655027	-0.218862	1.705050		
57415	H	-2.682762	0.117425	1.829435		
57416	H	-1.072062	0.124572	2.564082		
57417	H	-1.630949	-1.306143	1.683845		
57418	C	-2.299121	-0.540200	-1.063508		
57419	O	-2.714345	-1.570431	-0.811953		
57420	H	2.680559	-0.339800	-1.257718		
57421	H	0.394656	0.018349	-1.082766		
57422	O	0.443129	-1.428108	0.369816		
57423	O	1.521168	-1.979646	-0.373880		
57424	H	2.241827	-1.925043	0.270260		
57425	H	1.242317	1.848739	0.339244		
57426	H	1.202706	0.781229	1.772881		
57427	Rotational constants (GHz):			1.2415800	0.6764800	0.5592700
57428	Vibrational harmonic frequencies (cm-1):					
57429						

57430	i282.3562	46.6079	57.8572			
57431	89.0420	130.9283	147.7514			
57432	163.2635	168.0540	178.5161			
57433	193.2025	223.4715	245.0578			
57434	266.5549	273.0040	317.1144			
57435	378.9805	399.6896	415.3115			
57436	448.0506	472.3627	532.9190			
57437	537.1082	567.3980	606.3189			
57438	881.6708	902.1417	956.0488			
57439	974.5201	1032.9285	1043.2899			
57440	1054.2367	1100.7041	1136.4755			
57441	1145.7178	1262.1411	1299.6870			
57442	1304.9313	1340.1398	1378.6806			
57443	1405.2191	1412.5196	1425.5144			
57444	1435.2521	1444.9256	1467.2189			
57445	1475.6957	1489.1922	2092.5552			
57446	3049.6040	3080.7901	3093.5169			
57447	3128.2240	3141.2685	3168.7674			
57448	3729.5828	3743.1978	3782.7923			
57449	Zero-point correction (Hartree): 0.153179					
57450						
57451	TS.triHPacyl.COelim.pptp pptppd					
57452	-----					
57453	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16190436					
57454	Electronic state : 2-A					
57455	Cartesian coordinates (Angs):					
57456	O	-0.840805	2.141997	-0.964525		
57457	O	-1.334575	1.691254	0.287565		
57458	C	-1.088838	0.351040	0.432786		
57459	C	0.290937	-0.111710	0.028209		
57460	C	1.362896	0.722887	0.727662		
57461	O	2.660169	0.202556	0.486966		
57462	O	2.957052	0.413732	-0.890328		
57463	H	-1.473087	1.730756	-1.577469		
57464	C	-1.695787	-0.154504	1.696779		
57465	H	-2.713600	0.219363	1.793095		
57466	H	-1.123287	0.173129	2.569255		
57467	H	-1.708164	-1.241948	1.681501		
57468	C	-2.302817	-0.439260	-1.087068		
57469	O	-2.778102	-1.445188	-0.844668		
57470	H	3.633704	1.100251	-0.838439		
57471	H	0.425159	-0.050666	-1.051787		
57472	O	0.390432	-1.467978	0.425225		
57473	O	1.301792	-2.126167	-0.438311		
57474	H	2.158403	-1.833476	-0.092671		
57475	H	1.305153	1.767992	0.420958		
57476	H	1.249680	0.642243	1.809959		
57477	Rotational constants (GHz):			1.2217100	0.6787300	0.5596600
57478	Vibrational harmonic frequencies (cm-1):					
57479	i281.7146	45.0838	55.1449			
57480	69.6033	118.8636	146.3081			
57481	149.2945	161.9586	172.1351			
57482	190.3000	213.0556	238.4109			
57483	253.6001	271.3325	283.1880			
57484	317.6239	392.0315	415.0005			
57485	446.6086	452.9868	482.9240			
57486	535.6441	567.8737	600.5109			
57487	879.4245	898.7163	952.5821			
57488	973.0801	1038.4308	1041.1761			
57489	1053.3810	1093.1578	1132.1214			
57490	1149.3111	1256.4296	1298.5233			
57491	1303.2769	1334.6904	1375.7597			
57492	1393.7609	1409.3855	1415.0799			
57493	1437.2234	1442.9966	1465.1189			
57494	1475.9765	1488.8728	2093.8493			
57495	3047.2804	3077.9326	3107.7851			
57496	3127.1905	3139.1164	3170.4576			
57497	3719.6763	3767.5587	3819.9150			
57498	Zero-point correction (Hartree): 0.152543					
57499						
57500	TS.triHPacyl.COelim.ptmmmtmpmd					
57501	-----					

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57502 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15907495
57503 Electronic state : 2-A
57504 Cartesian coordinates (Angs):
57505 O -2.484586 -0.791652 -0.843307
57506 O -1.584112 0.123751 -1.462468
57507 C -0.538304 0.463401 -0.637984
57508 C 0.388719 -0.666802 -0.227642
57509 C 1.440904 -0.274814 0.810741
57510 O 2.508400 0.457191 0.243003
57511 O 3.183212 -0.400274 -0.670475
57512 H -2.105966 -1.646667 -1.094481
57513 C 0.119216 1.692209 -1.183233
57514 H -0.640570 2.411806 -1.481042
57515 H 0.735552 1.445202 -2.051751
57516 H 0.766986 2.139691 -0.432895
57517 C -1.495825 1.248289 1.061605
57518 O -0.933825 2.093384 1.581907
57519 H 4.015505 -0.557798 -0.208077
57520 H 0.917883 -0.994526 -1.131649
57521 O -0.286723 -1.843797 0.173339
57522 O -0.934262 -1.587887 1.412976
57523 H -1.766579 -1.177843 1.120245
57524 H 1.038647 0.388923 1.574704
57525 H 1.805442 -1.188213 1.284226
57526 Rotational constants (GHz): 1.1308900 0.7194300 0.6466200
57527 Vibrational harmonic frequencies (cm-1):
57528 i332.6758 37.4460 43.0926
57529 73.6063 140.4022 158.3020
57530 170.6856 176.8715 197.2987
57531 208.5069 217.7267 237.0340
57532 257.3077 264.7769 301.8480
57533 325.2231 366.1901 385.3152
57534 439.6389 470.0722 531.5955
57535 552.2903 595.5634 670.4338
57536 824.5794 937.5470 940.9293
57537 977.5544 1018.4598 1022.5247
57538 1088.5508 1094.0697 1113.2120
57539 1153.4204 1228.6846 1250.6847
57540 1278.8969 1329.6966 1368.1228
57541 1393.4746 1415.0778 1420.7808
57542 1428.9931 1448.3997 1475.8352
57543 1479.5206 1489.8724 2076.5906
57544 3037.5629 3053.1249 3078.8118
57545 3132.2591 3150.6961 3170.6538
57546 3695.4616 3783.5041 3825.0122
57547 Zero-point correction (Hartree): 0.152646
57548
57549 TS.triHPacyl.COelim.ptppmmtpm
57550 -----
57551 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16167340
57552 Electronic state : 2-A
57553 Cartesian coordinates (Angs):
57554 O -1.825295 1.728408 -0.633653
57555 O -1.901976 0.954647 0.561169
57556 C -0.927397 -0.002520 0.644027
57557 C 0.486867 0.506694 0.829448
57558 C 1.511197 -0.592548 1.072280
57559 O 1.528048 -1.602366 0.089377
57560 O 2.024157 -1.026805 -1.112772
57561 H -0.952109 2.149828 -0.577141
57562 C -1.383418 -1.100814 1.553280
57563 H -2.427014 -1.322554 1.343406
57564 H -1.293154 -0.808387 2.603515
57565 H -0.790732 -1.999513 1.388807
57566 C -1.014576 -0.905205 -1.229559
57567 O -2.033959 -1.367731 -1.435132
57568 H 1.191486 -0.829957 -1.577510
57569 H 0.498466 1.162356 1.712779
57570 O 0.781651 1.304672 -0.318770
57571 O 2.100079 1.803772 -0.222111
57572 H 2.586744 1.124010 -0.716653
57573 H 2.504068 -0.156349 1.181580

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57574      H      1.264562      -1.109846      1.999510
57575      Rotational constants (GHz):      1.1496300      0.8094100      0.6835600
57576      Vibrational harmonic frequencies (cm-1):
57577      i348.8932      49.2163      96.0628
57578      121.0711      126.6268      141.4107
57579      171.7549      190.8193      221.9325
57580      232.4298      246.0179      265.8870
57581      283.1670      314.1912      355.3948
57582      364.1134      391.9494      410.1219
57583      485.5334      518.9905      531.0502
57584      567.4542      579.5116      731.6394
57585      845.9288      882.4737      944.6320
57586      970.2590      1013.2171      1028.9435
57587      1050.7562      1098.8108      1123.0999
57588      1161.2237      1240.2868      1246.6174
57589      1295.5674      1363.6626      1371.8678
57590      1406.8711      1409.1560      1442.8202
57591      1453.9979      1475.8920      1481.1417
57592      1489.6356      1498.2345      2097.4615
57593      2998.8474      3045.1929      3093.2052
57594      3125.8187      3138.8212      3167.6466
57595      3670.6129      3722.9727      3727.5233
57596      Zero-point correction (Hartree): 0.153730
57597
57598      TS.triHPacyl.COelim.ptpppptomd
57599      -----
57600      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16265741
57601      Electronic state : 2-A
57602      Cartesian coordinates (Angs):
57603      O      -2.216358      -1.294640      -0.697250
57604      O      -2.154474      0.116328      -0.695743
57605      C      -0.896247      0.578964      -0.426160
57606      C      0.267145      -0.275524      -0.880625
57607      C      1.552217      0.518194      -1.073109
57608      O      1.972165      1.241476      0.065393
57609      O      2.409914      0.315898      1.052344
57610      H      -2.249414      -1.503951      0.249271
57611      C      -0.898194      2.060121      -0.642161
57612      H      -1.807089      2.481385      -0.215428
57613      H      -0.887655      2.295047      -1.709877
57614      H      -0.034507      2.513255      -0.163985
57615      C      -0.753487      0.446509      1.648821
57616      O      -1.697642      -0.020360      2.094694
57617      H      1.623091      0.265946      1.619778
57618      H      0.006875      -0.745419      -1.837105
57619      O      0.411547      -1.305097      0.100781
57620      O      1.494500      -2.139382      -0.257495
57621      H      2.217756      -1.727806      0.242385
57622      H      2.349946      -0.143003      -1.411143
57623      H      1.395191      1.281182      -1.836264
57624      Rotational constants (GHz):      1.1962200      0.7725600      0.7079800
57625      Vibrational harmonic frequencies (cm-1):
57626      i330.6523      70.5768      89.6144
57627      103.0671      110.4471      140.9501
57628      177.3834      203.0028      220.7519
57629      234.3896      247.9962      265.8487
57630      283.0529      300.3472      322.3141
57631      351.5241      354.4176      436.0068
57632      481.4262      494.2192      511.6076
57633      555.0445      573.7091      732.0015
57634      837.2091      882.1467      964.9161
57635      972.2018      1020.0457      1042.6991
57636      1074.4769      1086.2361      1118.5810
57637      1160.6132      1244.6027      1268.6538
57638      1299.7817      1345.5260      1382.2971
57639      1406.1504      1411.0564      1433.4120
57640      1435.6229      1447.7867      1481.8616
57641      1492.7590      1499.6012      2056.8003
57642      3035.0293      3051.2987      3090.9148
57643      3129.1118      3136.1012      3177.1317
57644      3718.5190      3734.4537      3759.5281
57645      Zero-point correction (Hartree): 0.153678

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57646
57647 TS.triHPacyl.COelim.ptpppttpmd
57648 -----
57649 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16289503
57650 Electronic state : 2-A
57651 Cartesian coordinates (Angs):
57652 O 2.449967 1.375714 0.150325
57653 O 2.391356 0.079543 -0.409600
57654 C 1.112726 -0.401196 -0.388579
57655 C 0.016823 0.592239 -0.726870
57656 C -1.195307 -0.036861 -1.399010
57657 O -1.843312 -1.023102 -0.620801
57658 O -2.576441 -0.371848 0.411168
57659 H 2.235538 1.204634 1.082630
57660 C 1.116556 -1.780300 -0.968678
57661 H 1.950555 -2.342074 -0.551524
57662 H 1.244479 -1.745006 -2.054020
57663 H 0.185552 -2.291866 -0.737216
57664 C 0.835589 -0.786155 1.633832
57665 O -0.084209 -1.413792 1.897272
57666 H -2.030669 -0.577107 1.185125
57667 H 0.437528 1.346229 -1.402592
57668 O -0.339318 1.236755 0.497605
57669 O -1.300954 2.236315 0.222187
57670 H -2.125474 1.747539 0.375034
57671 H -1.909152 0.735877 -1.684100
57672 H -0.883399 -0.561265 -2.302758
57673 Rotational constants (GHz): 1.1876700 0.8111200 0.7064500
57674 Vibrational harmonic frequencies (cm-1):
57675 i328.3844 79.2636 97.0169
57676 107.7826 122.4371 138.2352
57677 176.0300 191.9046 204.3597
57678 228.6413 241.2125 259.2044
57679 298.8438 321.9715 326.9196
57680 355.4489 373.5622 432.2857
57681 447.5079 478.2924 504.9123
57682 549.4394 570.8050 728.4202
57683 830.1711 885.2368 965.3944
57684 971.0454 1020.9250 1040.1891
57685 1069.0649 1079.5915 1116.8156
57686 1159.4639 1248.1436 1268.8350
57687 1299.1094 1346.2187 1382.4131
57688 1402.1385 1410.2108 1427.5527
57689 1442.6304 1445.5403 1480.3744
57690 1490.3770 1500.7312 2050.8000
57691 3039.5696 3050.3326 3091.4045
57692 3127.8999 3136.9927 3172.1872
57693 3721.8959 3727.4112 3768.6426
57694 Zero-point correction (Hartree): 0.153557
57695
57696 TS.triHPacyl.COelim.tmmmmmmmpd
57697 -----
57698 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16147051
57699 Electronic state : 2-A
57700 Cartesian coordinates (Angs):
57701 O 1.982171 -1.391265 -1.167533
57702 O 0.722017 -0.770216 -1.007444
57703 C 0.424232 -0.577818 0.311167
57704 C -0.979996 -0.061032 0.480168
57705 C -1.471681 0.828417 -0.656336
57706 O -0.681119 1.987417 -0.798134
57707 O -0.911498 2.806041 0.341332
57708 H 2.562873 -0.624165 -1.280637
57709 C 0.920695 -1.561571 1.315879
57710 H 2.004692 -1.635590 1.309666
57711 H 0.503012 -2.547789 1.096939
57712 H 0.581658 -1.256447 2.304409
57713 C 1.591804 1.140848 0.753364
57714 O 2.608684 1.060201 0.236039
57715 H -0.094122 2.668605 0.845219
57716 H -1.005051 0.506785 1.413358
57717 O -1.902296 -1.108693 0.749927

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57718      O      -1.908088      -1.980945      -0.380163
57719      H      -2.840737      -1.965380      -0.625601
57720      H      -1.389901      0.319537      -1.614664
57721      H      -2.511722      1.101054      -0.466326
57722      Rotational constants (GHz):      0.9642300      0.9320800      0.6038700
57723      Vibrational harmonic frequencies (cm-1):
57724      i271.2170      46.1988      86.2223
57725      96.6233      113.8633      146.6921
57726      150.4158      155.8145      173.8868
57727      191.3143      199.3630      232.0962
57728      244.0421      267.0318      285.9904
57729      313.9519      330.2309      363.9756
57730      427.7729      444.8389      491.1806
57731      515.1155      586.7877      728.5045
57732      786.4290      940.6912      949.7971
57733      976.2243      1024.6834      1050.9136
57734      1073.3415      1090.6425      1119.4384
57735      1150.2035      1244.0351      1280.9007
57736      1316.2145      1338.7888      1385.4827
57737      1398.6651      1409.8122      1417.5887
57738      1431.5191      1436.9176      1471.0442
57739      1487.8672      1491.9327      2052.1523
57740      3056.5847      3076.5410      3089.7537
57741      3133.5400      3156.9342      3170.2085
57742      3739.6322      3773.5683      3835.8656
57743      Zero-point correction (Hartree): 0.152523
57744
57745      TS.triHPacyl.COelim.tmmmmmmppd
57746      -----
57747      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16197760
57748      Electronic state : 2-A
57749      Cartesian coordinates (Angs):
57750      O      -2.464106      0.519158      -1.015993
57751      O      -1.051951      0.548189      -0.910213
57752      C      -0.639679      0.313700      0.374538
57753      C      0.851779      0.489467      0.486772
57754      C      1.667120      -0.103555      -0.658400
57755      O      1.490349      -1.498476      -0.765299
57756      O      2.075562      -2.098568      0.383304
57757      H      -2.617949      -0.400583      -1.278928
57758      C      -1.483406      0.825415      1.496075
57759      H      -2.491180      0.420843      1.461766
57760      H      -1.552741      1.916225      1.453234
57761      H      -1.016118      0.552053      2.440348
57762      C      -0.919004      -1.782791      0.591922
57763      O      -1.797721      -2.120609      -0.056169
57764      H      1.288185      -2.380100      0.873534
57765      H      1.158383      0.017326      1.422464
57766      O      1.198429      1.855162      0.702128
57767      O      1.069298      2.561469      -0.524162
57768      H      0.150693      2.861788      -0.506520
57769      H      1.342254      0.288120      -1.618860
57770      H      2.718749      0.140319      -0.501259
57771      Rotational constants (GHz):      0.9608100      0.9365200      0.6009200
57772      Vibrational harmonic frequencies (cm-1):
57773      i288.1495      35.9859      86.5981
57774      104.1521      118.8277      145.8526
57775      147.7108      163.8580      188.6911
57776      191.6705      215.2087      245.1375
57777      252.7516      272.6081      312.6428
57778      319.6664      329.9692      364.7372
57779      414.6316      436.0038      494.7129
57780      529.6357      588.0487      727.3594
57781      784.8886      938.9760      946.4612
57782      975.3323      1023.0838      1049.3721
57783      1068.3569      1081.6386      1119.3887
57784      1149.6452      1238.3401      1274.8496
57785      1310.3447      1334.7123      1397.4294
57786      1405.4558      1411.7766      1419.5163
57787      1428.9709      1434.2401      1470.8595
57788      1485.7378      1490.2254      2059.4671
57789      3049.3377      3089.7887      3099.2160

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57790          3131.3825          3168.5835          3171.9455
57791          3742.5843          3774.9448          3799.0525
57792 Zero-point correction (Hartree): 0.152665
57793
57794 TS.triHPacyl.COelim.tmmmtmpmd
57795 -----
57796 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16151219
57797 Electronic state : 2-A
57798 Cartesian coordinates (Angs):
57799 O          1.689124          -1.830221          1.361112
57800 O          1.094573          -0.569883          1.114643
57801 C          0.739219          -0.457469          -0.196491
57802 C          -0.034876          0.809436          -0.453626
57803 C          -0.871021          1.285997          0.728480
57804 O          -1.924993          0.388754          1.006610
57805 O          -2.907351          0.570155          -0.006865
57806 H          0.907720          -2.406686          1.367796
57807 C          1.703045          -0.901859          -1.245376
57808 H          2.002123          -1.936535          -1.103079
57809 H          2.594731          -0.270434          -1.205308
57810 H          1.245862          -0.784661          -2.226915
57811 C          -0.741870          -1.974652          -0.317795
57812 O          -1.521864          -1.805898          -1.138143
57813 H          -2.886673          -0.283274          -0.461208
57814 H          -0.700292          0.627341          -1.303430
57815 O          0.801893          1.843241          -0.955079
57816 O          1.769932          2.131050          0.054008
57817 H          1.615772          3.071800          0.201115
57818 H          -0.284119          1.320115          1.643289
57819 H          -1.272611          2.276029          0.506296
57820 Rotational constants (GHz):          1.0031900          0.8636500          0.6317700
57821 Vibrational harmonic frequencies (cm-1):
57822 i266.4395          55.9587          97.5257
57823 100.2660          120.8554          133.5139
57824 137.2251          161.9933          167.1487
57825 185.7366          205.6868          231.4346
57826 236.8823          289.9421          295.3152
57827 324.7723          343.0524          362.7293
57828 381.9751          446.6606          493.4400
57829 515.5785          575.8273          725.9229
57830 786.0313          939.0474          952.4850
57831 976.4968          1022.9129          1045.3468
57832 1068.1618          1085.1460          1117.4087
57833 1147.5160          1238.5778          1278.8158
57834 1320.8511          1341.1275          1382.2604
57835 1397.3955          1407.8975          1415.5281
57836 1430.8993          1440.8363          1469.3430
57837 1487.6851          1492.4120          2049.8878
57838 3054.6648          3075.5556          3083.4527
57839 3130.7324          3162.5881          3170.9868
57840 3735.4254          3803.1597          3833.7057
57841 Zero-point correction (Hartree): 0.152486
57842
57843 TS.triHPacyl.COelim.tmmmtmpmd
57844 -----
57845 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16049523
57846 Electronic state : 2-A
57847 Cartesian coordinates (Angs):
57848 O          -1.921067          -1.558383          -1.382523
57849 O          -1.272339          -0.342875          -1.047451
57850 C          -0.745047          -0.414642          0.216358
57851 C          0.114004          0.789628          0.504938
57852 C          0.984802          1.250230          -0.659733
57853 O          1.969945          0.289824          -0.976689
57854 O          2.878546          0.233497          0.118750
57855 H          -1.156379          -2.133251          -1.550748
57856 C          -1.632926          -0.901465          1.317493
57857 H          -2.068233          -1.867585          1.077376
57858 H          -2.445083          -0.189740          1.492249
57859 H          -1.054227          -0.984182          2.236199
57860 C          0.591646          -2.006143          0.070819
57861 O          1.260576          -2.142061          0.983600

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57862	H	3.678327	0.597219	-0.279943	
57863	H	0.757271	0.539473	1.352654	
57864	O	-0.664995	1.873678	1.006324	
57865	O	-1.404480	2.431583	-0.071707	
57866	H	-2.202602	1.885650	-0.097007	
57867	H	0.404311	1.358207	-1.572094	
57868	H	1.442257	2.206461	-0.400376	
57869	Rotational constants (GHz):		0.9865600	0.8798400	0.6269300
57870	Vibrational harmonic frequencies (cm-1):				
57871	i321.0755		24.9528		81.2144
57872	101.0768		118.6126		132.8268
57873	141.7462		149.7219		175.7246
57874	190.0023		206.9251		227.6102
57875	243.1279		258.8198		293.6668
57876	305.5230		351.5497		370.6292
57877	393.8721		448.9657		493.6408
57878	528.1341		577.7406		724.9434
57879	784.7527		933.8911		947.9637
57880	974.2908		1017.7255		1044.7952
57881	1061.6136		1076.2109		1109.6970
57882	1147.5327		1230.8878		1273.8500
57883	1310.9069		1330.1785		1387.1032
57884	1396.4939		1405.5914		1418.3001
57885	1422.6604		1439.3928		1474.1451
57886	1483.0560		1488.7494		2086.7092
57887	3047.0974		3085.4295		3088.7712
57888	3128.0174		3170.9445		3172.2965
57889	3730.0903		3788.1301		3828.0060
57890	Zero-point correction (Hartree): 0.152242				
57891					
57892	TS.triHPacyl.COelim.tmmmtmpd				
57893	-----				
57894	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16211285				
57895	Electronic state : 2-A				
57896	Cartesian coordinates (Angs):				
57897	O	-1.924267	-1.671991	-1.284798	
57898	O	-1.302091	-0.431073	-0.998047	
57899	C	-0.728786	-0.454343	0.243525	
57900	C	0.060593	0.804572	0.492500	
57901	C	0.900355	1.285399	-0.686774	
57902	O	1.951798	0.389430	-0.976102	
57903	O	2.914281	0.518690	0.064359	
57904	H	-1.155344	-2.213809	-1.524118	
57905	C	-1.525083	-1.010590	1.379520	
57906	H	-1.882490	-2.013644	1.163981	
57907	H	-2.390742	-0.372384	1.580402	
57908	H	-0.907709	-1.030271	2.276346	
57909	C	0.733068	-1.983493	0.023414	
57910	O	1.527314	-1.990155	0.845468	
57911	H	2.920546	-0.372732	0.439051	
57912	H	0.722075	0.614828	1.342151	
57913	O	-0.780559	1.847712	0.979791	
57914	O	-1.540886	2.355757	-0.107856	
57915	H	-2.323034	1.787021	-0.113462	
57916	H	0.315964	1.329002	-1.601799	
57917	H	1.295135	2.275770	-0.458189	
57918	Rotational constants (GHz):		1.0028300	0.8714900	0.6176100
57919	Vibrational harmonic frequencies (cm-1):				
57920	i284.0848		39.4159		95.2201
57921	113.7113		124.1593		132.4524
57922	142.4830		156.0337		178.6763
57923	196.6373		230.1453		231.4098
57924	267.9314		285.8088		312.4819
57925	324.3312		334.7789		348.2059
57926	370.3740		440.1281		493.9863
57927	527.7454		577.7760		724.0467
57928	783.3491		936.7680		949.2853
57929	975.4265		1018.5615		1045.6353
57930	1060.9885		1075.5688		1117.8738
57931	1144.9138		1230.0875		1273.4603
57932	1314.4667		1331.8001		1390.9391
57933	1404.1690		1410.5355		1418.4491

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57934      1430.5015          1432.5356          1472.8456
57935      1484.7872          1489.6353          2059.8431
57936      3046.9084          3087.7156          3095.6285
57937      3127.7965          3172.3033          3172.9356
57938      3744.4911          3790.5169          3794.7213
57939      Zero-point correction (Hartree): 0.152485
57940
57941      TS.triHPacyl.COelim.tmpmmtmmpd
57942      -----
57943      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16057499
57944      Electronic state : 2-A
57945      Cartesian coordinates (Angs):
57946      O      -1.293871      -1.292706      -1.849635
57947      O      -0.282293      -0.724817      -1.038337
57948      C      -0.786751      0.282734      -0.258297
57949      C      0.211882      0.754747      0.764021
57950      C      1.174256      -0.284524      1.336790
57951      O      2.226558      -0.620047      0.442677
57952      O      2.034354      -1.917568      -0.090821
57953      H      -1.816696      -1.777632      -1.188781
57954      C      -1.648116      1.313108      -0.907434
57955      H      -2.481762      0.860544      -1.437312
57956      H      -1.043135      1.883285      -1.616473
57957      H      -2.025954      1.996129      -0.148246
57958      C      -2.151928      -0.777651      0.904478
57959      O      -2.441046      -0.263419      1.881649
57960      H      1.383210      -1.756732      -0.790845
57961      H      -0.368302      1.150222      1.604849
57962      O      0.922868      1.904550      0.313658
57963      O      1.463662      1.650632      -0.975647
57964      H      2.198250      1.047733      -0.780389
57965      H      1.659599      0.165335      2.203632
57966      H      0.656870      -1.192374      1.647871
57967      Rotational constants (GHz):      1.0690200      0.7546900      0.7090600
57968      Vibrational harmonic frequencies (cm-1):
57969      i290.1294          45.8432          69.7128
57970      84.1183          113.5305          146.4494
57971      151.6870          168.5545          176.0511
57972      195.3585          220.7612          257.5550
57973      269.9790          316.8716          321.6700
57974      376.8799          397.5580          423.4541
57975      441.6411          473.7522          492.3180
57976      515.7622          590.4754          762.7316
57977      834.0031          901.0945          916.7270
57978      991.8871          999.6297          1044.1781
57979      1048.8693          1077.1055          1113.0741
57980      1142.8415          1230.7846          1278.3613
57981      1320.0733          1357.5333          1383.4473
57982      1407.6188          1410.4802          1444.8144
57983      1461.8328          1464.8127          1469.6792
57984      1471.2911          1489.7301          2075.0585
57985      3058.4499          3061.8068          3080.7092
57986      3135.5057          3136.3757          3171.7600
57987      3717.1321          3738.6936          3753.5141
57988      Zero-point correction (Hartree): 0.153096
57989
57990      TS.triHPacyl.COelim.tmpmmtmmpd
57991      -----
57992      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16116853
57993      Electronic state : 2-A
57994      Cartesian coordinates (Angs):
57995      O      2.003437      0.046315      1.737988
57996      O      0.787148      -0.128817      1.037525
57997      C      0.755827      0.624798      -0.106763
57998      C      -0.608311      0.523697      -0.735296
57999      C      -1.106674      -0.882372      -1.056787
58000      O      -1.097027      -1.806008      0.006687
58001      O      -1.994842      -1.340325      1.006242
58002      H      2.507585      -0.722523      1.433016
58003      C      1.424846      1.960193      -0.093374
58004      H      2.480933      1.877866      0.148622
58005      H      0.949055      2.605797      0.649213

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58006	H	1.317189	2.417211	-1.074825		
58007	C	2.004363	-0.458590	-1.446205		
58008	O	2.729781	-1.113410	-0.854494		
58009	H	-1.391735	-0.862542	1.596328		
58010	H	-0.570838	1.061039	-1.689309		
58011	O	-1.446729	1.240983	0.174660		
58012	O	-2.788287	1.194024	-0.276203		
58013	H	-3.112643	0.410547	0.196063		
58014	H	-2.106462	-0.813167	-1.487695		
58015	H	-0.441230	-1.322666	-1.800114		
58016	Rotational constants (GHz):			1.2951500	0.7021300	0.6315800
58017	Vibrational harmonic frequencies (cm-1):					
58018		i277.5767	25.5724			56.5300
58019		76.6139	124.3047			130.4117
58020		141.0367	154.3151			192.9662
58021		218.2952	225.8710			235.9984
58022		273.6058	299.0314			308.1439
58023		347.9561	356.0443			408.4550
58024		454.8670	470.3127			507.5756
58025		544.9411	625.5359			757.9856
58026		821.9735	869.4042			958.3203
58027		965.9013	1027.3554			1037.5763
58028		1060.6975	1077.8477			1109.8187
58029		1163.2195	1220.5599			1285.6895
58030		1313.5628	1350.2601			1393.5911
58031		1409.4253	1422.6053			1424.6013
58032		1434.2104	1441.9058			1473.7360
58033		1483.5519	1490.2778			2061.8738
58034		3048.6233	3057.7354			3084.9862
58035		3133.0547	3138.2899			3172.5063
58036		3741.1421	3757.7550			3778.1110
58037	Zero-point correction (Hartree): 0.152971					
58038						
58039	TS.triHPacyl.COelim.tmppmtmmmd					
58040	-----					
58041	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15964950					
58042	Electronic state : 2-A					
58043	Cartesian coordinates (Angs):					
58044	O	-1.347505	-0.728541	2.124052		
58045	O	-0.285229	-0.461583	1.226517		
58046	C	-0.730132	-0.474338	-0.068154		
58047	C	0.289710	0.036662	-1.052638		
58048	C	1.021918	1.349910	-0.725493		
58049	O	1.277268	1.664582	0.619928		
58050	O	2.199692	0.722026	1.143142		
58051	H	-1.813142	0.123821	2.119559		
58052	C	-1.553046	-1.644100	-0.500242		
58053	H	-2.380042	-1.819536	0.181683		
58054	H	-0.917997	-2.533756	-0.521613		
58055	H	-1.938356	-1.471567	-1.503831		
58056	C	-2.123196	1.090740	-0.053469		
58057	O	-2.373095	1.496875	-1.090499		
58058	H	1.599065	0.138057	1.634301		
58059	H	-0.268904	0.242074	-1.971959		
58060	O	1.165786	-0.994414	-1.502781		
58061	O	1.795543	-1.623316	-0.400326		
58062	H	2.473967	-0.979498	-0.142508		
58063	H	1.951927	1.356808	-1.301342		
58064	H	0.402269	2.185322	-1.054566		
58065	Rotational constants (GHz):			1.0777100	0.7805300	0.7475800
58066	Vibrational harmonic frequencies (cm-1):					
58067		i292.7199	35.3088			70.7649
58068		105.7965	126.4143			132.2790
58069		143.0939	170.1009			187.6025
58070		192.1380	217.6439			241.2956
58071		285.6321	288.3554			327.5852
58072		334.2273	358.3286			389.3125
58073		417.9352	468.4658			528.9298
58074		599.8746	619.8483			756.1056
58075		772.6732	904.3354			950.3275
58076		984.8155	1029.2753			1040.5258
58077		1052.0495	1067.3068			1111.9755

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58078      1165.5399      1210.7284      1289.2687
58079      1326.5159      1365.6456      1379.8220
58080      1406.1715      1413.6409      1435.2378
58081      1438.6260      1464.8792      1473.0922
58082      1477.8261      1491.0084      2073.9407
58083      3053.7538      3056.4936      3060.7135
58084      3121.0864      3134.0319      3175.4261
58085      3715.4164      3733.4644      3741.1717
58086      Zero-point correction (Hartree): 0.152897
58087
58088      TS.triHPacyl.COelim.tmtmmmmmd
58089      -----
58090      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16199486
58091      Electronic state : 2-A
58092      Cartesian coordinates (Angs):
58093      O      2.422547      0.649476      1.446404
58094      O      1.119701      0.236647      1.077756
58095      C      0.931972      0.334420      -0.274130
58096      C     -0.476857     -0.045386     -0.652022
58097      C     -1.100094     -1.043629      0.314610
58098      O     -2.395870     -1.431850     -0.100104
58099      O     -3.312769     -0.430394      0.333394
58100      H      2.896935     -0.195015      1.445277
58101      C      1.562686      1.463053     -1.014562
58102      H      2.641324      1.478595     -0.885736
58103      H      1.150863      2.409273     -0.654163
58104      H      1.322761      1.364648     -2.071570
58105      C      2.014101     -1.350657     -0.991914
58106      O      2.765798     -1.710352     -0.207345
58107      H     -3.853067     -0.930657      0.957033
58108      H     -0.441447     -0.494471     -1.648298
58109      O     -1.295133      1.091367     -0.873175
58110      O     -1.471483      1.773834      0.358687
58111      H     -2.324919      1.410908      0.640285
58112      H     -0.511533     -1.962916      0.308661
58113      H     -1.134088     -0.657002      1.331687
58114      Rotational constants (GHz): 1.4335800      0.6124100      0.5314600
58115      Vibrational harmonic frequencies (cm-1):
58116      i269.8932      41.5309      59.9946
58117      81.1589      121.1119      148.1116
58118      161.2247      169.3431      172.7710
58119      192.4386      216.7622      243.0127
58120      252.5832      271.8605      304.3058
58121      320.4477      333.8835      374.6481
58122      403.2772      479.3138      493.6784
58123      516.0207      610.3392      720.2973
58124      825.2060      887.3934      954.0497
58125      997.5695      1004.7911      1046.5756
58126      1054.3701      1103.9763      1115.5229
58127      1150.9048      1231.9156      1288.7504
58128      1315.2135      1347.5984      1376.8820
58129      1396.5497      1409.7904      1427.7397
58130      1434.3019      1442.8375      1469.1039
58131      1471.4067      1489.7830      2046.0455
58132      3057.6163      3081.1803      3086.9510
58133      3136.7887      3146.3542      3173.2772
58134      3766.9820      3777.9370      3826.7045
58135      Zero-point correction (Hartree): 0.152706
58136
58137      TS.triHPacyl.COelim.tmtmmmmmpd
58138      -----
58139      IRC pathway available
58140      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18824540
58141      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07117476
58142      T1 diagnostic: 0.016983
58143      E(MP2/Aug-CC-pVTZ) (Hartree): -721.03105939
58144      E(MP3/Aug-CC-pVTZ) (Hartree): -721.04963108
58145      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03640907
58146      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05314287
58147      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51322306
58148      E(UHF/Aug-CC-pVTZ) (Hartree): -718.50623255
58149      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16426877

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58150 Electronic state : 2-A
58151 Cartesian coordinates (Angs):
58152   O      2.448223      0.702922      1.381190
58153   O      1.139899      0.267326      1.063300
58154   C      0.914216      0.323428     -0.284787
58155   C     -0.497736     -0.087123     -0.607089
58156   C     -1.091820     -1.060632      0.401786
58157   O     -2.383852     -1.485448      0.017899
58158   O     -3.306933     -0.454762      0.357318
58159   H      2.926463     -0.138907      1.411685
58160   C      1.505316      1.440818     -1.074270
58161   H      2.586311      1.477374     -0.973170
58162   H      1.087022      2.390206     -0.730377
58163   H      1.242200      1.306810     -2.121898
58164   C      1.986749     -1.354258     -0.986704
58165   O      2.764823     -1.693185     -0.218789
58166   H     -3.447552     -0.032863     -0.501774
58167   H     -0.488853     -0.560257     -1.592953
58168   O     -1.345864      1.037450     -0.829614
58169   O     -1.441969      1.781957      0.374562
58170   H     -2.189028      1.347139      0.816315
58171   H     -0.489820     -1.970409      0.424467
58172   H     -1.121714     -0.642565      1.407158
58173 Rotational constants (GHz):  1.4419200      0.6189300      0.5346900
58174 Vibrational harmonic frequencies (cm-1):
58175   1278.5504      44.5674      62.1855
58176     86.8413      129.1074      151.1114
58177    162.6388      169.6613      177.7295
58178    196.4882      218.5516      247.1047
58179    277.5222      305.0062      320.7053
58180    335.9934      371.8657      405.8813
58181    408.7984      494.3321      506.2133
58182    533.6203      612.0881      724.8329
58183    828.3854      887.1414      951.9052
58184    998.9505     1004.9975     1047.8278
58185   1055.0343     1110.2089     1113.1949
58186   1140.5813     1231.3098     1292.0776
58187   1309.3991     1346.2925     1375.4195
58188   1407.2489     1411.9708     1425.4515
58189   1432.9509     1441.5143     1469.6879
58190   1478.4800     1489.9614     2046.7958
58191   3058.2338     3079.7303     3090.8224
58192   3136.9795     3143.1235     3173.3911
58193   3736.3446     3779.6627     3793.5642
58194 Zero-point correction (Hartree): 0.153165
58195
58196 TS.triHPacyl.COelim.tmtmmmpdp
58197 -----
58198 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16044600
58199 Electronic state : 2-A
58200 Cartesian coordinates (Angs):
58201   O      2.490055     -0.729610     -1.297372
58202   O      1.145779     -0.374840     -1.023210
58203   C      0.924342     -0.296821      0.325130
58204   C     -0.511856      0.047614      0.605766
58205   C     -1.132393      1.028499     -0.377827
58206   O     -2.402976      1.439776      0.078103
58207   O     -3.373735      0.519577     -0.397345
58208   H      2.885304      0.139494     -1.460519
58209   C      1.594989     -1.285983      1.220468
58210   H      2.676274     -1.248735      1.121247
58211   H      1.270102     -2.303363      0.983094
58212   H      1.318718     -1.070802      2.250754
58213   C      1.879090      1.490416      0.866721
58214   O      2.605032      1.834889      0.052415
58215   H     -3.279041     -0.222341      0.217386
58216   H     -0.550409      0.488351      1.605395
58217   O     -1.323020     -1.120828      0.772249
58218   O     -1.430044     -1.782894     -0.482231
58219   H     -0.801265     -2.509845     -0.386799
58220   H     -0.520832      1.932084     -0.416270
58221   H     -1.212610      0.604250     -1.376715

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58222 Rotational constants (GHz): 1.4031800 0.6269700 0.5317500
58223 Vibrational harmonic frequencies (cm-1):
58224 i296.8341 41.7526 53.5449
58225 77.4122 121.2308 132.0503
58226 137.6444 150.4860 170.5210
58227 175.5717 198.3182 217.4921
58228 249.5031 268.2731 303.4552
58229 318.9566 336.2759 373.8563
58230 394.6310 432.4005 499.2888
58231 510.8312 598.7665 725.6022
58232 828.1852 883.0733 957.4128
58233 995.3043 1002.1451 1043.5101
58234 1051.5202 1101.6032 1119.8769
58235 1140.7908 1227.0614 1288.7699
58236 1303.7099 1347.4489 1374.2383
58237 1397.3362 1412.2054 1418.7201
58238 1428.2725 1437.6533 1464.8002
58239 1467.5204 1490.1447 2051.1151
58240 3047.0517 3084.4715 3086.6245
58241 3132.3206 3151.4859 3173.7340
58242 3779.0688 3779.6187 3812.0083
58243 Zero-point correction (Hartree): 0.152106
58244
58245 TS.triHPacyl.COelim.tmtmmmtpm
58246 -----
58247 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16101698
58248 Electronic state : 2-A
58249 Cartesian coordinates (Angs):
58250 O 2.685821 0.244948 1.447551
58251 O 1.330316 -0.032444 1.150671
58252 C 0.984567 0.449291 -0.083605
58253 C -0.480336 0.220100 -0.335317
58254 C -0.964703 -1.105383 0.237271
58255 O -2.252376 -1.471695 -0.229520
58256 O -3.217854 -0.721638 0.498576
58257 H 3.116473 -0.570880 1.152078
58258 C 1.585627 1.729480 -0.555572
58259 H 2.668666 1.666763 -0.621052
58260 H 1.323090 2.536521 0.131711
58261 H 1.175979 1.964204 -1.536074
58262 C 1.879665 -0.965303 -1.396906
58263 O 2.707427 -1.539810 -0.854827
58264 H -3.670886 -1.409962 0.999397
58265 H -0.635917 0.229646 -1.416633
58266 O -1.174190 1.334803 0.218896
58267 O -2.298004 1.630465 -0.594725
58268 H -2.979384 1.057136 -0.210519
58269 H -0.320343 -1.913533 -0.114096
58270 H -0.955706 -1.086039 1.326986
58271 Rotational constants (GHz): 1.4247300 0.5795100 0.5073700
58272 Vibrational harmonic frequencies (cm-1):
58273 i274.1086 42.6987 53.6569
58274 59.6456 113.3501 121.2467
58275 144.3491 146.8375 160.7086
58276 174.0595 211.4334 233.8023
58277 235.5239 294.6673 309.8662
58278 322.3761 343.5254 367.2869
58279 404.4086 477.0319 494.5880
58280 526.0269 545.3220 696.0295
58281 852.5766 895.9116 965.4143
58282 996.6672 1025.9476 1055.7083
58283 1064.4963 1098.1322 1110.8289
58284 1134.3143 1224.8311 1291.9089
58285 1314.0568 1350.5463 1365.6900
58286 1384.7380 1410.5172 1429.0347
58287 1438.8849 1456.1151 1459.0898
58288 1470.1115 1487.8293 2048.5168
58289 3064.0456 3079.0430 3085.3949
58290 3138.1699 3138.9947 3169.6525
58291 3752.2254 3776.6432 3835.8753
58292 Zero-point correction (Hartree): 0.152296
58293

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58294 TS.triHPacyl.COelim.tmtmmtmmd
58295 -----
58296 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16218851
58297 Electronic state : 2-A
58298 Cartesian coordinates (Angs):
58299 O -2.415310 -1.068507 1.487996
58300 O -1.085714 -0.723083 1.146934
58301 C -1.024986 -0.269618 -0.141185
58302 C 0.352215 0.249769 -0.472942
58303 C 1.105699 0.746839 0.754263
58304 O 2.370353 1.277686 0.408078
58305 O 3.281649 0.189186 0.281614
58306 H -2.820737 -0.190286 1.577161
58307 C -1.748066 -1.024521 -1.205564
58308 H -2.803633 -1.133606 -0.972964
58309 H -1.302527 -2.017781 -1.304237
58310 H -1.632737 -0.503441 -2.154686
58311 C -2.168004 1.475834 0.009454
58312 O -1.949230 2.250653 -0.800507
58313 H 3.897112 0.377273 1.000664
58314 H 0.242313 1.078176 -1.179863
58315 O 1.098129 -0.680882 -1.238872
58316 O 1.361364 -1.821963 -0.437256
58317 H 2.251341 -1.610375 -0.116587
58318 H 0.557455 1.579507 1.198607
58319 H 1.220331 -0.034004 1.503863
58320 Rotational constants (GHz): 1.2788800 0.6399700 0.5597300
58321 Vibrational harmonic frequencies (cm-1):
58322 i280.0020 43.3797 70.0075
58323 78.6533 109.3826 131.5479
58324 151.6323 164.0746 181.1251
58325 185.3154 217.7115 255.3519
58326 266.2843 297.4968 310.5512
58327 322.4335 360.2066 387.7012
58328 416.4622 473.1234 487.6295
58329 516.4374 612.2732 713.3738
58330 824.6938 888.7200 954.8534
58331 996.9792 1004.7188 1039.2842
58332 1052.9258 1103.8341 1115.8866
58333 1150.8680 1230.2113 1289.9301
58334 1315.2136 1345.1525 1383.1351
58335 1396.3140 1407.1646 1431.6445
58336 1437.0452 1441.3173 1469.7294
58337 1470.9638 1488.6070 2070.3166
58338 3057.2850 3069.3161 3087.0820
58339 3133.7758 3146.8891 3172.7444
58340 3726.6714 3752.9641 3825.3926
58341 Zero-point correction (Hartree): 0.152714
58342 -----
58343 TS.triHPacyl.COelim.tmtmmtmmpd
58344 -----
58345 IRC pathway available
58346 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18833837
58347 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07107073
58348 T1 diagnostic: 0.016967
58349 E(MP2/Aug-CC-pVTZ) (Hartree): -721.03164745
58350 E(MP3/Aug-CC-pVTZ) (Hartree): -721.04974718
58351 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03703264
58352 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05322866
58353 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51180403
58354 E(UHF/Aug-CC-pVTZ) (Hartree): -718.50470929
58355 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16437035
58356 Electronic state : 2-A
58357 Cartesian coordinates (Angs):
58358 O -2.455775 -1.080685 1.417470
58359 O -1.114725 -0.735646 1.126817
58360 C -1.011386 -0.257821 -0.149484
58361 C 0.376748 0.262035 -0.420624
58362 C 1.103355 0.727480 0.834387
58363 O 2.369052 1.276183 0.528980
58364 O 3.276818 0.199125 0.315340
58365 H -2.853916 -0.203282 1.539577

```

58366	C	-1.699140	-0.991363	-1.251861	
58367	H	-2.761121	-1.105147	-1.053603	
58368	H	-1.250345	-1.982545	-1.355593	
58369	H	-1.556457	-0.450800	-2.186314	
58370	C	-2.142334	1.483873	-0.013646	
58371	O	-1.907891	2.261513	-0.816748	
58372	H	3.323242	0.176362	-0.650598	
58373	H	0.298088	1.102373	-1.117813	
58374	O	1.152298	-0.664404	-1.177206	
58375	O	1.324591	-1.845481	-0.410219	
58376	H	2.127449	-1.637906	0.094180	
58377	H	0.543765	1.542634	1.295705	
58378	H	1.210889	-0.071753	1.566373	
58379	Rotational constants (GHz):		1.2799800	0.6474100	0.5636000
58380	Vibrational harmonic frequencies (cm-1):				
58381		1288.4228	45.1276		71.5516
58382		82.9920	116.1325		133.6500
58383		156.0617	166.4969		180.5482
58384		199.3292	220.6434		259.9160
58385		291.8697	308.9208		325.0086
58386		358.6751	385.1686		406.0656
58387		420.8694	484.4478		508.2499
58388		536.8409	612.6222		717.1621
58389		828.1127	888.6512		952.7796
58390		997.4651	1005.1584		1040.2689
58391		1052.5472	1111.3119		1112.3709
58392		1140.7781	1229.2702		1293.7863
58393		1309.1547	1343.5058		1382.3376
58394		1403.9289	1413.1827		1425.3506
58395		1437.7097	1441.6360		1470.0472
58396		1476.1712	1488.7298		2069.5038
58397		3057.7665	3066.5014		3090.8504
58398		3134.0190	3143.8530		3173.7704
58399		3730.5216	3731.6058		3794.7280
58400	Zero-point correction (Hartree): 0.153151				
58401	TS.triHPacyl.COelim.tmtmmtmpd				
58402	-----				
58403	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16037765				
58404	Electronic state : 2-A				
58405	Cartesian coordinates (Angs):				
58406	O	2.477199	-1.062138	-1.379910	
58407	O	1.119464	-0.807381	-1.064909	
58408	C	1.019963	-0.230923	0.170755	
58409	C	-0.393332	0.201921	0.449365	
58410	C	-1.139844	0.735228	-0.764642	
58411	O	-2.374924	1.292832	-0.371823	
58412	O	-3.352636	0.263690	-0.363722	
58413	H	2.772984	-0.181884	-1.661854	
58414	C	1.806210	-0.819639	1.297545	
58415	H	2.867547	-0.853659	1.067389	
58416	H	1.472583	-1.841464	1.501667	
58417	H	1.646870	-0.225821	2.195994	
58418	C	1.996438	1.578161	-0.109625	
58419	O	1.805633	2.348575	0.710584	
58420	H	-3.176480	-0.187268	0.474631	
58421	H	-0.357476	0.988241	1.209511	
58422	O	-1.140159	-0.814531	1.127635	
58423	O	-1.336947	-1.903490	0.234121	
58424	H	-0.677897	-2.541672	0.536612	
58425	H	-0.567107	1.552871	-1.206978	
58426	H	-1.298681	-0.038285	-1.513188	
58427	Rotational constants (GHz):		1.2576300	0.6569300	0.5532700
58428	Vibrational harmonic frequencies (cm-1):				
58429		1307.4600	45.8303		61.7240
58430		79.4031	102.7915		128.6127
58431		139.9598	144.2367		170.4891
58432		176.2052	207.7404		217.9434
58433		252.2385	289.3504		306.4584
58434		318.8888	355.8076		382.9151
58435		400.6665	418.6138		493.9842
58436		510.8711	599.7630		716.4648
58437					


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58438      827.6189      883.9292      958.0955
58439      993.9005      1001.0565      1035.7237
58440      1050.4940      1101.2802      1119.3639
58441      1139.4992      1224.1244      1291.2829
58442      1307.2398      1345.6682      1377.7584
58443      1396.6759      1411.6644      1419.1290
58444      1431.3430      1437.0225      1465.6485
58445      1468.1668      1490.2725      2074.8258
58446      3045.7255      3073.0769      3082.7587
58447      3129.1915      3151.2218      3172.9554
58448      3747.2334      3781.0016      3809.6385
58449 Zero-point correction (Hartree): 0.152103
58450
58451 TS.triHPacyl.COelim.tmtmmttppmd
58452 -----
58453 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16100791
58454 Electronic state : 2-A
58455 Cartesian coordinates (Angs):
58456 O      -2.751744      0.236042      -1.607038
58457 O      -1.359615      0.173282      -1.360836
58458 C      -1.102061      0.349333      -0.029441
58459 C      0.362571      0.146453      0.252786
58460 C      0.971019      -0.939649      -0.624955
58461 O      2.248088      -1.362517      -0.178111
58462 O      3.204228      -0.386972      -0.574350
58463 H      -3.040561      -0.629569      -1.275072
58464 C      -1.810719      1.439644      0.703443
58465 H      -2.889624      1.316374      0.659480
58466 H      -1.549249      2.404077      0.262852
58467 H      -1.484883      1.438272      1.742304
58468 C      -1.993218      -1.356024      0.792649
58469 O      -1.628813      -1.616638      1.842140
58470 H      3.707582      -0.858156      -1.248721
58471 H      0.468930      -0.130269      1.305602
58472 O      0.996610      1.409595      0.071378
58473 O      2.046782      1.540691      1.015596
58474 H      2.789582      1.129638      0.546558
58475 H      0.361284      -1.843380      -0.566663
58476 H      1.027116      -0.613376      -1.663454
58477 Rotational constants (GHz): 1.2687400      0.5890200      0.5597400
58478 Vibrational harmonic frequencies (cm-1):
58479 1286.8783      44.4898      56.4585
58480 67.0292      100.9709      122.4500
58481 124.6299      142.0075      165.5156
58482 172.1981      216.3376      232.2377
58483 261.7348      278.7058      313.4416
58484 344.5284      360.6917      380.4045
58485 407.7888      473.5770      493.7176
58486 517.9212      537.5781      688.1454
58487 852.7966      897.2017      965.7021
58488 994.9788      1024.6365      1048.3337
58489 1063.5805      1098.5166      1110.2838
58490 1133.7562      1224.7125      1295.6936
58491 1313.2882      1349.1124      1367.5567
58492 1385.2398      1408.3295      1434.0910
58493 1436.9572      1454.9465      1457.4543
58494 1469.8029      1487.3117      2075.8863
58495 3063.9898      3072.0609      3080.1412
58496 3136.6202      3137.5088      3169.9858
58497 3734.0786      3746.3169      3829.9762
58498 Zero-point correction (Hartree): 0.152235
58499
58500 TS.triHPacyl.COelim.tmtmpmmmd
58501 -----
58502 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16023555
58503 Electronic state : 2-A
58504 Cartesian coordinates (Angs):
58505 O      -2.320071      -0.778043      1.589395
58506 O      -0.972468      -0.585605      1.172372
58507 C      -0.950979      -0.209717      -0.145997
58508 C      0.430745      0.251680      -0.538702
58509 C      1.181321      0.903681      0.614136

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58510      O      2.445604      1.388664      0.202642
58511      O      3.358607      0.293225      0.210120
58512      H      -2.323820      -1.723477      1.785939
58513      C      -1.698505      -1.054553      -1.123166
58514      H      -2.756723      -1.096484      -0.879209
58515      H      -1.277841      -2.063646      -1.124806
58516      H      -1.584001      -0.638730      -2.122541
58517      C      -1.970777      1.583523      -0.139333
58518      O      -2.951980      1.583003      -0.722518
58519      H      3.979083      0.574348      0.893435
58520      H      0.327314      0.984629      -1.344612
58521      O      1.173444      -0.774004      -1.178183
58522      O      1.445622      -1.797074      -0.232563
58523      H      2.331631      -1.533470      0.059815
58524      H      0.623672      1.781306      0.942474
58525      H      1.299787      0.226518      1.457759
58526      Rotational constants (GHz):      1.4320100      0.5886500      0.5357400
58527      Vibrational harmonic frequencies (cm-1):
58528      i324.8761      36.4801      59.2126
58529      79.6129      96.2789      130.6026
58530      158.7680      164.5908      168.4234
58531      192.8388      205.4137      216.1828
58532      252.8464      275.0295      287.6723
58533      313.4177      318.3274      378.1743
58534      419.6639      474.0539      492.2899
58535      514.7317      608.7313      713.6948
58536      827.4825      888.6342      952.0996
58537      996.2268      1003.4071      1023.5059
58538      1055.7039      1100.5575      1114.0880
58539      1146.9783      1222.7077      1282.8254
58540      1312.8212      1332.7145      1373.2019
58541      1394.9749      1402.6307      1414.4621
58542      1431.2797      1443.5351      1471.9354
58543      1472.4820      1488.9755      2071.6352
58544      3055.3672      3069.2456      3096.9804
58545      3137.1859      3152.1286      3171.5647
58546      3765.8640      3821.5173      3826.9501
58547      Zero-point correction (Hartree): 0.152361
58548
58549      TS.triHPacyl.COelim.tmtmpmmmpd
58550      -----
58551      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16236299
58552      Electronic state : 2-A
58553      Cartesian coordinates (Angs):
58554      O      -2.359686      -0.795929      1.528000
58555      O      -0.998030      -0.604017      1.158547
58556      C      -0.936653      -0.204679      -0.151121
58557      C      0.453333      0.271262      -0.487011
58558      C      1.178441      0.892059      0.698466
58559      O      2.441935      1.405079      0.325783
58560      O      3.353645      0.312915      0.236907
58561      H      -2.360606      -1.733211      1.760187
58562      C      -1.647364      -1.035022      -1.167852
58563      H      -2.711526      -1.090156      -0.954958
58564      H      -1.219367      -2.040807      -1.176871
58565      H      -1.508740      -0.597074      -2.154743
58566      C      -1.956849      1.576307      -0.145358
58567      O      -2.918506      1.588859      -0.760252
58568      H      3.405447      0.183773      -0.720143
58569      H      0.375134      1.021195      -1.280295
58570      O      1.226514      -0.742654      -1.125983
58571      O      1.422585      -1.809658      -0.210884
58572      H      2.225722      -1.522493      0.253113
58573      H      0.608034      1.751716      1.050513
58574      H      1.292802      0.190725      1.523499
58575      Rotational constants (GHz):      1.4341400      0.5945900      0.5396900
58576      Vibrational harmonic frequencies (cm-1):
58577      i332.0122      36.4453      61.4854
58578      82.3818      101.6760      135.1854
58579      164.1991      173.8660      189.9166
58580      200.0056      207.3743      217.8423
58581      259.2372      280.3957      303.3969

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58582      324.7236      377.9483      400.4942
58583      423.5967      481.7647      504.7707
58584      549.0688      610.9368      717.6137
58585      830.8051      888.8742      949.9765
58586      997.7488      1003.8458     1025.9415
58587      1056.1233     1107.6283     1111.3897
58588      1137.2656     1221.8159     1286.4757
58589      1307.5420     1331.1337     1371.0849
58590      1403.2529     1407.7995     1415.2354
58591      1429.5098     1443.6632     1473.2347
58592      1477.6059     1489.8828     2071.0663
58593      3056.6916     3066.7767     3098.7449
58594      3137.3953     3150.5773     3172.5102
58595      3737.4624     3797.9987     3824.9677
58596      Zero-point correction (Hartree): 0.152834
58597
58598      TS.triHPacyl.COelim.tmtmppmmpd
58599      -----
58600      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16167776
58601      Electronic state : 2-A
58602      Cartesian coordinates (Angs):
58603      O      -2.568678      -0.545715      1.323188
58604      O      -1.190855      -0.322277      1.052444
58605      C      -0.977946      -0.336907     -0.300720
58606      C      0.442841      0.066558     -0.605610
58607      C      1.042941      1.013308      0.425668
58608      O      2.341790      1.430556      0.054994
58609      O      3.252145      0.381489      0.373902
58610      H      -2.529634     -1.376843      1.813580
58611      C      -1.554214     -1.457910     -1.098662
58612      H      -2.634423     -1.501695     -0.991106
58613      H      -1.113025     -2.404937     -0.778288
58614      H      -1.311523     -1.303062     -2.148159
58615      C      -1.992614      1.315394     -0.992647
58616      O      -2.189825      2.114321     -0.201496
58617      H      3.403004     -0.012497     -0.496416
58618      H      0.453708      0.553829     -1.585612
58619      O      1.277784     -1.066731     -0.841867
58620      O      1.368593     -1.823801      0.355131
58621      H      2.122676     -1.400087      0.796366
58622      H      0.449908      1.927185      0.469827
58623      H      1.065616      0.572727      1.421263
58624      Rotational constants (GHz):      1.3539300      0.6589100      0.5505000
58625      Vibrational harmonic frequencies (cm-1):
58626      i328.0514      33.2492      61.5572
58627      83.6519      98.2919      133.5645
58628      162.4681      169.3032      183.4327
58629      191.8663      198.5093      214.8153
58630      259.8958      269.3567      303.6388
58631      319.7990      368.2296      401.6785
58632      409.5287      503.7955      506.6136
58633      547.0487      610.4488      721.1289
58634      829.2986      886.2270      950.0541
58635      997.3958      1004.1361     1032.7403
58636      1056.4756     1107.1208     1111.9416
58637      1135.1789     1223.9298     1283.9176
58638      1311.1193     1334.1805     1377.0741
58639      1405.3372     1407.9418     1418.3886
58640      1432.0936     1444.4033     1472.8874
58641      1479.4131     1491.0264     2070.8284
58642      3059.6799     3067.0478     3098.9109
58643      3140.7956     3149.7135     3173.4574
58644      3729.9664     3794.7188     3819.7234
58645      Zero-point correction (Hartree): 0.152749
58646
58647      TS.triHPacyl.COelim.tmtpmmmrmd
58648      -----
58649      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16273946
58650      Electronic state : 2-A
58651      Cartesian coordinates (Angs):
58652      O      -2.630958      0.773223      -1.092253
58653      O      -1.263726      0.426599      -0.977320

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58654	C	-0.903399	0.270576	0.332886			
58655	C	0.561377	-0.041464	0.465107			
58656	C	1.135060	-0.839122	-0.707605			
58657	O	2.537952	-0.696312	-0.776531			
58658	O	3.094048	-1.187587	0.433888			
58659	H	-3.035045	-0.095201	-1.237037			
58660	C	-1.506624	1.170876	1.357616			
58661	H	-2.591145	1.109154	1.360868			
58662	H	-1.215028	2.203778	1.151432			
58663	H	-1.124584	0.893074	2.338180			
58664	C	-1.742825	-1.597973	0.816938			
58665	O	-2.565065	-1.883168	0.073524			
58666	H	3.167170	-0.375269	0.956026			
58667	H	0.680887	-0.607580	1.391652			
58668	O	1.351022	1.115492	0.726489			
58669	O	1.361592	1.932658	-0.433895			
58670	H	2.137917	1.592284	-0.903312			
58671	H	0.853612	-1.890567	-0.615380			
58672	H	0.785755	-0.454280	-1.663310			
58673	Rotational constants (GHz):				1.3847000	0.6316200	0.5409600
58674	Vibrational harmonic frequencies (cm-1):						
58675		i285.6055		39.3585		52.2131	
58676		74.9555		118.9221		134.1085	
58677		143.4549		156.2879		165.2104	
58678		198.9763		217.3136		235.9140	
58679		268.9598		310.5630		332.1784	
58680		342.7049		372.1416		399.1678	
58681		422.2970		449.1096		486.3838	
58682		499.5757		682.5698		716.3937	
58683		814.4842		899.4439		959.9247	
58684		993.3621		1008.0766		1045.3256	
58685		1055.4342		1086.6539		1115.4083	
58686		1160.5370		1239.1306		1294.6828	
58687		1301.5211		1353.6161		1383.4584	
58688		1406.8737		1414.0015		1424.8418	
58689		1430.8045		1432.6203		1470.2705	
58690		1490.0901		1490.6298		2046.3780	
58691		3059.2220		3074.6212		3092.0834	
58692		3137.3048		3154.9517		3173.4647	
58693		3766.5738		3771.7995		3772.6755	
58694	Zero-point correction (Hartree):				0.152954		
58695							
58696	TS.triHPacyl.COelim.tmtpmtpmd						
58697	-----						
58698	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16329283						
58699	Electronic state : 2-A						
58700	Cartesian coordinates (Angs):						
58701	O	2.847766	0.507427	1.123643			
58702	O	1.455424	0.262972	1.076484			
58703	C	0.969729	0.420306	-0.193840			
58704	C	-0.519779	0.231304	-0.203694			
58705	C	-0.989412	-0.865188	0.742786			
58706	O	-2.399440	-0.956294	0.789016			
58707	O	-2.857939	-1.376313	-0.487004			
58708	H	3.201400	-0.390348	1.036193			
58709	C	1.550202	1.487237	-1.060739			
58710	H	2.615434	1.341058	-1.217954			
58711	H	1.397157	2.464811	-0.598570			
58712	H	1.038483	1.473072	-2.021012			
58713	C	1.618392	-1.327895	-1.165736			
58714	O	2.482378	-1.813167	-0.593995			
58715	H	-3.023615	-0.528142	-0.927012			
58716	H	-0.801854	-0.004428	-1.232592			
58717	O	-1.095452	1.493138	0.138677			
58718	O	-2.433537	1.524848	-0.349054			
58719	H	-2.930806	1.283691	0.445527			
58720	H	-0.559106	-1.827288	0.453471			
58721	H	-0.705486	-0.627899	1.767148			
58722	Rotational constants (GHz):				1.3976100	0.6049500	0.5176400
58723	Vibrational harmonic frequencies (cm-1):						
58724		i292.1256		50.6064		54.2328	
58725		98.2837		130.4221		144.4518	

58726	151.4161	161.9601	169.4119
58727	214.6751	219.2280	232.8119
58728	270.4988	307.7477	329.1802
58729	348.7485	365.6067	397.2106
58730	432.2555	480.4244	490.8496
58731	519.0157	567.6325	698.5199
58732	868.1097	889.8531	961.3548
58733	1001.0414	1018.9764	1052.5710
58734	1060.7517	1093.7398	1113.9295
58735	1154.1351	1236.2141	1298.0193
58736	1305.8164	1357.8114	1370.6012
58737	1410.7727	1417.0382	1431.1395
58738	1439.0363	1441.4056	1469.8068
58739	1470.6546	1490.6359	2050.5633
58740	3064.3634	3066.5409	3082.3059
58741	3140.0763	3145.1638	3170.9253
58742	3744.9175	3776.1773	3785.8735

58743 Zero-point correction (Hartree): 0.153128

58744
58745 TS.triHPacyl.COelim.tmtpmmtppd

58746 -----
58747 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16174598

58748 Electronic state : 2-A

58749 Cartesian coordinates (Angs):

58750	O	2.867498	0.428437	1.113740
58751	O	1.467950	0.224206	1.078375
58752	C	0.968952	0.426239	-0.180677
58753	C	-0.524592	0.280719	-0.172711
58754	C	-1.011381	-0.805552	0.774237
58755	O	-2.426338	-0.887444	0.772193
58756	O	-2.827160	-1.364132	-0.509910
58757	H	3.194584	-0.474611	0.987772
58758	C	1.566689	1.493173	-1.033540
58759	H	2.624945	1.321905	-1.211690
58760	H	1.446759	2.464013	-0.547675
58761	H	1.037772	1.514761	-1.984290
58762	C	1.560170	-1.340573	-1.198550
58763	O	2.408881	-1.859666	-0.633323
58764	H	-3.186471	-2.231380	-0.285841
58765	H	-0.843468	0.064057	-1.193914
58766	O	-1.081693	1.536906	0.209887
58767	O	-2.331241	1.696503	-0.445416
58768	H	-2.914928	1.138014	0.089151
58769	H	-0.575210	-1.776721	0.527118
58770	H	-0.766187	-0.542555	1.802451

58771 Rotational constants (GHz): 1.3420700 0.6125900 0.5168000

58772 Vibrational harmonic frequencies (cm-1):

58773	i278.6311	44.8552	52.2939
58774	79.6211	115.3771	132.6247
58775	142.4622	148.0786	164.8803
58776	190.9606	209.3608	233.4321
58777	240.0047	274.7098	305.4754
58778	326.2072	347.4791	373.6471
58779	402.1226	453.2500	489.8343
58780	500.4345	556.1716	698.0439
58781	865.4145	889.7568	957.2994
58782	1002.5236	1022.9081	1053.3391
58783	1063.7954	1085.9611	1109.3213
58784	1148.5841	1231.5607	1295.4221
58785	1305.0761	1350.8744	1363.7206
58786	1398.1419	1411.4277	1429.8454
58787	1437.4026	1438.7372	1467.1191
58788	1470.9239	1488.8620	2048.3918
58789	3063.6059	3065.6397	3096.5537
58790	3139.2297	3144.8735	3170.5768
58791	3771.7276	3778.2089	3826.3402

58792 Zero-point correction (Hartree): 0.152351

58793
58794 TS.triHPacyl.COelim.tmtptmmd

58795 -----
58796 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16274899

58797 Electronic state : 2-A

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58798 Cartesian coordinates (Angs):
58799 O 2.694007 -0.972268 -1.146673
58800 O 1.297088 -0.812233 -0.988559
58801 C 1.021571 -0.186960 0.194875
58802 C -0.442686 0.138235 0.324614
58803 C -1.146899 0.375861 -1.013087
58804 O -2.541221 0.198461 -0.885831
58805 O -3.023373 1.138656 0.062604
58806 H 2.961867 -0.068278 -1.379877
58807 C 1.728351 -0.645910 1.427506
58808 H 2.807353 -0.605445 1.308487
58809 H 1.436591 -1.676627 1.644374
58810 H 1.429176 -0.020951 2.267497
58811 C 1.877703 1.677486 -0.122270
58812 O 1.473862 2.503332 0.555732
58813 H -3.024667 0.610709 0.874312
58814 H -0.524338 1.030665 0.951275
58815 O -1.146944 -0.822294 1.105672
58816 O -1.194036 -2.044627 0.386238
58817 H -2.022041 -1.947373 -0.107616
58818 H -0.912518 1.375647 -1.385733
58819 H -0.854736 -0.362821 -1.756023
58820 Rotational constants (GHz): 1.2339400 0.6746800 0.5661200
58821 Vibrational harmonic frequencies (cm-1):
58822 i296.1993 44.2370 60.6353
58823 74.5388 114.9106 129.1233
58824 136.9033 148.9704 179.6274
58825 200.7376 220.1049 238.5820
58826 306.3342 322.0440 337.0469
58827 365.8883 383.0176 404.7033
58828 420.8111 449.3288 480.5177
58829 498.4692 676.0092 713.5414
58830 813.6435 902.3347 960.0645
58831 994.0305 1006.6143 1038.6501
58832 1055.2162 1086.1759 1116.2780
58833 1159.9926 1235.9352 1297.5242
58834 1301.3096 1352.7354 1392.1781
58835 1405.4584 1412.4910 1425.6085
58836 1428.0829 1439.2961 1470.6724
58837 1490.5002 1490.5796 2068.6754
58838 3058.1818 3074.3937 3079.5554
58839 3134.2354 3157.4535 3173.4951
58840 3731.5034 3763.3600 3776.7452
58841 Zero-point correction (Hartree): 0.153091
58842
58843 TS.triHPacyl.COelim.tmtpttprm
58844 -----
58845 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16313037
58846 Electronic state : 2-A
58847 Cartesian coordinates (Angs):
58848 O -2.949661 -0.552360 1.193301
58849 O -1.537247 -0.594110 1.131331
58850 C -1.108514 -0.300286 -0.133445
58851 C 0.390716 -0.203860 -0.169609
58852 C 0.978333 0.408810 1.094439
58853 O 2.391627 0.407330 1.073412
58854 O 2.819509 1.271971 0.032073
58855 H -3.107740 0.404264 1.240200
58856 C -1.798082 -0.944049 -1.291808
58857 H -2.859995 -0.713818 -1.300822
58858 H -1.675594 -2.027727 -1.233522
58859 H -1.342466 -0.594989 -2.216893
58860 C -1.701662 1.675094 -0.343906
58861 O -1.201364 2.231282 -1.205729
58862 H 2.911668 0.656657 -0.711731
58863 H 0.654838 0.394919 -1.045797
58864 O 0.882880 -1.528200 -0.380717
58865 O 2.192585 -1.437582 -0.933630
58866 H 2.740284 -1.547340 -0.143179
58867 H 0.603517 1.425863 1.235716
58868 H 0.724102 -0.198730 1.961672
58869 Rotational constants (GHz): 1.2584500 0.6288000 0.5631400

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58870 Vibrational harmonic frequencies (cm-1):
58871 i306.1396 45.2161 59.0024
58872 86.3770 119.9334 129.6624
58873 134.8327 157.9565 169.6450
58874 198.9305 216.5755 245.8398
58875 260.5728 306.5459 342.2929
58876 350.7696 380.0918 393.3051
58877 414.5916 475.2630 486.9380
58878 509.2444 567.9385 689.4355
58879 872.5264 889.0610 960.8687
58880 1000.6321 1017.6757 1045.6554
58881 1058.7138 1091.9705 1114.1164
58882 1152.7504 1234.3825 1300.9319
58883 1305.9428 1357.7562 1373.2349
58884 1408.6915 1415.2359 1435.2342
58885 1437.2871 1439.6363 1469.3019
58886 1470.7070 1490.1523 2075.3088
58887 3063.7489 3068.2840 3071.3894
58888 3137.5929 3146.3903 3170.6850
58889 3741.5087 3742.2608 3785.3193
58890 Zero-point correction (Hartree): 0.152833
58891
58892 TS.triHPacyl.COelim.tmtptmtpd
58893 -----
58894 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16175012
58895 Electronic state : 2-A
58896 Cartesian coordinates (Angs):
58897 O -2.970354 -0.343942 1.224098
58898 O -1.560334 -0.449693 1.176235
58899 C -1.113579 -0.301092 -0.107802
58900 C 0.387597 -0.273073 -0.141035
58901 C 0.994020 0.410470 1.074979
58902 O 2.409523 0.399308 1.010617
58903 O 2.795635 1.238693 -0.074677
58904 H -3.090253 0.615018 1.129884
58905 C -1.824058 -1.021140 -1.205523
58906 H -2.875395 -0.749570 -1.248375
58907 H -1.746266 -2.098469 -1.043147
58908 H -1.346049 -0.782249 -2.154102
58909 C -1.628040 1.685047 -0.496471
58910 O -1.059094 2.159162 -1.364713
58911 H 3.229075 1.964509 0.390980
58912 H 0.696962 0.236392 -1.056921
58913 O 0.846381 -1.621391 -0.215007
58914 O 2.055867 -1.648171 -0.958335
58915 H 2.702114 -1.334197 -0.308510
58916 H 0.626575 1.434112 1.184207
58917 H 0.766611 -0.158543 1.975355
58918 Rotational constants (GHz): 1.2202600 0.6359300 0.5647700
58919 Vibrational harmonic frequencies (cm-1):
58920 i290.5287 47.6162 57.9142
58921 73.2644 116.3620 117.2454
58922 128.8493 146.1312 167.7523
58923 186.1659 215.4774 220.6421
58924 256.8516 268.8030 314.5088
58925 344.8892 360.6655 386.4101
58926 408.7458 433.5304 485.7066
58927 495.7794 556.3922 690.3251
58928 869.4699 889.8801 957.1670
58929 1001.7068 1021.0787 1046.5067
58930 1062.5870 1084.9335 1110.8414
58931 1147.7532 1231.9715 1299.3261
58932 1306.0663 1351.4178 1369.7381
58933 1398.3194 1409.4960 1434.4280
58934 1435.7931 1438.4096 1465.5324
58935 1471.5620 1488.6196 2075.3563
58936 3063.2259 3066.3868 3086.7996
58937 3137.1056 3145.6832 3170.8951
58938 3736.1521 3769.8545 3825.8091
58939 Zero-point correction (Hartree): 0.152295
58940
58941 TS.triHPacyl.COelim.tmtppmmmmmd

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58942 -----
58943 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16042418
58944 Electronic state : 2-A
58945 Cartesian coordinates (Angs):
58946 O 2.534890 -0.953093 -1.211764
58947 O 1.135886 -0.847147 -0.967285
58948 C 0.933565 -0.161441 0.201444
58949 C -0.516246 0.210084 0.361923
58950 C -1.219738 0.559337 -0.952631
58951 O -2.617541 0.390416 -0.832494
58952 O -3.085098 1.272790 0.177194
58953 H 2.649896 -1.911711 -1.226315
58954 C 1.654674 -0.642185 1.418288
58955 H 2.731118 -0.617690 1.272313
58956 H 1.337566 -1.662833 1.647529
58957 H 1.401929 -0.007852 2.266027
58958 C 1.749426 1.679286 -0.177574
58959 O 2.651585 1.953028 0.466358
58960 H -3.076929 0.696447 0.955332
58961 H -0.559310 1.066042 1.040601
58962 O -1.254713 -0.768309 1.090109
58963 O -1.365886 -1.939001 0.294919
58964 H -2.177674 -1.756578 -0.202441
58965 H -0.970057 1.578895 -1.247673
58966 H -0.939608 -0.124680 -1.750357
58967 Rotational constants (GHz): 1.3611700 0.6178600 0.5427500
58968 Vibrational harmonic frequencies (cm-1):
58969 i337.8982 30.7792 48.5557
58970 67.5143 88.9359 130.0082
58971 137.2008 157.2092 179.8382
58972 184.2380 205.8419 220.6128
58973 241.7709 288.8866 320.7471
58974 341.9344 375.3418 418.2620
58975 429.7989 470.2594 481.5376
58976 490.1744 675.0069 717.2076
58977 813.6715 901.2189 957.3588
58978 991.4939 1009.3586 1023.9720
58979 1055.3412 1082.6679 1111.6040
58980 1153.6836 1228.0786 1288.9335
58981 1296.7431 1341.2834 1377.1878
58982 1402.7361 1404.6611 1418.2764
58983 1429.9502 1431.5172 1473.8243
58984 1489.4021 1491.3335 2069.3675
58985 3056.2713 3078.7363 3094.0981
58986 3136.8214 3162.3028 3172.6014
58987 3759.6443 3771.7975 3824.0444
58988 Zero-point correction (Hartree): 0.152641
58989
58990 TS.triHPacyl.COelim.tmtppmtpmd
58991 -----
58992 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16052552
58993 Electronic state : 2-A
58994 Cartesian coordinates (Angs):
58995 O -2.782695 -0.519200 1.314433
58996 O -1.368810 -0.608133 1.184393
58997 C -1.013693 -0.291573 -0.101738
58998 C 0.480054 -0.142405 -0.190034
58999 C 1.085950 0.552223 1.021610
59000 O 2.499717 0.584880 0.955527
59001 O 2.873132 1.411053 -0.137184
59002 H -3.004360 -1.418545 1.587229
59003 C -1.710792 -1.009653 -1.212216
59004 H -2.779983 -0.817007 -1.193288
59005 H -1.530211 -2.083578 -1.127026
59006 H -1.311751 -0.670873 -2.166464
59007 C -1.634977 1.652717 -0.323175
59008 O -2.372279 1.836065 -1.174365
59009 H 2.959809 0.764629 -0.854648
59010 H 0.698269 0.420255 -1.102137
59011 O 1.010177 -1.460368 -0.352120
59012 O 2.302899 -1.359841 -0.940518
59013 H 2.871134 -1.382217 -0.157045

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59014      H      0.682976      1.561194      1.119370
59015      H      0.877734      -0.017361      1.925981
59016      Rotational constants (GHz):      1.3314700      0.5839700      0.5370000
59017      Vibrational harmonic frequencies (cm-1):
59018      i335.5673      24.4458      54.6570
59019      83.1775      102.4347      132.5838
59020      145.4803      158.4661      170.2928
59021      181.5746      208.4245      216.6254
59022      260.0665      261.7578      312.0473
59023      344.0121      382.8862      407.6579
59024      434.5169      469.7125      481.9676
59025      520.3081      566.7054      688.4367
59026      870.6348      891.0380      959.2833
59027      998.6759      1020.6275      1036.3685
59028      1059.0072      1089.0575      1112.6259
59029      1149.2899      1224.9903      1289.2757
59030      1301.7672      1346.0969      1364.8264
59031      1404.8632      1415.3034      1419.4476
59032      1439.7350      1442.3615      1472.7824
59033      1474.0106      1487.9389      2074.6099
59034      3061.8772      3066.8719      3088.5834
59035      3139.8775      3153.2491      3172.1724
59036      3752.9036      3782.1159      3824.6532
59037      Zero-point correction (Hartree): 0.152626
59038
59039      TS.triHPacyl.COelim.tpmmmmpppd
59040      -----
59041      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16318951
59042      Electronic state : 2-A
59043      Cartesian coordinates (Angs):
59044      O      1.280178      -2.346920      0.243614
59045      O      0.460125      -1.412353      -0.434429
59046      C      0.412236      -0.206596      0.227585
59047      C      -0.560748      0.665484      -0.544998
59048      C      -1.940187      0.709184      0.113566
59049      O      -2.394404      -0.583918      0.447914
59050      O      -2.568903      -1.305696      -0.766364
59051      H      2.109358      -2.257896      -0.249303
59052      C      0.423420      -0.243083      1.721931
59053      H      1.349838      -0.668402      2.099704
59054      H      -0.407163      -0.856300      2.079934
59055      H      0.308913      0.767428      2.104577
59056      C      2.303062      0.627172      -0.188222
59057      O      2.972509      -0.146969      -0.697496
59058      H      -1.796550      -1.889316      -0.758551
59059      H      -0.659098      0.240995      -1.545454
59060      O      -0.088754      1.971624      -0.807975
59061      O      0.173748      2.625651      0.424540
59062      H      1.130983      2.487409      0.501198
59063      H      -1.893415      1.242890      1.062324
59064      H      -2.645551      1.208879      -0.552036
59065      Rotational constants (GHz):      1.1025300      0.8369700      0.5805700
59066      Vibrational harmonic frequencies (cm-1):
59067      i293.7092      57.2100      81.5665
59068      98.6106      138.7390      155.0577
59069      179.4137      187.2983      193.1161
59070      221.8937      238.8584      259.8007
59071      270.8414      316.8862      321.8370
59072      342.4304      365.1339      395.8979
59073      410.5002      476.9319      498.1492
59074      532.4044      605.0725      687.8727
59075      811.4403      938.0966      950.2272
59076      979.8256      1023.7495      1038.4941
59077      1055.8997      1109.4424      1128.8992
59078      1138.1527      1216.9096      1263.3925
59079      1310.0402      1336.1099      1380.6605
59080      1400.6575      1415.1955      1426.0776
59081      1429.0737      1439.5643      1478.9424
59082      1487.3482      1496.1889      2060.5785
59083      3063.4250      3082.2615      3103.5702
59084      3142.9911      3148.0795      3180.3679
59085      3742.3078      3775.0229      3777.9523

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59086 Zero-point correction (Hartree): 0.153472
59087
59088 TS.triHPacyl.COelim.tpmmmpmpd
59089 -----
59090 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16325236
59091 Electronic state : 2-A
59092 Cartesian coordinates (Angs):
59093 O 0.833886 -2.468748 -0.079765
59094 O 0.234331 -1.289455 -0.580203
59095 C 0.374040 -0.234117 0.287414
59096 C -0.528552 0.886552 -0.181958
59097 C -1.946925 0.745693 0.393364
59098 O -2.430554 -0.572628 0.343629
59099 O -2.603263 -0.912301 -1.026178
59100 H 1.712187 -2.425172 -0.487117
59101 C 0.472243 -0.508260 1.749637
59102 H 1.348429 -1.102141 1.996656
59103 H -0.414739 -1.053776 2.083748
59104 H 0.528177 0.446363 2.270712
59105 C 2.382731 0.346874 -0.123076
59106 O 2.975191 -0.576430 -0.446195
59107 H -1.824671 -1.466387 -1.183166
59108 H -0.562388 0.902996 -1.271359
59109 O -0.089970 2.141275 0.297875
59110 O 0.780242 2.735574 -0.648957
59111 H 1.642549 2.393339 -0.368311
59112 H -1.932809 0.997508 1.454891
59113 H -2.616839 1.428524 -0.129995
59114 Rotational constants (GHz): 1.0590700 0.8355200 0.5662300
59115 Vibrational harmonic frequencies (cm-1):
59116 i276.8210 48.5032 80.0568
59117 89.7125 133.4236 144.8841
59118 163.4646 190.6937 201.4680
59119 226.7832 234.6538 260.9362
59120 271.9390 293.4275 332.8835
59121 352.5969 368.4609 421.9834
59122 426.0286 447.7993 478.4970
59123 507.6755 596.0217 662.7490
59124 808.9981 930.1820 960.6397
59125 1014.2356 1015.0626 1048.7946
59126 1055.1265 1100.0102 1133.0149
59127 1171.5992 1229.7359 1271.2270
59128 1307.6436 1327.1335 1380.1543
59129 1398.8878 1414.2493 1433.5686
59130 1437.5244 1444.4971 1473.9244
59131 1484.8817 1494.2806 2053.1028
59132 3051.7519 3079.7114 3108.2685
59133 3132.8257 3137.3294 3165.7794
59134 3736.5422 3771.3242 3773.6577
59135 Zero-point correction (Hartree): 0.153276
59136
59137 TS.triHPacyl.COelim.tpmmmtmpd
59138 -----
59139 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16225258
59140 Electronic state : 2-A
59141 Cartesian coordinates (Angs):
59142 O -0.151665 2.808892 -0.007806
59143 O 0.365474 1.582578 -0.490372
59144 C -0.252114 0.512831 0.118103
59145 C 0.285287 -0.734766 -0.555766
59146 C 1.454296 -1.349872 0.217720
59147 O 2.397937 -0.373322 0.594809
59148 O 2.965111 0.161832 -0.595563
59149 H -0.914079 2.929692 -0.594460
59150 C -0.441526 0.586201 1.598847
59151 H -1.037030 1.451891 1.876878
59152 H 0.535736 0.672142 2.082450
59153 H -0.929831 -0.318756 1.950226
59154 C -2.237730 0.745270 -0.586072
59155 O -2.998758 0.015033 -0.147661
59156 H 2.522962 1.021778 -0.649021
59157 H 0.629287 -0.444320 -1.549530

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59158      O      -0.691689      -1.715289      -0.848561
59159      O      -1.207745      -2.238707      0.370419
59160      H      -2.111076      -1.892665      0.353130
59161      H      1.105527      -1.775753      1.157734
59162      H      1.919906      -2.130132      -0.386522
59163      Rotational constants (GHz):      1.1300700      0.8369700      0.5735000
59164      Vibrational harmonic frequencies (cm-1):
59165      i292.9777      67.5019      95.9636
59166      102.5201      117.8867      148.1462
59167      149.4371      165.9759      181.5617
59168      212.3462      216.9544      233.3205
59169      287.1682      307.0976      327.1198
59170      354.2495      362.2873      383.4497
59171      397.3294      428.5841      485.3053
59172      531.1975      600.7197      679.0736
59173      802.6032      937.9065      950.2341
59174      977.4999      1020.9894      1035.4637
59175      1052.7060      1109.8913      1126.6157
59176      1140.6330      1217.7242      1263.9061
59177      1307.6178      1332.9298      1381.1150
59178      1396.9929      1413.2077      1423.5849
59179      1433.1797      1436.7540      1474.8897
59180      1486.0137      1496.5710      2064.8607
59181      3055.7473      3079.3570      3108.0716
59182      3142.2069      3148.4234      3181.8283
59183      3761.4753      3775.7075      3789.5507
59184      Zero-point correction (Hartree): 0.153005
59185
59186      TS.triHPacyl.COelim.tpmmtmpmpd
59187      -----
59188      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16132318
59189      Electronic state : 2-A
59190      Cartesian coordinates (Angs):
59191      O      0.064100      2.716862      -0.396307
59192      O      0.443380      1.379674      -0.659453
59193      C      -0.205360      0.509414      0.181954
59194      C      0.212530      -0.895081      -0.198071
59195      C      1.509035      -1.315790      0.514650
59196      O      2.483325      -0.304580      0.524861
59197      O      2.897018      -0.096223      -0.819403
59198      H      -0.755284      2.779988      -0.912038
59199      C      -0.303119      0.859682      1.630509
59200      H      -0.840694      1.791315      1.786019
59201      H      0.701844      0.968928      2.047912
59202      H      -0.824325      0.055917      2.149128
59203      C      -2.197671      0.851158      -0.405858
59204      O      -2.996120      0.281194      0.179888
59205      H      2.427617      0.723190      -1.035792
59206      H      0.340903      -0.956463      -1.278313
59207      O      -0.724784      -1.868254      0.220653
59208      O      -1.648904      -2.094489      -0.835167
59209      H      -2.476583      -1.798248      -0.435219
59210      H      1.297167      -1.509065      1.567400
59211      H      1.892740      -2.225341      0.051231
59212      Rotational constants (GHz):      1.1341100      0.7993000      0.5669300
59213      Vibrational harmonic frequencies (cm-1):
59214      i291.6596      49.6827      71.2731
59215      91.4622      124.6903      143.0359
59216      158.3179      172.8774      184.6153
59217      214.9741      223.3320      234.8408
59218      273.2517      294.5722      324.6415
59219      354.4017      362.8921      366.0589
59220      429.1289      452.2711      470.3389
59221      506.6602      592.6437      658.4042
59222      805.5851      929.6182      961.3853
59223      1008.7013      1014.4231      1042.3404
59224      1054.4068      1101.8020      1132.4494
59225      1164.1986      1227.5589      1266.9700
59226      1302.2099      1325.7559      1379.0315
59227      1395.9626      1414.2090      1420.9589
59228      1427.9443      1438.3907      1471.9604
59229      1483.1109      1496.3733      2062.3561

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59230          3051.5396          3078.1522          3113.7829
59231          3131.7545          3136.6157          3166.4322
59232          3749.7923          3768.8147          3817.9621
59233 Zero-point correction (Hartree): 0.152858
59234
59235 TS.triHPacyl.COelim.tpppmtpmd
59236 -----
59237 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16068598
59238 Electronic state : 2-A
59239 Cartesian coordinates (Angs):
59240 O      2.643162      -1.492834      -0.179081
59241 O      1.481994      -0.921914      -0.753092
59242 C      0.790532      -0.178796      0.169206
59243 C     -0.398299      0.407750     -0.554962
59244 C     -1.352206     -0.659110     -1.099061
59245 O     -1.954203     -1.440232     -0.086925
59246 O     -2.981268     -0.665539      0.525796
59247 H      3.314456     -0.841503     -0.431246
59248 C      0.653472     -0.703105      1.559027
59249 H      1.629355     -0.884014      2.001902
59250 H      0.091948     -1.641380      1.556268
59251 H      0.125171      0.033975      2.159751
59252 C      2.040195      1.510822      0.421949
59253 O      3.004839      1.388401     -0.180560
59254 H     -2.544280     -0.368976      1.336497
59255 H     -0.040926      1.001655     -1.403935
59256 O     -1.033202      1.259352      0.384075
59257 O     -2.067397      1.954324     -0.287720
59258 H     -2.821362      1.357494     -0.154262
59259 H     -2.122830     -0.204443     -1.722919
59260 H     -0.785102     -1.370642     -1.698964
59261 Rotational constants (GHz): 1.4608300      0.6404800      0.5282300
59262 Vibrational harmonic frequencies (cm-1):
59263 1299.9552          23.5980          40.5837
59264 73.8904           133.3599          146.2754
59265 159.9478          178.9751          206.9733
59266 211.2510          224.6683          232.4923
59267 262.8996          289.3250          331.6677
59268 359.1982          379.2957          409.3818
59269 419.8077          459.9507          500.4900
59270 547.9315          622.1278          759.0035
59271 816.2217          879.5818          948.7486
59272 972.3093          1026.0997         1037.9704
59273 1060.1273         1080.5915         1114.7206
59274 1168.5666         1237.6256         1289.0178
59275 1322.0013         1342.7241         1377.9657
59276 1400.0068         1406.6082         1413.9869
59277 1430.2191         1454.0585         1476.9763
59278 1480.8687         1489.0112         2050.5348
59279 3042.0941         3052.6104         3084.6175
59280 3138.8443         3142.1698         3171.2348
59281 3738.7985         3774.2988         3787.9946
59282 Zero-point correction (Hartree): 0.153053
59283
59284 TS.triHPacyl.COelim.tpppmttpmd
59285 -----
59286 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16113197
59287 Electronic state : 2-A
59288 Cartesian coordinates (Angs):
59289 O      2.754408      -1.546292      -0.224151
59290 O      1.455672      -1.266913      -0.717836
59291 C      0.867853      -0.276354      0.026655
59292 C     -0.372793      0.150699     -0.718563
59293 C     -1.403422     -0.970711     -0.866977
59294 O     -1.925423     -1.422506      0.366068
59295 O     -2.860299     -0.456230      0.838126
59296 H      3.286342     -0.926497     -0.745149
59297 C      0.857973     -0.417872      1.512990
59298 H      1.864989     -0.585477      1.886159
59299 H      0.229200     -1.264274      1.802702
59300 H      0.463525      0.493083      1.959053
59301 C      2.157866      1.336800     -0.285157

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59302      O      2.148966      2.140889      0.521611
59303      H      -2.335427      0.015907      1.499818
59304      H      -0.081694      0.474839     -1.723683
59305      O      -0.885644      1.257132      0.007285
59306      O      -1.965190      1.801186     -0.728956
59307      H      -2.716554      1.303032     -0.368634
59308      H      -2.218605     -0.659219     -1.521599
59309      H      -0.916559     -1.844894     -1.299527
59310      Rotational constants (GHz):      1.2810400      0.6963700      0.5487300
59311      Vibrational harmonic frequencies (cm-1):
59312      i310.0748      26.0990      45.3821
59313      68.5277      114.5574      136.3949
59314      156.2286      170.5456      195.8394
59315      201.3746      222.7987      226.8163
59316      275.7366      288.6427      317.1053
59317      336.7555      377.1841      393.9321
59318      410.3130      466.6471      495.6818
59319      550.6690      619.7122      754.7805
59320      814.8673      879.1427      951.2141
59321      972.3968      1018.4588     1036.3306
59322      1055.7493     1079.7328     1114.0689
59323      1166.4001     1235.9834     1289.6183
59324      1317.5672     1346.8102     1379.4987
59325      1399.1851     1405.4173     1412.6336
59326      1419.5758     1456.6881     1477.9458
59327      1480.0764     1489.1226     2090.1975
59328      3047.7418     3051.3906     3082.0600
59329      3136.8703     3139.1974     3172.0525
59330      3730.2330     3772.7453     3788.3156
59331      Zero-point correction (Hartree): 0.152776
59332
59333      TS.triHPacyl.COelim.tpppmttppd
59334      -----
59335      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15950336
59336      Electronic state : 2-A
59337      Cartesian coordinates (Angs):
59338      O      2.752311      -1.584673      -0.233890
59339      O      1.461430      -1.275219      -0.730365
59340      C      0.884212      -0.287585      0.028609
59341      C      -0.350102      0.164239      -0.712443
59342      C      -1.405574      -0.936581      -0.839903
59343      O      -1.948437      -1.340179      0.402668
59344      O      -2.929021      -0.380489      0.791243
59345      H      3.295265      -0.952158      -0.727526
59346      C      0.871328      -0.446913      1.512020
59347      H      1.881801      -0.570850      1.893159
59348      H      0.277964      -1.322881      1.785942
59349      H      0.419587      0.434002      1.961938
59350      C      2.197840      1.312483      -0.267350
59351      O      2.221627      2.096580      0.558486
59352      H      -3.722657      -0.928606      0.819492
59353      H      -0.056284      0.454384      -1.728117
59354      O      -0.817322      1.294000      -0.004350
59355      O      -1.926607      1.825521      -0.704844
59356      H      -2.657085      1.423739      -0.210103
59357      H      -2.206502      -0.623711      -1.510347
59358      H      -0.930146      -1.832101      -1.241616
59359      Rotational constants (GHz):      1.2988000      0.6810100      0.5387600
59360      Vibrational harmonic frequencies (cm-1):
59361      i307.9856      19.2920      46.7953
59362      63.4192      109.2629      131.1323
59363      150.3801      171.2323      182.2924
59364      192.8717      212.0862      223.6536
59365      266.2968      280.6928      298.7774
59366      314.3849      335.1537      388.9432
59367      396.2148      466.6241      482.1327
59368      505.8391      619.2637      750.5138
59369      810.9228      876.7142      949.1721
59370      977.3678      1019.9322     1035.1474
59371      1056.7522     1082.1041     1111.1568
59372      1174.4979     1232.3504     1293.0184
59373      1321.0679     1348.8012     1381.4642

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59374      1392.7479          1408.5992          1416.1439
59375      1419.7247          1452.7112          1470.4096
59376      1476.0693          1484.5437          2090.2912
59377      3038.1531          3057.9625          3082.4530
59378      3137.2260          3141.0006          3176.2323
59379      3754.9041          3771.7548          3826.8956
59380      Zero-point correction (Hartree): 0.152354
59381
59382      TS.triHPacyl.COelim.tptmmmmmpd
59383      -----
59384      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16037006
59385      Electronic state : 2-A
59386      Cartesian coordinates (Angs):
59387      O      -2.717365          1.256978          0.830092
59388      O      -1.433512          1.212939          0.236442
59389      C      -0.902833          -0.054657          0.263771
59390      C      0.455764          0.026741          -0.403748
59391      C      1.347828          1.111285          0.200245
59392      O      2.533679          1.307298          -0.544043
59393      O      3.434358          0.238365          -0.265976
59394      H      -3.287228          1.105170          0.061231
59395      C      -1.142328          -0.914865          1.456636
59396      H      -2.204833          -0.965982          1.678989
59397      H      -0.622078          -0.519631          2.333964
59398      H      -0.761791          -1.911677          1.253676
59399      C      -2.036259          -1.048418          -1.225096
59400      O      -2.990468          -0.461724          -1.461101
59401      H      3.371607          -0.283787          -1.077403
59402      H      0.311885          0.273114          -1.460399
59403      O      1.091281          -1.237535          -0.461899
59404      O      1.578890          -1.590117          0.825743
59405      H      2.468092          -1.201027          0.801604
59406      H      0.831014          2.067530          0.138626
59407      H      1.585410          0.906137          1.244801
59408      Rotational constants (GHz):      1.5567900      0.5557100      0.5166400
59409      Vibrational harmonic frequencies (cm-1):
59410      i293.3690          31.6492          38.7100
59411      92.5642          122.9143          158.7948
59412      169.8667          184.5900          195.0638
59413      216.9976          222.1924          263.0756
59414      271.5700          308.1898          341.4884
59415      361.0882          375.0461          379.0007
59416      412.9538          480.7340          500.7002
59417      576.3607          628.9428          692.8574
59418      832.4910          895.4232          947.8299
59419      989.2522          997.6793          1040.7648
59420      1047.7250          1112.2655          1117.8722
59421      1148.1933          1239.3968          1284.9469
59422      1313.7518          1326.6061          1381.2947
59423      1398.6529          1411.2005          1413.8833
59424      1433.9286          1453.9474          1475.9894
59425      1478.6236          1487.3109          2043.2541
59426      3048.2909          3059.5443          3092.3738
59427      3142.7927          3154.1752          3186.3814
59428      3724.7390          3770.2043          3799.7458
59429      Zero-point correction (Hartree): 0.153266
59430
59431      TS.triHPacyl.COelim.tptmmtmmpd
59432      -----
59433      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16089342
59434      Electronic state : 2-A
59435      Cartesian coordinates (Angs):
59436      O      2.780523          -1.658958          0.190298
59437      O      1.410479          -1.482850          -0.119203
59438      C      0.997084          -0.214035          0.205900
59439      C      -0.381071          -0.029928          -0.397818
59440      C      -1.337466          -1.167604          -0.037146
59441      O      -2.555899          -1.089859          -0.749013
59442      O      -3.361402          -0.065850          -0.170976
59443      H      3.198490          -1.179257          -0.543111
59444      C      1.340601          0.327143          1.553316
59445      H      2.402772          0.201504          1.746640

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59446	H	0.778025	-0.196042	2.331516	
59447	H	1.078913	1.381215	1.597987	
59448	C	2.203505	0.930858	-1.040157	
59449	O	1.965909	2.045273	-1.070752	
59450	H	-3.294831	0.631917	-0.836979	
59451	H	-0.286085	-0.020011	-1.488607	
59452	O	-0.917752	1.250119	-0.115572	
59453	O	-1.338443	1.306021	1.240673	
59454	H	-2.255069	0.994115	1.164301	
59455	H	-0.898272	-2.111428	-0.355941	
59456	H	-1.527173	-1.211775	1.035972	
59457	Rotational constants (GHz):		1.3609100	0.6228500	0.5298900
59458	Vibrational harmonic frequencies (cm-1):				
59459	i309.1965		7.3678		52.5030
59460	87.1596		117.3070		144.0029
59461	159.4313		193.9037		198.3325
59462	221.4257		227.0981		254.5159
59463	284.6143		324.4467		330.6412
59464	338.6748		377.4100		380.4296
59465	406.3796		481.5426		502.0201
59466	575.3429		629.1744		687.6852
59467	830.8802		895.3471		948.5852
59468	990.7180		998.8682		1037.1270
59469	1042.9688		1112.0715		1117.3483
59470	1147.0923		1242.9088		1285.8100
59471	1306.9112		1323.8624		1380.0458
59472	1396.8410		1410.0158		1411.3382
59473	1436.6261		1456.6549		1474.3250
59474	1477.2468		1485.8694		2083.4444
59475	3050.4552		3057.0794		3091.6251
59476	3139.3941		3153.3344		3180.3190
59477	3722.8090		3736.6409		3799.3046
59478	Zero-point correction (Hartree):		0.153105		
59479	TS.triHPacyl.COelim.tptpmttmd				
59480	-----				
59481	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16021833				
59482	Electronic state : 2-A				
59483	Cartesian coordinates (Angs):				
59484	O	2.703605	-1.691389	-0.436420	
59485	O	1.303677	-1.463890	-0.479971	
59486	C	0.997458	-0.307708	0.190127	
59487	C	-0.450655	0.000107	-0.094260	
59488	C	-1.375919	-1.044751	0.528289	
59489	O	-2.740047	-0.687365	0.425361	
59490	O	-3.096790	-0.715765	-0.947971	
59491	H	2.975772	-1.320066	-1.287931	
59492	C	1.542989	-0.122577	1.567844	
59493	H	2.627746	-0.188528	1.561786	
59494	H	1.157782	-0.896273	2.238983	
59495	H	1.247253	0.854420	1.943887	
59496	C	1.998173	1.153890	-0.924799	
59497	O	2.397399	2.039208	-0.330005	
59498	H	-2.916163	0.197448	-1.220002	
59499	H	-0.588161	0.036621	-1.177398	
59500	O	-0.689777	1.291032	0.449149	
59501	O	-1.858437	1.821649	-0.160313	
59502	H	-2.530902	1.617099	0.505363	
59503	H	-1.201372	-2.019692	0.069676	
59504	H	-1.201262	-1.102639	1.603779	
59505	Rotational constants (GHz):		1.3466500	0.6202800	0.5019500
59506	Vibrational harmonic frequencies (cm-1):				
59507	i307.6225		23.8374		47.4637
59508	89.7747		99.6856		116.6160
59509	147.5725		163.3061		180.8630
59510	197.0950		217.6509		225.6822
59511	269.4241		273.1843		295.8938
59512	356.6797		376.1478		404.0582
59513	414.8559		457.8608		490.8374
59514	522.2454		557.7280		683.3087
59515	866.1471		896.0762		957.2677
59516	1000.4457		1015.6446		1043.9012

```

59518      1048.9789      1100.2238      1137.3989
59519      1143.2919      1237.1214      1298.7583
59520      1313.4399      1339.2660      1379.9181
59521      1407.6284      1412.4742      1413.4956
59522      1426.5294      1443.1277      1468.9801
59523      1475.5542      1490.2557      2091.6057
59524      3044.5063      3074.6011      3082.6744
59525      3134.5085      3137.7271      3176.6684
59526      3751.2009      3783.5131      3786.3420
59527      Zero-point correction (Hartree): 0.152617
59528
59529      TS.triHPacyl.COelim.ttpmmtpm
59530      -----
59531      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16335179
59532      Electronic state : 2-A
59533      Cartesian coordinates (Angs):
59534      O      -3.082136      -0.380910      -0.405780
59535      O      -1.768913      -0.827548      -0.681685
59536      C      -0.848321      0.174362      -0.517739
59537      C      0.497179      -0.388905      -0.906805
59538      C      1.585949      0.664758      -1.053480
59539      O      1.769393      1.490047      0.075070
59540      O      2.322686      0.695635      1.116148
59541      H      -3.191598      -0.671597      0.511552
59542      C      -1.230983      1.560131      -0.924282
59543      H      -2.199099      1.824491      -0.509961
59544      H      -1.299838      1.631888      -2.014832
59545      H      -0.484409      2.264392      -0.566087
59546      C      -0.719379      0.345496      1.585952
59547      O      -1.686835      -0.020028      2.073100
59548      H      1.522684      0.490092      1.629465
59549      H      0.403138      -0.895777      -1.877297
59550      O      0.785518      -1.371980      0.084806
59551      O      2.045039      -1.950089      -0.192501
59552      H      2.626863      -1.395112      0.351097
59553      H      2.525999      0.183982      -1.324080
59554      H      1.311572      1.351574      -1.854987
59555      Rotational constants (GHz):      1.3139200      0.6808900      0.6601000
59556      Vibrational harmonic frequencies (cm-1):
59557      i313.1538      51.6230      99.0816
59558      118.2952      130.0273      153.6453
59559      165.3275      174.6285      204.1838
59560      237.2867      238.7281      254.7306
59561      281.3998      324.5428      330.4773
59562      364.1371      379.0797      408.5347
59563      477.5716      478.8598      504.8185
59564      550.9224      612.5180      739.3691
59565      845.8721      874.9555      950.8875
59566      978.8516      1018.3767      1046.9678
59567      1049.7968      1088.6214      1123.9524
59568      1168.8525      1230.7544      1289.0832
59569      1302.1282      1357.3961      1382.5006
59570      1406.7222      1410.4937      1433.9860
59571      1439.2735      1450.3503      1477.1496
59572      1493.3921      1496.8816      2058.0930
59573      3011.3882      3037.6584      3091.3553
59574      3135.9136      3143.1138      3184.8415
59575      3690.1394      3735.0366      3780.2743
59576      Zero-point correction (Hartree): 0.153696
59577
59578      TS.triHPacyl.COelim.ttpmmtpm
59579      -----
59580      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16261168
59581      Electronic state : 2-A
59582      Cartesian coordinates (Angs):
59583      O      -3.247507      0.379679      -0.217043
59584      O      -2.027580      1.000512      0.135197
59585      C      -1.061631      0.062941      0.399005
59586      C      0.233390      0.815704      0.606101
59587      C      1.292756      0.047754      1.381886
59588      O      1.694585      -1.162707      0.777495
59589      O      2.537801      -0.845845      -0.325151

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59590      H      -3.079832      0.152762      -1.145603
59591      C      -1.428130      -1.078891      1.293181
59592      H      -2.361652      -1.527664      0.966443
59593      H      -1.565179      -0.725500      2.320350
59594      H      -0.641503      -1.830415      1.279212
59595      C      -0.928342      -0.901082      -1.442173
59596      O      -0.019335      -1.570507      -1.620904
59597      H      1.953089      -1.054952      -1.069170
59598      H      0.011450      1.733407      1.167738
59599      O      0.668815      1.185021      -0.699232
59600      O      1.825176      1.990520      -0.575670
59601      H      2.525514      1.322656      -0.648402
59602      H      2.162280      0.682808      1.551099
59603      H      0.891934      -0.245035      2.352803
59604      Rotational constants (GHz):      1.3201700      0.7131700      0.6580100
59605      Vibrational harmonic frequencies (cm-1):
59606      i328.5681      77.6765      96.4360
59607      122.5099      137.8783      153.3169
59608      157.4500      182.8283      215.6965
59609      224.1427      230.2289      252.7515
59610      281.0711      326.9556      344.9792
59611      359.4080      371.9162      412.4339
59612      445.8099      467.1625      489.9271
59613      552.7886      611.8289      735.0300
59614      841.7830      876.2378      949.3504
59615      980.8662      1019.1475      1044.0105
59616      1049.0402      1080.4776      1122.1933
59617      1166.3167      1223.2660      1283.7128
59618      1302.8843      1353.5888      1385.8407
59619      1403.4930      1407.0586      1431.2466
59620      1439.1331      1447.2907      1475.8875
59621      1490.6644      1496.7180      2059.7451
59622      3012.4139      3039.8487      3091.3444
59623      3135.5113      3137.1004      3179.3286
59624      3740.6907      3744.2986      3770.0065
59625      Zero-point correction (Hartree): 0.153618
59626
59627
59628
59629      (2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)
59630      =====
59631
59632      triHPacyl.mmmmmmtmpu
59633      -----
59634      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17432340
59635      Electronic state : 2-A
59636      Cartesian coordinates (Angs):
59637      O      -2.264666      -1.032644      1.358050
59638      O      -1.848404      0.203983      0.778097
59639      C      -0.977098      -0.087491      -0.303745
59640      C      0.266246      -0.828987      0.206875
59641      C      0.957825      -0.091659      1.342664
59642      O      1.333805      1.229672      1.011888
59643      O      2.426751      1.166511      0.100293
59644      H      -3.215940      -1.002323      1.198286
59645      C      -1.677177      -0.833209      -1.432290
59646      H      -2.582529      -0.296535      -1.712480
59647      H      -1.931286      -1.836151      -1.095021
59648      H      -1.020724      -0.912536      -2.295153
59649      C      -0.593153      1.293099      -0.873705
59650      O      -1.235142      2.268879      -0.858771
59651      H      1.978088      1.316373      -0.746964
59652      H      -0.043642      -1.810866      0.575701
59653      O      1.078661      -0.991958      -0.945783
59654      O      2.262983      -1.671300      -0.575532
59655      H      2.848330      -0.924858      -0.367989
59656      H      0.251923      0.023701      2.164934
59657      H      1.824012      -0.652452      1.693953
59658      Rotational constants (GHz):      1.2087100      0.7811500      0.6849000
59659      Vibrational harmonic frequencies (cm-1):
59660      47.4079      102.3708      103.8136
59661      131.2776      152.8255      180.8859

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59662      185.6678      206.7562      221.8861
59663      236.9128      249.2872      294.4187
59664      313.6819      344.6525      375.8483
59665      403.9394      436.9919      474.6563
59666      503.2881      548.1020      559.5050
59667      629.3448      723.7792      765.6036
59668      872.1202      894.0890      953.6614
59669      977.5983      1016.8696     1046.9968
59670      1050.0549     1115.1485     1139.3198
59671      1157.2653     1195.6013     1245.1530
59672      1295.4668     1369.2444     1383.3419
59673      1392.7971     1399.6640     1409.6710
59674      1431.2797     1450.8679     1477.9984
59675      1490.2312     1497.8311     1991.4374
59676      3072.5579     3079.2719     3093.6935
59677      3145.9584     3160.1565     3172.9064
59678      3729.1503     3745.0101     3827.2952
59679      Zero-point correction (Hartree): 0.155992
59680
59681      triHPacyl.mmmmttmpu
59682      -----
59683      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17614486
59684      Electronic state : 2-A
59685      Cartesian coordinates (Angs):
59686      O      2.604342      -1.174820      -0.691282
59687      O      1.948285      0.064351      -0.931268
59688      C      1.065074      0.313045      0.158641
59689      C      0.002750      -0.799977      0.222266
59690      C     -0.738325     -0.975127     -1.093539
59691      O     -1.376591      0.201590     -1.545893
59692      O     -2.499869      0.452377     -0.708246
59693      H      3.524757     -0.892719     -0.627728
59694      C      1.802945      0.500680      1.475324
59695      H      2.563670      1.272518      1.365745
59696      H      2.275230     -0.437571      1.760142
59697      H      1.099728      0.791999      2.251197
59698      C      0.444566      1.666104     -0.224018
59699      O     -0.389506      2.254776      0.354648
59700      H     -2.172540      1.182265     -0.157006
59701      H      0.516031     -1.739570      0.450911
59702      O     -0.833961     -0.439789      1.308184
59703      O     -1.858397     -1.407553      1.431826
59704      H     -2.550711     -1.014240      0.875568
59705      H     -0.014084     -1.208837     -1.873532
59706      H     -1.458570     -1.789656     -1.021093
59707      Rotational constants (GHz):      1.2638700      0.7706100      0.7404500
59708      Vibrational harmonic frequencies (cm-1):
59709      60.3244      117.8786      131.1070
59710      153.4955      162.0485      186.3290
59711      205.7044      221.5460      226.7057
59712      239.4721      245.3035      287.7869
59713      326.8478      338.4230      366.0719
59714      412.6137      450.7162      467.1555
59715      481.8886      532.1610      564.0572
59716      616.6912      713.9756      777.2012
59717      869.7285      896.7102      952.3705
59718      976.9969      1038.3318     1044.4609
59719      1053.7518     1119.1185     1143.9266
59720      1163.9151     1203.4521     1226.3796
59721      1295.0105     1358.7470     1376.5332
59722      1398.0617     1405.3974     1406.4251
59723      1445.7908     1456.4187     1478.2459
59724      1488.8831     1498.1993     1973.0410
59725      3059.6426     3078.4214     3096.2964
59726      3147.7086     3156.9677     3175.7100
59727      3720.8712     3730.7955     3829.4313
59728      Zero-point correction (Hartree): 0.156171
59729
59730      triHPacyl.mpmmpmpu
59731      -----
59732      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17387377
59733      Electronic state : 2-A

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59734 Cartesian coordinates (Angs):
59735 O 0.237456 1.935165 -1.082096
59736 O -0.610594 0.815212 -1.256545
59737 C -1.094398 0.348997 0.000084
59738 C -0.107386 -0.597466 0.717209
59739 C 1.116615 0.026657 1.382057
59740 O 2.036636 0.664759 0.513066
59741 O 3.064807 -0.240706 0.156500
59742 H 1.074431 1.539965 -0.768363
59743 C -1.630191 1.466537 0.877279
59744 H -2.399604 2.014227 0.335881
59745 H -0.838365 2.162929 1.137663
59746 H -2.065192 1.042348 1.781070
59747 C -2.294320 -0.543249 -0.413352
59748 O -2.987231 -1.128736 0.323257
59749 H 2.622547 -0.775862 -0.527744
59750 H -0.680889 -1.052784 1.531538
59751 O 0.182150 -1.724673 -0.098129
59752 O 1.013054 -1.365620 -1.196994
59753 H 0.424196 -0.835203 -1.759396
59754 H 0.780597 0.795857 2.079372
59755 H 1.650137 -0.743546 1.937854
59756 Rotational constants (GHz): 1.4056300 0.7619300 0.6666700
59757 Vibrational harmonic frequencies (cm-1):
59758 34.8183 65.7642 104.9346
59759 150.3992 183.8709 194.3784
59760 220.0960 232.3659 256.8731
59761 267.4256 292.2988 315.3126
59762 330.5498 351.5391 434.2793
59763 448.2923 455.6147 500.8455
59764 535.9319 609.3691 626.3479
59765 664.4521 692.9089 789.0111
59766 869.7759 911.9819 941.0515
59767 956.3082 1022.2083 1039.9360
59768 1066.6279 1120.4382 1126.4834
59769 1159.9436 1184.3123 1235.4789
59770 1314.4531 1349.8050 1370.9374
59771 1402.1249 1407.4665 1460.3395
59772 1464.0226 1479.5783 1481.1963
59773 1506.7260 1511.7148 1994.6618
59774 3064.6882 3081.3447 3085.8223
59775 3139.2896 3157.8389 3177.2329
59776 3580.7968 3639.3364 3711.2022
59777 Zero-point correction (Hartree): 0.156676
59778
59779 triHPacyl.pmmmpmpppu
59780 -----
59781 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17464676
59782 Electronic state : 2-A
59783 Cartesian coordinates (Angs):
59784 O -1.915797 -1.096562 -1.111046
59785 O -2.026857 0.237107 -0.641758
59786 C -0.832827 0.602585 0.028831
59787 C 0.365440 0.575149 -0.948310
59788 C 0.991921 -0.796864 -1.236425
59789 O 1.001362 -1.730656 -0.178500
59790 O 2.060278 -1.416676 0.717575
59791 H -2.278309 -1.599682 -0.366572
59792 C -1.103125 2.008577 0.546751
59793 H -2.020544 2.000921 1.131910
59794 H -1.219820 2.680914 -0.300950
59795 H -0.273341 2.348012 1.159037
59796 C -0.655258 -0.300950 1.267990
59797 O -1.469672 -1.005919 1.730976
59798 H 1.564710 -1.094645 1.488260
59799 H -0.043648 0.936267 -1.895797
59800 O 1.328685 1.572011 -0.661572
59801 O 1.864949 1.373847 0.637585
59802 H 2.522711 0.676173 0.494462
59803 H 0.399670 -1.296003 -1.999879
59804 H 2.008086 -0.648163 -1.609581
59805 Rotational constants (GHz): 1.1504600 0.9081900 0.7565200

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59806 Vibrational harmonic frequencies (cm-1):
59807      61.2117      105.8553      130.2165
59808      147.4851      155.0543      198.4700
59809      204.9054      215.0049      228.9494
59810      235.6362      245.1735      296.6513
59811      326.9696      362.6105      387.8292
59812      420.7053      429.6386      441.8759
59813      530.6702      551.4603      556.5081
59814      639.5181      724.0003      774.4383
59815      820.4049      929.3973      950.5004
59816      985.0144      1023.1138      1049.1241
59817      1061.8190      1126.1892      1130.1158
59818      1169.5842      1186.8462      1225.1096
59819      1305.8066      1354.3408      1375.7174
59820      1403.2871      1409.7106      1422.0969
59821      1434.2454      1455.8537      1472.1281
59822      1489.6517      1494.8986      1971.0222
59823      3073.7479      3083.3092      3086.1679
59824      3155.8368      3164.6508      3188.6580
59825      3718.1080      3752.8036      3768.0915
59826 Zero-point correction (Hartree): 0.156301
59827
59828 triHPacyl.pmmmpmtmpu
59829 -----
59830 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17810022
59831 Electronic state : 2-A
59832 Cartesian coordinates (Angs):
59833 O      -1.928448      -1.035098      -1.227204
59834 O      -1.938647      0.346787      -0.909415
59835 C      -0.897358      0.666086      -0.006012
59836 C      0.487636      0.622329      -0.673276
59837 C      0.943277      -0.759111      -1.116893
59838 O      0.898608      -1.720852      -0.081502
59839 O      1.961698      -1.446534      0.827297
59840 H      -2.498458      -1.402462      -0.535445
59841 C      -1.238281      2.073412      0.474513
59842 H      -2.237796      2.073707      0.904047
59843 H      -1.214082      2.747869      -0.380153
59844 H      -0.515115      2.407398      1.212243
59845 C      -0.950380      -0.241582      1.239929
59846 O      -1.863969      -0.887441      1.588745
59847 H      1.492504      -0.984739      1.539965
59848 H      0.447780      1.273279      -1.553452
59849 O      1.349359      1.195929      0.304641
59850 O      2.676191      1.198648      -0.183313
59851 H      3.003870      0.351299      0.159256
59852 H      0.264814      -1.138290      -1.876304
59853 H      1.948770      -0.706363      -1.533707
59854 Rotational constants (GHz): 1.2720700      0.8149400      0.6959400
59855 Vibrational harmonic frequencies (cm-1):
59856      58.7778      97.9658      133.7427
59857      150.8845      175.3798      191.7221
59858      209.1570      219.9166      224.9829
59859      263.7764      297.9253      311.1794
59860      341.7180      390.1298      393.1293
59861      418.2349      431.1083      450.7395
59862      491.7553      552.2919      582.4851
59863      651.5293      729.5685      763.7552
59864      869.7571      912.9730      940.9844
59865      971.3345      1042.0350      1049.6249
59866      1057.0748      1113.2565      1125.1024
59867      1174.7563      1192.5739      1233.0327
59868      1292.3626      1357.5752      1381.1124
59869      1404.5130      1410.7239      1429.4051
59870      1433.8795      1449.1252      1480.8308
59871      1490.1052      1496.4448      1976.8227
59872      3052.2768      3083.0212      3103.6415
59873      3161.0602      3171.4981      3186.3605
59874      3732.9687      3743.5301      3772.1431
59875 Zero-point correction (Hartree): 0.156792
59876
59877 triHPacyl.pmmmpptppu

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59878 -----
59879 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17417989
59880 Electronic state : 2-A
59881 Cartesian coordinates (Angs):
59882 O -1.911384 -1.740805 -0.352870
59883 O -2.231778 -0.369237 -0.191217
59884 C -1.046118 0.355862 0.092307
59885 C -0.062585 0.234313 -1.104250
59886 C 0.796858 -1.035868 -1.169947
59887 O 1.219487 -1.584293 0.060947
59888 O 2.367948 -0.881276 0.516721
59889 H -1.922188 -2.061118 0.561613
59890 C -1.513868 1.789016 0.300150
59891 H -2.281219 1.810654 1.071296
59892 H -1.932091 2.162953 -0.632497
59893 H -0.672919 2.409080 0.594675
59894 C -0.510884 -0.165552 1.443852
59895 O 0.324262 0.275944 2.139316
59896 H 2.038797 -0.497621 1.346327
59897 H -0.712823 0.216535 -1.983830
59898 O 0.681930 1.413547 -1.322163
59899 O 1.476347 1.697239 -0.181365
59900 H 2.219073 1.079680 -0.271579
59901 H 0.204017 -1.834170 -1.609138
59902 H 1.664435 -0.841579 -1.804494
59903 Rotational constants (GHz): 1.1502300 0.9144700 0.7985800
59904 Vibrational harmonic frequencies (cm-1):
59905 73.8842 109.6351 154.6382
59906 164.3141 176.5269 205.5215
59907 215.7941 225.2190 235.5984
59908 238.8326 264.4081 274.0389
59909 293.8789 335.1084 366.6905
59910 400.4044 435.9278 482.9440
59911 506.9845 553.2327 558.2443
59912 622.5935 657.6211 770.5848
59913 821.7925 939.5608 950.7373
59914 977.3282 1023.2068 1051.2418
59915 1060.1965 1127.7397 1129.9556
59916 1169.2676 1186.3844 1208.4702
59917 1300.3232 1345.9813 1374.8894
59918 1404.3106 1409.1758 1414.4349
59919 1444.4803 1460.6543 1476.7713
59920 1487.6886 1495.9880 1973.8798
59921 3075.4815 3080.4680 3086.0696
59922 3159.3162 3162.7454 3193.2843
59923 3724.6865 3742.4122 3764.1670
59924 Zero-point correction (Hartree): 0.156159
59925
59926 triHPacyl.pmmmpptmpu
59927 -----
59928 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17837354
59929 Electronic state : 2-A
59930 Cartesian coordinates (Angs):
59931 O -2.000795 -1.567579 -0.687423
59932 O -2.170692 -0.159998 -0.713348
59933 C -1.111989 0.478830 -0.026884
59934 C 0.191632 0.449080 -0.852464
59935 C 0.775766 -0.934367 -1.090546
59936 O 1.000149 -1.663637 0.098980
59937 O 2.130125 -1.101421 0.759144
59938 H -2.441132 -1.808671 0.140127
59939 C -1.602884 1.905702 0.192183
59940 H -2.522046 1.893297 0.773984
59941 H -1.804787 2.355570 -0.779028
59942 H -0.842241 2.484521 0.707370
59943 C -0.949910 -0.158266 1.366883
59944 O -0.154246 0.093094 2.190339
59945 H 1.707472 -0.597183 1.473289
59946 H -0.044262 0.892398 -1.827454
59947 O 1.072031 1.306680 -0.138974
59948 O 2.318849 1.352857 -0.803823
59949 H 2.797959 0.641399 -0.348644

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59950      H      0.067635      -1.534063      -1.655793
59951      H      1.702348      -0.853101      -1.658056
59952 Rotational constants (GHz):      1.2211400      0.8444200      0.7541400
59953 Vibrational harmonic frequencies (cm-1):
59954      70.1647      104.6924      139.8872
59955      154.5767      168.0406      193.6495
59956      201.4977      221.2880      227.8027
59957      248.0950      281.2882      283.5436
59958      335.7987      361.8446      366.3731
59959      396.5603      432.3141      470.6777
59960      508.1920      536.5534      560.3353
59961      632.0212      693.5384      776.0419
59962      866.7483      912.3722      943.4213
59963      973.0122      1043.1924      1046.3427
59964      1057.6410      1116.3419      1126.0755
59965      1174.2580      1197.7999      1223.2353
59966      1292.1230      1352.4156      1374.3840
59967      1402.8090      1408.0462      1417.8120
59968      1442.5416      1453.5500      1481.0364
59969      1487.6187      1495.5985      1978.6426
59970      3036.5138      3082.3883      3105.4354
59971      3159.1038      3170.4953      3187.3347
59972      3728.0730      3738.2880      3779.6100
59973 Zero-point correction (Hartree): 0.156326
59974
59975 triHPacyl.pmtmppppmu
59976 -----
59977 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17328177
59978 Electronic state : 2-A
59979 Cartesian coordinates (Angs):
59980      O      -1.444464      -1.938007      -0.627779
59981      O      -1.830316      -0.641734      -1.054158
59982      C      -1.120238      0.329152      -0.304050
59983      C      0.414185      0.134271      -0.458036
59984      C      1.053580      -0.731688      0.629103
59985      O      2.458500      -0.593383      0.642269
59986      O      2.948175      -1.068373      -0.605589
59987      H      -2.108033      -2.122708      0.053445
59988      C      -1.583766      1.663621      -0.863413
59989      H      -2.669765      1.718040      -0.811972
59990      H      -1.264291      1.747019      -1.899826
59991      H      -1.145111      2.474728      -0.289341
59992      C      -1.560183      0.260655      1.173368
59993      O      -2.305189      -0.512698      1.647103
59994      H      3.374981      -1.893610      -0.343837
59995      H      0.554207      -0.333770      -1.433699
59996      O      1.097137      1.358654      -0.597639
59997      O      1.137504      2.004901      0.668293
59998      H      2.027636      1.767400      0.965823
59999      H      0.757385      -0.395489      1.623490
60000      H      0.760732      -1.772570      0.494077
60001 Rotational constants (GHz):      1.2822000      0.7156100      0.6112600
60002 Vibrational harmonic frequencies (cm-1):
60003      24.4955      65.6451      77.5073
60004      124.0319      135.6753      164.7383
60005      203.2398      211.1368      233.4810
60006      253.1299      264.4872      314.3322
60007      328.4136      348.8294      379.2250
60008      402.4083      415.8508      425.9419
60009      437.9685      493.0960      566.8182
60010      685.1492      699.6654      742.6581
60011      868.8445      924.0536      961.6905
60012      980.9922      994.3517      1049.9364
60013      1088.0581      1127.4274      1142.1250
60014      1170.6595      1192.0861      1213.8686
60015      1303.5042      1318.0784      1378.2774
60016      1396.9836      1408.0173      1410.6914
60017      1422.4570      1424.4495      1484.8361
60018      1486.6257      1494.3811      1969.7932
60019      3084.9543      3086.0214      3110.4993
60020      3142.1311      3164.8387      3184.1725
60021      3768.9986      3781.6344      3820.3428

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60022 Zero-point correction (Hartree): 0.155721
60023
60024 triHPacyl.pmtmpppppu
60025 -----
60026 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17567796
60027 Electronic state : 2-A
60028 Cartesian coordinates (Angs):
60029 O -1.571312 -1.873988 -0.605157
60030 O -1.883886 -0.563439 -1.049224
60031 C -1.101196 0.366980 -0.323509
60032 C 0.405858 0.061181 -0.509087
60033 C 1.001074 -0.984963 0.451690
60034 O 2.374276 -0.736011 0.677320
60035 O 3.054578 -0.906852 -0.557064
60036 H -2.240749 -2.011599 0.081569
60037 C -1.477948 1.724682 -0.891252
60038 H -2.557733 1.850655 -0.837148
60039 H -1.160215 1.780268 -1.930562
60040 H -0.986448 2.509576 -0.323650
60041 C -1.515616 0.342920 1.163359
60042 O -2.321942 -0.357443 1.649249
60043 H 3.040139 -0.005717 -0.912601
60044 H 0.501679 -0.284717 -1.540312
60045 O 1.193698 1.236601 -0.500952
60046 O 1.178795 1.786854 0.809365
60047 H 1.922505 1.319539 1.221465
60048 H 0.560442 -0.920705 1.447719
60049 H 0.853674 -1.987877 0.058029
60050 Rotational constants (GHz): 1.3570700 0.7067400 0.6218600
60051 Vibrational harmonic frequencies (cm-1):
60052 51.7879 67.2114 85.4313
60053 154.3357 164.0877 173.8404
60054 205.1734 219.1126 243.6479
60055 262.0877 318.1411 322.4601
60056 360.7825 378.1324 398.6363
60057 418.4801 433.7593 461.7352
60058 490.9776 501.9803 567.3688
60059 681.9868 711.0861 763.8976
60060 857.7029 925.5508 958.4797
60061 984.7265 1006.4419 1049.0580
60062 1080.8161 1120.0311 1138.2744
60063 1175.8842 1194.3874 1220.8176
60064 1300.5432 1330.6322 1377.9003
60065 1403.1791 1410.0833 1422.3887
60066 1425.6583 1435.2025 1481.6489
60067 1487.7827 1495.1024 1971.4266
60068 3084.8476 3091.1282 3100.7389
60069 3155.8279 3163.3558 3184.4995
60070 3747.3438 3768.6469 3770.0300
60071 Zero-point correction (Hartree): 0.156638
60072
60073 triHPacyl.pmtpppppmu
60074 -----
60075 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17670044
60076 Electronic state : 2-A
60077 Cartesian coordinates (Angs):
60078 O -1.849458 -1.654842 -0.834816
60079 O -2.050398 -0.259432 -0.985230
60080 C -1.107777 0.446447 -0.194336
60081 C 0.342736 0.052443 -0.585287
60082 C 0.950365 -1.059651 0.263040
60083 O 2.227411 -1.444796 -0.201410
60084 O 3.181763 -0.484151 0.243653
60085 H -2.462692 -1.862252 -0.114085
60086 C -1.408397 1.910564 -0.469312
60087 H -2.459431 2.103302 -0.262271
60088 H -1.200467 2.126375 -1.514936
60089 H -0.786271 2.541593 0.157750
60090 C -1.379498 0.174706 1.300424
60091 O -2.184409 -0.556247 1.741397
60092 H 3.360924 -0.000122 -0.574159
60093 H 0.289919 -0.282808 -1.623613

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60094	O	1.203608	1.174313	-0.660319		
60095	O	1.391815	1.696794	0.647921		
60096	H	2.162668	1.188228	0.948947		
60097	H	1.009927	-0.779852	1.316810		
60098	H	0.338187	-1.954642	0.168817		
60099	Rotational constants (GHz):			1.3775000	0.6963200	0.6022700
60100	Vibrational harmonic frequencies (cm-1):					
60101		48.2018	71.1823		103.7286	
60102		157.7609	170.9508		199.2113	
60103		213.5227	224.0616		253.0819	
60104		263.3171	299.4223		322.7937	
60105		335.2690	377.6465		381.2139	
60106		410.0738	416.0013		438.0621	
60107		508.7223	553.4568		578.5888	
60108		636.3537	712.2360		733.2319	
60109		888.2405	917.7084		948.7047	
60110		983.1797	1001.2410		1050.7026	
60111		1103.6426	1122.6179		1130.7069	
60112		1163.5955	1186.2495		1215.6854	
60113		1299.5951	1318.2764		1378.0855	
60114		1405.8827	1410.4749		1415.4687	
60115		1422.5431	1440.8426		1482.0062	
60116		1490.5955	1496.3188		1971.4217	
60117		3079.4430	3087.5131		3097.7427	
60118		3155.3109	3166.0408		3189.8697	
60119		3731.3724	3769.9286		3800.3530	
60120	Zero-point correction (Hartree): 0.156577					
60121	triHPacyl.pmtppppppu					
60122	-----					
60123	-----					
60124	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17489122					
60125	Electronic state : 2-A					
60126	Cartesian coordinates (Angs):					
60127	O	-1.858400	-1.651185	-0.849563		
60128	O	-2.089379	-0.255383	-0.945197		
60129	C	-1.129319	0.441484	-0.166683		
60130	C	0.315639	0.093349	-0.624118		
60131	C	0.965911	-1.035329	0.170264		
60132	O	2.249948	-1.357700	-0.326390		
60133	O	3.189294	-0.435539	0.220524		
60134	H	-2.437197	-1.892248	-0.111099		
60135	C	-1.464289	1.908532	-0.378408		
60136	H	-2.508321	2.078140	-0.121332		
60137	H	-1.301872	2.162960	-1.423311		
60138	H	-0.824129	2.527070	0.243247		
60139	C	-1.342050	0.115193	1.326153		
60140	O	-2.111796	-0.650516	1.772435		
60141	H	3.747433	-1.025782	0.741214		
60142	H	0.229998	-0.213982	-1.668649		
60143	O	1.143097	1.231447	-0.699720		
60144	O	1.396597	1.702848	0.617127		
60145	H	2.256909	1.288969	0.788129		
60146	H	1.030502	-0.794623	1.232782		
60147	H	0.376429	-1.941654	0.042039		
60148	Rotational constants (GHz):			1.3730400	0.6914700	0.5996900
60149	Vibrational harmonic frequencies (cm-1):					
60150		47.8583	72.5637		94.8677	
60151		146.5617	171.6743		194.5347	
60152		215.7673	222.5094		256.0034	
60153		258.8308	275.2977		299.5409	
60154		329.4836	338.5796		385.8081	
60155		407.7339	427.4114		436.0101	
60156		506.0468	513.8864		575.4770	
60157		636.3558	707.1138		733.4034	
60158		884.9425	917.2009		949.0983	
60159		982.2600	1001.3052		1049.9232	
60160		1098.3026	1122.7528		1137.0961	
60161		1163.2654	1189.7104		1214.0764	
60162		1304.6614	1321.4494		1378.6214	
60163		1393.1485	1411.1105		1420.5588	
60164		1424.9344	1444.4912		1477.0114	
60165		1489.8410	1496.3976		1968.5189	


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60166          3081.5814              3087.2144              3100.6999
60167          3151.2296              3166.4724              3188.5341
60168          3760.9372              3771.1169              3827.2805
60169 Zero-point correction (Hartree): 0.156349
60170
60171 triHPacyl.pmtpptppmu
60172 -----
60173 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17503387
60174 Electronic state : 2-A
60175 Cartesian coordinates (Angs):
60176 O      1.813401      2.068001      -0.159266
60177 O      2.137430      0.815401      -0.740974
60178 C      1.246828      -0.165465      -0.239621
60179 C      -0.221768      0.231665      -0.570282
60180 C      -0.978143      0.923747      0.558358
60181 O      -2.249406      1.374394      0.136486
60182 O      -3.143270      0.264360      0.130020
60183 H      2.406048      2.088882      0.605603
60184 C      1.683006      -1.457560      -0.909868
60185 H      2.737434      -1.630569      -0.704260
60186 H      1.534984      -1.367770      -1.983972
60187 H      1.090676      -2.285069      -0.531751
60188 C      1.495284      -0.294671      1.283207
60189 O      1.064817      -1.098174      2.014861
60190 H      -3.216684      0.084042      -0.817242
60191 H      -0.153202      0.920772      -1.415500
60192 O      -0.964828      -0.846833      -1.105972
60193 O      -1.183908      -1.809059      -0.083714
60194 H      -2.015046      -1.492487      0.306512
60195 H      -1.087302      0.283689      1.434443
60196 H      -0.442018      1.827507      0.843880
60197 Rotational constants (GHz):      1.2794400      0.7353900      0.6341600
60198 Vibrational harmonic frequencies (cm-1):
60199      48.7665      66.1979      98.4840
60200      134.7326      157.7207      175.3764
60201      199.8769      219.9072      249.3243
60202      254.9957      268.2157      290.8412
60203      322.0238      331.3603      362.1483
60204      379.3943      413.8549      481.6273
60205      516.8086      556.0489      569.1925
60206      591.9515      666.3296      745.0198
60207      887.9334      924.7355      948.8377
60208      974.8245      999.9648      1048.9136
60209      1098.5191      1120.2095      1130.7579
60210      1162.6291      1178.5980      1211.8008
60211      1296.0566      1315.8664      1375.1851
60212      1406.1854      1407.1504      1408.6795
60213      1415.2657      1442.2681      1481.6154
60214      1489.3869      1495.7529      1996.2881
60215      3087.4860      3087.7905      3096.9556
60216      3157.4181      3165.6232      3190.9502
60217      3702.7989      3779.8428      3799.1994
60218 Zero-point correction (Hartree): 0.155794
60219
60220 triHPacyl.ppmmpmpmu
60221 -----
60222 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17371940
60223 Electronic state : 2-A
60224 Cartesian coordinates (Angs):
60225 O      -0.197559      0.463662      1.788182
60226 O      -0.877580      -0.672339      1.288015
60227 C      -1.158410      -0.555321      -0.088167
60228 C      0.072420      -0.415186      -1.026850
60229 C      1.296684      -1.209097      -0.572405
60230 O      1.938151      -0.748957      0.602211
60231 O      2.977847      0.147887      0.248943
60232 H      0.725749      0.155612      1.724307
60233 C      -1.926078      -1.833714      -0.396266
60234 H      -2.765990      -1.926486      0.288952
60235 H      -1.280153      -2.700949      -0.270407
60236 H      -2.303050      -1.801216      -1.415707
60237 C      -2.074929      0.661743      -0.405640

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60238	O	-2.168586	1.655353	0.204614		
60239	H	2.479510	0.965014	0.063193		
60240	H	-0.233990	-0.861818	-1.976901		
60241	O	0.329047	0.915214	-1.452132		
60242	O	0.873096	1.719147	-0.419375		
60243	H	0.115882	1.901642	0.164581		
60244	H	0.977947	-2.228621	-0.348631		
60245	H	2.030638	-1.233463	-1.377088		
60246	Rotational constants (GHz):			1.3579000	0.8202700	0.7395200
60247	Vibrational harmonic frequencies (cm-1):					
60248		58.6333	94.2372			113.9529
60249		163.4838	191.2832			206.1038
60250		222.7851	238.8567			249.6523
60251		262.5405	291.4036			302.3619
60252		328.6612	364.3920			389.5733
60253		404.1037	492.9208			510.3409
60254		525.5121	608.2090			612.3383
60255		670.2903	687.0325			793.1795
60256		854.5105	907.0849			936.1324
60257		960.3111	1016.7628			1044.1626
60258		1068.8289	1125.9090			1135.4095
60259		1163.7677	1184.7184			1227.0057
60260		1321.4612	1336.6556			1387.9035
60261		1400.4575	1413.9277			1459.3080
60262		1466.9998	1482.3662			1484.5570
60263		1499.6755	1503.8164			1987.5251
60264		3075.6606	3081.2919			3086.9622
60265		3138.0178	3162.1392			3171.2881
60266		3623.0875	3645.7425			3695.2644
60267	Zero-point correction (Hartree):			0.156808		
60268						
60269	triHPacyl.ppmmtmpmu					
60270	-----					
60271	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.17550486		
60272	Electronic state : 2-A					
60273	Cartesian coordinates (Angs):					
60274	O	-0.006982	-1.005322	1.796383		
60275	O	0.025296	0.381487	1.493863		
60276	C	0.655938	0.609439	0.257791		
60277	C	-0.033589	-0.040177	-0.963104		
60278	C	-1.389589	0.564950	-1.312759		
60279	O	-2.225700	0.873585	-0.217118		
60280	O	-2.529001	-0.326553	0.476293		
60281	H	-0.903006	-1.225664	1.493563		
60282	C	0.689849	2.129069	0.125954		
60283	H	1.322355	2.550070	0.904396		
60284	H	-0.317619	2.522608	0.240861		
60285	H	1.098920	2.404509	-0.844571		
60286	C	2.137873	0.146650	0.315510		
60287	O	2.954754	0.387407	-0.487657		
60288	H	-3.421139	-0.525873	0.165901		
60289	H	0.635030	0.120741	-1.817313		
60290	O	-0.269316	-1.428990	-0.829390		
60291	O	0.970278	-2.082256	-0.634325		
60292	H	1.011956	-2.120515	0.336892		
60293	H	-1.247089	1.530106	-1.798084		
60294	H	-1.896926	-0.110437	-2.006390		
60295	Rotational constants (GHz):			1.3007800	0.8286900	0.7475300
60296	Vibrational harmonic frequencies (cm-1):					
60297		101.9589	109.6957			135.3369
60298		140.6948	157.5720			180.2273
60299		206.1231	221.3735			245.7897
60300		253.6851	283.2147			291.4488
60301		310.9544	337.4966			381.2649
60302		396.9245	451.6999			495.8023
60303		527.8317	544.4262			597.2027
60304		643.0925	662.6506			833.9913
60305		850.5678	895.9449			947.1186
60306		977.3038	1029.8689			1052.8139
60307		1072.6240	1120.3186			1139.1419
60308		1152.9624	1188.3386			1254.4261
60309		1316.7875	1364.5547			1380.9234

60310	1389.9447	1400.0422	1422.9488		
60311	1440.8102	1461.3072	1469.1237		
60312	1485.5818	1513.5848	1978.8140		
60313	3039.1621	3066.3431	3082.4207		
60314	3136.2896	3162.8406	3172.2531		
60315	3697.7453	3743.2690	3819.1380		
60316	Zero-point correction (Hartree): 0.156592				
60317					
60318	triHPacyl.ppmmtmpu				
60319	-----				
60320	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17521570				
60321	Electronic state : 2-A				
60322	Cartesian coordinates (Angs):				
60323	O	0.144424	-0.375401	1.932776	
60324	O	-0.620858	-1.200020	1.072063	
60325	C	-1.100024	-0.475123	-0.035922	
60326	C	-0.012239	0.086539	-0.992498	
60327	C	1.230925	-0.796107	-1.103146	
60328	O	2.051170	-0.860932	0.048786	
60329	O	3.065256	0.125631	-0.041297	
60330	H	1.044000	-0.577949	1.613314	
60331	C	-1.998035	-1.468681	-0.759585	
60332	H	-2.714614	-1.891736	-0.059720	
60333	H	-1.399577	-2.278176	-1.176368	
60334	H	-2.536259	-0.962744	-1.557607	
60335	C	-1.944281	0.740146	0.454998	
60336	O	-2.889427	1.177722	-0.073603	
60337	H	2.581010	0.930412	0.218937	
60338	H	-0.468668	0.084777	-1.986388	
60339	O	0.237066	1.475246	-0.835765	
60340	O	0.938438	1.764012	0.362900	
60341	H	0.281301	1.606583	1.063911	
60342	H	0.904898	-1.821677	-1.285418	
60343	H	1.841292	-0.460203	-1.940621	
60344	Rotational constants (GHz):		1.4522400	0.7539550	0.6903300
60345	Vibrational harmonic frequencies (cm-1):				
60346	68.6929	86.6337	108.4309		
60347	162.8811	184.8439	205.8125		
60348	227.1762	240.8972	251.8352		
60349	262.5318	281.9284	315.5547		
60350	325.4107	346.6977	382.0196		
60351	448.1929	487.7665	495.4654		
60352	535.3057	610.5203	624.6066		
60353	670.2474	677.8811	805.4666		
60354	852.3215	914.5596	943.5991		
60355	960.4115	1015.9199	1044.4583		
60356	1064.0273	1126.4555	1134.3491		
60357	1158.4961	1175.2638	1231.8855		
60358	1323.0536	1338.7739	1389.0323		
60359	1400.7425	1411.8981	1457.0229		
60360	1459.0880	1480.4355	1483.8857		
60361	1497.0153	1501.4834	1998.0578		
60362	3076.9371	3078.2710	3086.3014		
60363	3138.1874	3157.4933	3173.7656		
60364	3618.1504	3659.6870	3686.3953		
60365	Zero-point correction (Hartree): 0.156839				
60366					
60367	triHPacyl.ppmppmmpu				
60368	-----				
60369	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17688888				
60370	Electronic state : 2-A				
60371	Cartesian coordinates (Angs):				
60372	O	0.930642	-0.671711	1.652438	
60373	O	0.339193	0.538352	1.194214	
60374	C	0.508544	0.697729	-0.214062	
60375	C	-0.407971	-0.223706	-1.038995	
60376	C	-1.883333	0.175994	-1.003267	
60377	O	-2.352695	0.638557	0.239695	
60378	O	-2.419067	-0.459113	1.132876	
60379	H	1.792791	-0.354997	1.960164	
60380	C	0.213097	2.173146	-0.477321	
60381	H	0.979969	2.792763	-0.017172	

60382	H	-0.754923	2.422467	-0.050594	
60383	H	0.204652	2.359889	-1.550100	
60384	C	1.980209	0.510967	-0.615395	
60385	O	2.906349	0.434477	0.100717	
60386	H	-1.549111	-0.418982	1.559119	
60387	H	-0.063935	-0.170386	-2.078433	
60388	O	-0.354311	-1.565464	-0.608531	
60389	O	0.969754	-2.031547	-0.812629	
60390	H	1.291528	-2.048046	0.101383	
60391	H	-2.044571	1.017343	-1.677696	
60392	H	-2.478598	-0.673246	-1.342666	
60393	Rotational constants (GHz):			1.3410200	0.8161900 0.7354500
60394	Vibrational harmonic frequencies (cm-1):				
60395		85.1327	101.3935		130.7452
60396		169.7229	188.4725		196.2033
60397		212.0978	237.4603		247.8882
60398		256.8556	292.0360		319.5411
60399		352.1892	375.9307		387.5501
60400		419.0728	435.6499		441.3486
60401		465.1567	504.4337		591.4013
60402		619.2453	717.5608		843.5437
60403		854.3660	886.9870		939.4865
60404		986.1376	1029.9341		1036.1840
60405		1067.7181	1125.1934		1136.6013
60406		1159.5930	1191.9264		1244.1212
60407		1314.5441	1357.8570		1379.8590
60408		1399.2335	1413.1984		1418.6165
60409		1434.4126	1436.8410		1466.4519
60410		1488.3801	1511.8999		1968.8092
60411		3041.4716	3080.0223		3082.7052
60412		3134.0520	3159.5764		3179.1488
60413		3760.1987	3767.9751		3773.2503
60414	Zero-point correction (Hartree):			0.156778	
60415	triHPacyl.ppmmpptmpu				
60416	-----				
60418	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.17712396	
60419	Electronic state : 2-A				
60420	Cartesian coordinates (Angs):				
60421	O	-0.408290	-0.264325	1.814243	
60422	O	-1.037515	-1.039571	0.813163	
60423	C	-1.100005	-0.332002	-0.407498	
60424	C	0.246452	0.156468	-0.959309	
60425	C	1.369877	-0.875914	-0.929784	
60426	O	1.761050	-1.326365	0.344027	
60427	O	2.362101	-0.240055	1.038967	
60428	H	-1.133678	0.300694	2.123030	
60429	C	-1.791018	-1.300083	-1.358025	
60430	H	-2.758457	-1.583733	-0.948768	
60431	H	-1.188123	-2.198525	-1.471148	
60432	H	-1.938848	-0.829751	-2.327118	
60433	C	-2.017890	0.912380	-0.260250	
60434	O	-2.529102	1.272192	0.730617	
60435	H	1.609812	0.048681	1.582004	
60436	H	0.082758	0.421250	-2.010583	
60437	O	0.548595	1.345802	-0.246371	
60438	O	1.729144	1.905493	-0.786532	
60439	H	2.400029	1.501749	-0.210919	
60440	H	1.043031	-1.778910	-1.447030	
60441	H	2.231120	-0.471918	-1.465179	
60442	Rotational constants (GHz):			1.3058400	0.7925000 0.7377300
60443	Vibrational harmonic frequencies (cm-1):				
60444		72.4817	101.1313		128.6071
60445		165.5483	187.8258		194.4211
60446		206.9985	227.2375		242.4987
60447		261.1084	305.1830		314.3073
60448		348.5060	377.8778		408.0492
60449		412.8691	439.0775		472.1825
60450		520.6700	584.4962		587.7933
60451		643.4168	692.8016		822.6029
60452		847.9667	891.0798		938.5267
60453		978.2114	1036.7847		1049.9896

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60454      1064.7094      1125.1521      1133.6725
60455      1159.1057      1206.5406      1251.9863
60456      1307.8096      1367.0970      1379.2116
60457      1405.4026      1413.8467      1425.7946
60458      1451.9765      1463.4737      1477.2112
60459      1485.1613      1506.2392      1979.2106
60460      3037.1554      3077.2911      3086.3176
60461      3127.3004      3164.8188      3174.7623
60462      3716.4396      3728.5497      3752.2664
60463 Zero-point correction (Hartree): 0.157031
60464
60465 triHPacyl.ppmptmpu
60466 -----
60467 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17699389
60468 Electronic state : 2-A
60469 Cartesian coordinates (Angs):
60470 O      0.532085      -1.136962      1.769283
60471 O      0.042660      0.164289      1.467964
60472 C      0.565780      0.631112      0.228164
60473 C     -0.139933     -0.016147     -0.983606
60474 C     -1.554220      0.517968     -1.221785
60475 O     -2.311079      0.752097     -0.059428
60476 O     -2.659158     -0.496841      0.511453
60477 H      1.254536     -0.933044      2.379155
60478 C      0.393957      2.146119      0.260335
60479 H      1.047886      2.580302      1.013815
60480 H     -0.638620      2.386460      0.500455
60481 H      0.657599      2.557437     -0.712962
60482 C      2.085728      0.382105      0.176441
60483 O      2.805880      0.696387     -0.689398
60484 H     -1.916373     -0.650080      1.115895
60485 H      0.464196      0.202187     -1.871368
60486 O     -0.266687     -1.412141     -0.842723
60487 O      1.036108     -1.972537     -0.865866
60488 H      1.153831     -2.183576      0.072450
60489 H     -1.492939      1.494642     -1.702087
60490 H     -2.076458     -0.175607     -1.882925
60491 Rotational constants (GHz):      1.2697400      0.8158500      0.7447700
60492 Vibrational harmonic frequencies (cm-1):
60493      87.1714      100.5640      138.0001
60494      156.2202      165.5543      189.5583
60495      205.8493      221.8661      245.4727
60496      257.7779      286.2995      306.0680
60497      318.6791      360.1933      382.0046
60498      393.1734      446.7929      464.3871
60499      467.4546      507.5223      551.0671
60500      632.5448      662.7926      841.9169
60501      854.6550      897.2745      938.0306
60502      987.8900      1029.3931      1038.3459
60503      1068.8483      1124.8011      1132.9123
60504      1158.8837      1189.3208      1236.1817
60505      1312.1625      1354.1769      1374.5226
60506      1397.6783      1409.8881      1410.6423
60507      1436.7964      1438.7495      1466.1804
60508      1486.6184      1509.8980      1990.0666
60509      3048.5600      3079.5285      3081.9638
60510      3136.7038      3159.2195      3174.9956
60511      3751.9454      3769.9188      3795.2041
60512 Zero-point correction (Hartree): 0.156353
60513
60514 triHPacyl.ppmptmpu
60515 -----
60516 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17603508
60517 Electronic state : 2-A
60518 Cartesian coordinates (Angs):
60519 O     -0.063637     -1.103193     -1.695009
60520 O      0.706834     -1.518879     -0.584367
60521 C      1.105945     -0.405856      0.181511
60522 C     -0.034703      0.486323      0.694840
60523 C     -1.203232     -0.267101      1.326446
60524 O     -1.913930     -1.127796      0.470637
60525 O     -2.590402     -0.337842     -0.500349

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60526	H	0.609141	-0.752005	-2.299086			
60527	C	1.928680	-1.004032	1.313673			
60528	H	2.755805	-1.577732	0.901100			
60529	H	1.308540	-1.673953	1.906132			
60530	H	2.324344	-0.209499	1.941604			
60531	C	2.051737	0.488259	-0.677397			
60532	O	2.722899	1.357681	-0.281063			
60533	H	-1.969980	-0.416721	-1.243721			
60534	H	0.392340	1.129953	1.473003			
60535	O	-0.418081	1.308020	-0.397866			
60536	O	-1.392652	2.226873	0.055173			
60537	H	-2.208541	1.738544	-0.146202			
60538	H	-0.827242	-0.919558	2.115391			
60539	H	-1.883223	0.456512	1.780097			
60540	Rotational constants (GHz):				1.3043400	0.8104500	0.6932000
60541	Vibrational harmonic frequencies (cm-1):						
60542		65.0681		100.5651		122.6256	
60543		159.6386		165.5637		190.0734	
60544		201.1576		211.0036		243.6737	
60545		256.8589		274.4198		302.2396	
60546		308.5089		346.5595		377.6764	
60547		390.5280		464.5022		511.3015	
60548		520.6469		540.1324		586.9077	
60549		607.4304		683.7191		820.6036	
60550		844.9381		893.0653		945.5204	
60551		976.3381		1037.5453		1049.7731	
60552		1064.8029		1120.1007		1126.8549	
60553		1156.1799		1198.1002		1257.1995	
60554		1308.8824		1365.0839		1377.7276	
60555		1403.2281		1412.7358		1418.0204	
60556		1449.5526		1461.3939		1476.5663	
60557		1483.4507		1505.9402		1999.5363	
60558		3039.0924		3078.0519		3084.4899	
60559		3129.0017		3162.5256		3174.0326	
60560		3707.0483		3719.6107		3747.0574	
60561	Zero-point correction (Hartree):				0.156339		
60562	triHPacyl.pppmmmpmu						
60563	-----						
60564	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17617674						
60565	Electronic state : 2-A						
60566	Cartesian coordinates (Angs):						
60567	O	-0.363104	0.155437	1.824987			
60568	O	-0.071511	-0.933051	0.963708			
60569	C	-0.464407	-0.649046	-0.371811			
60570	C	0.163437	0.626044	-0.961103			
60571	C	1.687079	0.653323	-0.945310			
60572	O	2.218878	0.523219	0.364037			
60573	O	2.650816	-0.814619	0.564202			
60574	H	0.432594	0.706024	1.717388			
60575	C	-0.041421	-1.885615	-1.162677			
60576	H	-0.571160	-2.756689	-0.781787			
60577	H	1.029095	-2.048949	-1.062721			
60578	H	-0.294406	-1.754715	-2.212980			
60579	C	-2.005269	-0.609042	-0.504333			
60580	O	-2.788904	-0.872597	0.322262			
60581	H	1.876756	-1.204129	1.002519			
60582	H	-0.191241	0.696718	-1.995536			
60583	O	-0.167971	1.820016	-0.268495			
60584	O	-1.570214	1.923643	-0.131179			
60585	H	-1.700278	1.602916	0.776552			
60586	H	2.117706	-0.108373	-1.591546			
60587	H	2.000502	1.636840	-1.296656			
60588	Rotational constants (GHz):				1.3340900	0.8426500	0.7236600
60589	Vibrational harmonic frequencies (cm-1):						
60590		80.3990		100.1692		118.2014	
60591		137.9466		175.4146		201.0297	
60592		211.5927		226.0515		269.2042	
60593		288.4351		291.8579		326.3368	
60594		343.1538		370.3348		424.2486	
60595		446.4832		506.3150		509.9718	
60596		555.9961		579.6589		600.0247	

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60598          627.8318          693.6429          812.0494
60599          842.0394          906.8444          945.5795
60600          962.7691          1018.8879         1053.2918
60601          1076.3741         1119.7218         1134.4994
60602          1148.4277         1170.9550         1245.2583
60603          1306.7070         1344.3741         1380.7316
60604          1399.5633         1411.9112         1438.9144
60605          1454.9414         1469.1339         1476.8741
60606          1489.0593         1513.3464         1986.9819
60607          3048.3340         3083.7821         3095.0248
60608          3152.8021         3162.7351         3173.7690
60609          3682.2558         3719.4769         3730.6625
60610 Zero-point correction (Hartree): 0.157290
60611
60612 triHPacyl.pmpmtmpmu
60613 -----
60614 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17739024
60615 Electronic state : 2-A
60616 Cartesian coordinates (Angs):
60617 O      -0.064904      -0.595746      1.929639
60618 O      -0.211484      0.661626      1.289656
60619 C       0.491696      0.695874      0.059073
60620 C       0.065711     -0.396540     -0.943334
60621 C      -1.415872     -0.379865     -1.307493
60622 O      -2.253651     -0.551545     -0.176231
60623 O      -2.757099      0.712196      0.230940
60624 H      -0.784164     -1.107573      1.520200
60625 C       0.228916      2.092978     -0.495587
60626 H       0.639321      2.838132      0.182777
60627 H      -0.839749      2.263534     -0.604451
60628 H       0.719934      2.194574     -1.461271
60629 C       2.016210      0.622402      0.328302
60630 O       2.855537      0.878870     -0.445532
60631 H      -2.122395      0.958094      0.923243
60632 H       0.665393     -0.241551     -1.847481
60633 O       0.246447     -1.722796     -0.475953
60634 O       1.584049     -1.910152     -0.061313
60635 H       1.510326     -1.780997      0.898963
60636 H      -1.695977      0.527852     -1.837461
60637 H      -1.603815     -1.240786     -1.949937
60638 Rotational constants (GHz): 1.3205100 0.8240600 0.7193300
60639 Vibrational harmonic frequencies (cm-1):
60640      82.8859          102.3701          113.7038
60641     147.8907          187.8738          201.9401
60642     216.9720          228.6946          267.9332
60643     284.4919          290.9284          306.8558
60644     329.8212          357.6182          423.7903
60645     488.4023          492.1849          507.0548
60646     539.3443          561.7228          576.3221
60647     630.4753          665.8921          807.8572
60648     848.7825          919.5640          950.1404
60649     961.1192          1019.1499         1054.3714
60650    1075.3964          1116.1027         1136.5893
60651    1146.3410          1169.8463         1241.3192
60652    1307.6544          1340.3424         1378.0371
60653    1397.8501          1410.6696         1436.9972
60654    1453.3899          1468.1320         1473.5487
60655    1487.7716          1512.9633         1981.4142
60656    3047.8084          3084.1857         3094.0974
60657    3153.1408          3164.7608         3172.7243
60658    3702.1181          3721.3864         3727.3377
60659 Zero-point correction (Hartree): 0.157121
60660
60661 triHPacyl.pmpmttpmu
60662 -----
60663 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17563250
60664 Electronic state : 2-A
60665 Cartesian coordinates (Angs):
60666 O       0.297516      -0.624338      1.996953
60667 O       0.413014      -1.368012      0.798625
60668 C      -0.481409     -0.872659     -0.171123
60669 C      -0.251199      0.593122     -0.576190

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60670	C	1.175601	0.971510	-0.951577			
60671	O	2.107567	0.698573	0.081326			
60672	O	2.792347	-0.509147	-0.218485			
60673	H	0.861127	0.148356	1.813730			
60674	C	-0.325810	-1.813348	-1.359484			
60675	H	-0.549661	-2.831383	-1.047688			
60676	H	0.699232	-1.775949	-1.725790			
60677	H	-1.009773	-1.524495	-2.154397			
60678	C	-1.939124	-1.008392	0.337079			
60679	O	-2.883406	-0.572922	-0.200834			
60680	H	2.244951	-1.162278	0.247773			
60681	H	-0.904008	0.780855	-1.433580			
60682	O	-0.694305	1.404591	0.505968			
60683	O	-0.933721	2.702974	-0.019311			
60684	H	-1.896754	2.752639	0.040821			
60685	H	1.501607	0.484890	-1.869688			
60686	H	1.192829	2.052229	-1.097357			
60687	Rotational constants (GHz):				1.1413500	0.8807400	0.6803300
60688	Vibrational harmonic frequencies (cm-1):						
60689		66.2646	73.9510			98.5332	
60690		135.2356	166.6969			182.0089	
60691		207.0828	215.9712			231.9437	
60692		245.5582	254.4181			286.6803	
60693		299.6564	320.2455			367.4461	
60694		398.3059	477.7240			504.1996	
60695		521.9975	556.1785			577.7263	
60696		597.5390	688.6679			823.6590	
60697		854.9157	922.7473			944.0830	
60698		971.9608	1028.2154			1055.1211	
60699		1069.0004	1120.8461			1124.5568	
60700		1142.6952	1182.2631			1257.4806	
60701		1305.0952	1352.1338			1376.3465	
60702		1399.6613	1408.0850			1412.2363	
60703		1459.9720	1470.6150			1477.1413	
60704		1488.9130	1506.6699			1982.4937	
60705		3068.8977	3080.2564			3091.7054	
60706		3143.7415	3159.9798			3169.8530	
60707		3691.6783	3714.6426			3810.2960	
60708	Zero-point correction (Hartree):				0.156150		
60709	triHPacyl.pppppmpmpu						
60710	-----						
60711	-----						
60712	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.17551525		
60713	Electronic state : 2-A						
60714	Cartesian coordinates (Angs):						
60715	O	-2.090333	0.772652	1.018196			
60716	O	-1.208229	-0.313157	1.245167			
60717	C	-0.540611	-0.707796	0.051980			
60718	C	0.484982	0.295970	-0.503529			
60719	C	1.593764	0.670491	0.476012			
60720	O	2.543339	-0.367917	0.626087			
60721	O	3.179965	-0.563437	-0.630955			
60722	H	-2.875600	0.331480	0.658737			
60723	C	0.103198	-2.039466	0.429260			
60724	H	-0.670682	-2.779030	0.624399			
60725	H	0.704899	-1.903634	1.324022			
60726	H	0.749566	-2.385045	-0.374512			
60727	C	-1.557615	-1.013295	-1.064232			
60728	O	-2.727330	-1.008862	-0.974523			
60729	H	4.055545	-0.192743	-0.465642			
60730	H	0.942554	-0.192651	-1.366296			
60731	O	-0.120711	1.447107	-1.060759			
60732	O	-0.273602	2.444760	-0.060471			
60733	H	-1.113619	2.182533	0.351435			
60734	H	2.071620	1.586006	0.126388			
60735	H	1.208631	0.828486	1.482593			
60736	Rotational constants (GHz):				1.3307400	0.7269900	0.5995500
60737	Vibrational harmonic frequencies (cm-1):						
60738		38.0737	59.4784			100.0581	
60739		152.0158	167.9008			196.6737	
60740		217.4844	230.1302			241.5255	
60741		266.5146	267.6939			284.0147	


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60742      319.9187      346.0294      361.0848
60743      391.4501      433.6164      468.2376
60744      528.4099      561.5315      601.3149
60745      618.5578      694.8295      768.3690
60746      856.2959      922.9939      942.8635
60747      979.5383      1036.3923      1048.8941
60748      1102.2826      1114.1946      1134.9706
60749      1146.5628      1187.2900      1247.1419
60750      1289.4751      1337.0763      1388.3593
60751      1394.0928      1414.4542      1422.3631
60752      1427.7136      1460.6542      1474.8793
60753      1481.4975      1500.6206      1975.0672
60754      3085.9326      3087.5043      3099.8921
60755      3150.0162      3167.1565      3179.0080
60756      3688.5191      3751.9684      3820.8552
60757 Zero-point correction (Hartree): 0.156354
60758
60759 triHPacyl.ppppptompu
60760 -----
60761 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17526168
60762 Electronic state : 2-A
60763 Cartesian coordinates (Angs):
60764 O      2.301229      0.841305      -0.891515
60765 O      1.293834      -0.023974      -1.387525
60766 C      0.598952      -0.655643      -0.323317
60767 C      -0.350504      0.256337      0.477395
60768 C      -1.454355      0.894491      -0.364339
60769 O      -2.466072      -0.031110      -0.710073
60770 O      -3.088655      -0.467952      0.492100
60771 H      3.005621      0.223550      -0.642694
60772 C      -0.128629      -1.816969      -0.989680
60773 H      0.594272      -2.545505      -1.351763
60774 H      -0.709619      -1.442965      -1.829318
60775 H      -0.804575      -2.287691      -0.279163
60776 C      1.627908      -1.269037      0.655904
60777 O      1.387918      -1.834898      1.649171
60778 H      -3.944553      -0.025120      0.440292
60779 H      -0.816575      -0.382175      1.230716
60780 O      0.330651      1.229927      1.243484
60781 O      0.549787      2.391950      0.454784
60782 H      1.392260      2.177857      0.022383
60783 H      -1.870009      1.735279      0.192500
60784 H      -1.076583      1.249716      -1.322138
60785 Rotational constants (GHz):      1.1459800      0.7728900      0.6495800
60786 Vibrational harmonic frequencies (cm-1):
60787      40.0260      64.8372      106.4810
60788      137.0110      177.3453      181.4130
60789      202.5944      242.8687      246.3447
60790      264.4674      267.4930      279.3141
60791      298.5486      320.6124      341.8085
60792      375.6076      417.1013      480.3321
60793      526.5273      540.3039      590.3228
60794      623.2765      651.7683      759.6281
60795      856.3221      932.2137      944.2239
60796      977.7619      1037.4918      1048.4025
60797      1095.3087      1115.3455      1131.5624
60798      1143.3770      1180.2860      1246.4686
60799      1290.2037      1334.0860      1385.8139
60800      1395.6379      1412.3838      1415.3492
60801      1420.2985      1456.4440      1473.9821
60802      1481.5867      1499.0566      2001.0137
60803      3082.2635      3084.0287      3101.1883
60804      3148.2388      3163.7446      3173.9522
60805      3717.3417      3755.6270      3824.4316
60806 Zero-point correction (Hartree): 0.155967
60807
60808 triHPacyl.pptmpptompu
60809 -----
60810 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17620193
60811 Electronic state : 2-A
60812 Cartesian coordinates (Angs):
60813 O      -1.428202      0.165078      1.823567

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60814 O -1.594055 -0.898615 0.904135
60815 C -1.084799 -0.519529 -0.356755
60816 C 0.373563 -0.046670 -0.323182
60817 C 1.211017 -0.861222 0.651813
60818 O 2.539371 -0.381982 0.722181
60819 O 3.153800 -0.597682 -0.539704
60820 H -2.220117 0.700124 1.659974
60821 C -1.265629 -1.753893 -1.229675
60822 H -2.308403 -2.064208 -1.209176
60823 H -0.651520 -2.568503 -0.851906
60824 H -0.981016 -1.527735 -2.254320
60825 C -1.936934 0.624040 -0.966050
60826 O -2.840480 1.157880 -0.446138
60827 H 2.994595 0.249905 -0.982997
60828 H 0.761965 -0.137592 -1.339447
60829 O 0.386145 1.333910 0.017842
60830 O 1.590915 1.897416 -0.486751
60831 H 2.126802 1.939992 0.317935
60832 H 0.824516 -0.737693 1.662263
60833 H 1.209925 -1.918697 0.379712
60834 Rotational constants (GHz): 1.4710100 0.6549100 0.6027600
60835 Vibrational harmonic frequencies (cm-1):
60836 68.6890 86.0648 104.5979
60837 141.2432 162.7099 177.0581
60838 198.7719 201.1434 225.2514
60839 238.4169 286.9082 317.4828
60840 342.6597 379.2064 392.2357
60841 405.4242 429.8950 435.7187
60842 475.7519 516.0085 560.2412
60843 603.4082 692.9181 776.8882
60844 895.5188 911.3896 964.1295
60845 991.3443 1029.0684 1060.9648
60846 1084.3379 1122.8729 1139.0170
60847 1163.3282 1191.5281 1254.0578
60848 1300.7733 1332.4310 1389.7490
60849 1411.5865 1417.8440 1426.3847
60850 1432.2579 1440.6631 1469.3669
60851 1486.2102 1502.7593 1982.4077
60852 3076.4467 3085.1434 3090.3944
60853 3153.9340 3165.1050 3173.4324
60854 3745.9062 3760.7405 3789.5439
60855 Zero-point correction (Hartree): 0.156417
60856
60857 triHPacyl.ptmmmtmpmu
60858 -----
60859 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17526869
60860 Electronic state : 2-A
60861 Cartesian coordinates (Angs):
60862 O 2.231923 -1.521662 -0.510550
60863 O 1.547039 -1.093035 0.656160
60864 C 0.947465 0.159354 0.393408
60865 C -0.080732 0.024779 -0.763251
60866 C -1.193542 1.066528 -0.769825
60867 O -2.085579 1.007846 0.319814
60868 O -3.138467 0.114659 -0.002589
60869 H 1.543276 -2.025943 -0.971052
60870 C 0.426344 0.649332 1.738109
60871 H 1.255731 0.681395 2.442357
60872 H -0.351408 -0.011548 2.110152
60873 H 0.001084 1.644837 1.636131
60874 C 2.038092 1.168089 -0.040239
60875 O 1.852700 2.176803 -0.605519
60876 H -2.783953 -0.731652 0.310273
60877 H 0.457876 0.150632 -1.706788
60878 O -0.531573 -1.320398 -0.882679
60879 O -1.137150 -1.752218 0.327122
60880 H -0.370283 -2.048879 0.841682
60881 H -0.730456 2.054888 -0.727906
60882 H -1.758785 0.981820 -1.698129
60883 Rotational constants (GHz): 1.3148600 0.8055900 0.6323600
60884 Vibrational harmonic frequencies (cm-1):
60885 72.7264 93.3327 102.2661

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60886	151.0026	168.1263	208.5052		
60887	228.4836	230.7467	245.2714		
60888	252.9825	274.9072	321.6861		
60889	355.5061	384.8204	420.8022		
60890	460.9042	490.6414	507.7517		
60891	514.1884	532.5340	541.2473		
60892	649.5897	677.8227	823.3676		
60893	846.3480	899.7836	954.3386		
60894	961.4896	1013.2340	1033.8296		
60895	1058.9208	1114.4778	1138.5056		
60896	1158.8363	1186.7081	1246.8484		
60897	1324.3202	1350.1474	1391.0519		
60898	1409.1493	1412.8361	1422.6269		
60899	1437.8508	1451.9732	1466.3963		
60900	1478.9851	1491.7546	1979.0332		
60901	3074.0996	3082.5885	3088.6926		
60902	3132.0051	3169.1671	3181.6904		
60903	3748.7557	3751.8624	3758.9966		
60904	Zero-point correction (Hartree): 0.157026				
60905	triHPacyl.ptmmttmpu				
60906	-----				
60907	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17504777				
60908	Electronic state : 2-A				
60909	Cartesian coordinates (Angs):				
60910	O	-2.002307	1.868404	-0.113922	
60911	O	-1.678207	0.970355	0.933033	
60912	C	-1.082969	-0.175732	0.379618	
60913	C	0.114265	0.193789	-0.524192	
60914	C	1.077772	-0.952382	-0.816491	
60915	O	1.854513	-1.352129	0.296003	
60916	O	2.900481	-0.402400	0.481226	
60917	H	-1.232526	2.457151	-0.098383	
60918	C	-0.778514	-1.061404	1.578529	
60919	H	-1.695647	-1.207953	2.145939	
60920	H	-0.042502	-0.571068	2.211937	
60921	H	-0.390530	-2.025628	1.260908	
60922	C	-2.122952	-0.924723	-0.496063	
60923	O	-1.899545	-1.766711	-1.279459	
60924	H	2.598518	0.062744	1.273668	
60925	H	-0.274631	0.555903	-1.479427	
60926	O	0.763798	1.276810	0.130540	
60927	O	1.692392	1.839678	-0.783397	
60928	H	2.484622	1.305116	-0.609688	
60929	H	0.517764	-1.841655	-1.105374	
60930	H	1.740340	-0.683954	-1.640179	
60931	Rotational constants (GHz): 1.2419900			0.7864300	0.6250400
60932	Vibrational harmonic frequencies (cm-1):				
60933	53.4352	77.7249	90.7709		
60934	144.3522	154.6871	185.6304		
60935	202.5387	224.4275	254.4259		
60936	260.3280	280.1457	306.5388		
60937	319.4808	336.6443	378.7624		
60938	422.0390	445.9937	476.2829		
60939	518.2613	529.1690	578.3558		
60940	639.2432	714.0553	786.3803		
60941	841.6852	892.7185	955.4368		
60942	972.4516	1027.4231	1040.9892		
60943	1065.5874	1105.5401	1137.2032		
60944	1165.7931	1197.5141	1254.7168		
60945	1311.7888	1372.6717	1385.6006		
60946	1400.4270	1408.6269	1411.9447		
60947	1422.4576	1450.6706	1479.9426		
60948	1482.0218	1499.0772	1977.8610		
60949	3073.9624	3085.0038	3088.2425		
60950	3142.8483	3163.8119	3177.6164		
60951	3721.3118	3763.1089	3795.8763		
60952	Zero-point correction (Hartree): 0.156400				
60953	triHPacyl.ptmmpmmpu				
60954	-----				
60955	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17553006				
60956					
60957					

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60958 Electronic state : 2-A
60959 Cartesian coordinates (Angs):
60960 O -2.274848 1.246980 -0.381627
60961 O -1.642483 0.653146 0.743741
60962 C -0.765590 -0.378883 0.308434
60963 C 0.343442 0.199069 -0.590901
60964 C 1.410294 -0.816859 -0.996395
60965 O 2.292774 -1.130427 0.061240
60966 O 3.362771 -0.197897 0.057149
60967 H -3.105736 0.750783 -0.420401
60968 C -0.258622 -1.017778 1.592407
60969 H -1.107947 -1.296116 2.213459
60970 H 0.365544 -0.302329 2.122855
60971 H 0.336555 -1.899099 1.368896
60972 C -1.557499 -1.451556 -0.464320
60973 O -2.722799 -1.522468 -0.563469
60974 H 2.950936 0.593070 0.436827
60975 H -0.111005 0.624017 -1.486992
60976 O 1.006271 1.235150 0.116539
60977 O 0.366734 2.475139 -0.120381
60978 H -0.389194 2.438604 0.485033
60979 H 0.934699 -1.756439 -1.283214
60980 H 1.986631 -0.433440 -1.837354
60981 Rotational constants (GHz): 1.3943900 0.7205800 0.5670400
60982 Vibrational harmonic frequencies (cm-1):
60983 55.1562 72.8237 98.1752
60984 138.0882 152.3839 184.8375
60985 186.1681 213.7238 249.1856
60986 253.5025 285.2241 304.0465
60987 339.6014 368.6190 388.2765
60988 408.2010 432.0651 449.8677
60989 472.1118 505.1739 547.2635
60990 620.7496 733.8627 762.1440
60991 860.0910 910.3478 942.3021
60992 1000.8937 1014.5723 1045.9927
60993 1071.6610 1122.3154 1143.5202
60994 1152.0530 1173.1742 1237.2130
60995 1315.6027 1344.3092 1383.0199
60996 1399.6050 1412.6542 1419.4454
60997 1439.5052 1460.8844 1471.4762
60998 1484.5458 1495.6945 1983.1048
60999 3081.4232 3086.8856 3103.7618
61000 3138.2001 3167.7691 3180.9019
61001 3757.8747 3768.7770 3777.2533
61002 Zero-point correction (Hartree): 0.156210
61003
61004 triHPacyl.ptmmpmpu
61005 -----
61006 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17506500
61007 Electronic state : 2-A
61008 Cartesian coordinates (Angs):
61009 O -2.469775 1.105362 -0.422362
61010 O -1.763714 0.693750 0.741516
61011 C -0.862985 -0.345975 0.384009
61012 C 0.213357 0.200635 -0.581467
61013 C 1.366940 -0.762502 -0.858182
61014 O 2.253092 -0.873955 0.237501
61015 O 3.249026 0.131650 0.130075
61016 H -3.295003 0.607832 -0.334780
61017 C -0.320323 -0.864091 1.706228
61018 H -1.148811 -1.139186 2.355894
61019 H 0.269172 -0.080854 2.178179
61020 H 0.318336 -1.727393 1.539098
61021 C -1.677798 -1.473298 -0.278446
61022 O -1.275496 -2.425702 -0.826874
61023 H 2.770051 0.928171 0.404282
61024 H -0.262400 0.480477 -1.522151
61025 O 0.786715 1.362622 0.000224
61026 O 0.070987 2.516260 -0.396846
61027 H -0.680543 2.512721 0.214852
61028 H 0.983132 -1.765512 -1.043147
61029 H 1.924245 -0.424760 -1.730957

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61030 Rotational constants (GHz): 1.202000 0.8124700 0.5945900
61031 Vibrational harmonic frequencies (cm-1):
61032 55.3306 73.5375 96.7532
61033 146.2532 153.0927 173.2586
61034 192.2639 206.5720 244.4363
61035 254.8348 275.2308 291.5578
61036 315.1717 336.4132 368.6424
61037 422.8658 437.7119 451.1732
61038 493.2582 505.2584 548.4003
61039 626.8214 678.4215 768.1101
61040 861.1657 908.9233 945.5735
61041 1001.8132 1010.5577 1045.0987
61042 1071.7050 1118.4294 1141.3797
61043 1145.0095 1175.0921 1232.6132
61044 1316.8287 1341.7807 1376.5066
61045 1402.1739 1404.3426 1410.2329
61046 1435.0180 1460.3558 1475.5295
61047 1481.5584 1495.4169 1991.7276
61048 3085.0819 3092.9549 3108.2070
61049 3149.3962 3165.3273 3178.7423
61050 3760.5064 3772.7416 3788.4309
61051 Zero-point correction (Hartree): 0.155976
61052
61053 triHPacyl.ptppmmmpmu
61054 -----
61055 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17585716
61056 Electronic state : 2-A
61057 Cartesian coordinates (Angs):
61058 O 1.871105 1.012079 -1.192655
61059 O 1.652998 0.893118 0.206109
61060 C 0.307648 0.519993 0.424194
61061 C 0.020177 -0.870275 -0.162903
61062 C -1.307494 -1.475433 0.301266
61063 O -2.388132 -0.580095 0.227710
61064 O -2.680208 -0.377344 -1.147429
61065 H 2.151861 0.111712 -1.424076
61066 C 0.097174 0.605583 1.924745
61067 H 0.469087 1.563410 2.280798
61068 H 0.638054 -0.203570 2.414055
61069 H -0.962564 0.525665 2.159751
61070 C -0.602712 1.600925 -0.252603
61071 O -0.487059 2.754488 -0.124678
61072 H -2.310069 0.510049 -1.290210
61073 H 0.049102 -0.828664 -1.252830
61074 O 0.970045 -1.816675 0.296934
61075 O 2.168616 -1.702574 -0.461582
61076 H 2.766377 -1.310420 0.190272
61077 H -1.514126 -2.375085 -0.277968
61078 H -1.235397 -1.741840 1.356744
61079 Rotational constants (GHz): 1.0816500 0.8845300 0.6362600
61080 Vibrational harmonic frequencies (cm-1):
61081 50.7484 95.8876 102.4304
61082 133.8423 172.9774 180.2562
61083 198.8607 225.0416 244.7781
61084 263.9778 278.3890 316.5235
61085 337.9251 358.8883 392.0018
61086 402.6687 434.4791 441.0057
61087 505.7543 547.2571 579.6025
61088 618.8064 673.1656 737.3098
61089 848.1665 938.5928 959.4171
61090 1009.2205 1017.1254 1047.5029
61091 1102.4569 1122.4334 1140.0368
61092 1164.8587 1194.1463 1265.9746
61093 1294.5265 1342.8838 1387.1360
61094 1405.3563 1415.1701 1416.4477
61095 1438.2271 1445.2644 1483.3063
61096 1495.8449 1504.5957 2002.8087
61097 3078.0103 3085.7732 3097.2684
61098 3139.4639 3159.0709 3169.8019
61099 3668.4665 3720.8515 3793.6291
61100 Zero-point correction (Hartree): 0.156388
61101

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61102 triHPacyl.ptppmtpmu
61103 -----
61104 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17640935
61105 Electronic state : 2-A
61106 Cartesian coordinates (Angs):
61107 O 2.012125 1.217478 -0.983744
61108 O 1.814778 0.850591 0.374382
61109 C 0.439429 0.572902 0.565553
61110 C 0.039492 -0.719346 -0.190082
61111 C -1.254219 -1.363583 0.317244
61112 O -2.340264 -0.476986 0.384999
61113 O -2.850427 -0.328290 -0.932370
61114 H 2.172411 0.354467 -1.400135
61115 C 0.254189 0.478510 2.067679
61116 H 0.700950 1.351264 2.537532
61117 H 0.742631 -0.422369 2.437220
61118 H -0.805353 0.443138 2.314993
61119 C -0.314693 1.824196 0.044528
61120 O -1.174561 1.900918 -0.747420
61121 H -2.533479 0.558986 -1.159688
61122 H -0.027858 -0.525410 -1.262294
61123 O 0.988153 -1.745876 0.049108
61124 O 2.121635 -1.574501 -0.792092
61125 H 2.796714 -1.331111 -0.142961
61126 H -1.498877 -2.215654 -0.315480
61127 H -1.103833 -1.716044 1.338379
61128 Rotational constants (GHz): 1.2356300 0.8065400 0.6591300
61129 Vibrational harmonic frequencies (cm-1):
61130 66.6736 75.1259 96.6991
61131 154.1442 183.1370 204.2090
61132 214.3571 239.4550 248.7097
61133 267.3623 278.9892 324.6101
61134 359.0897 365.6152 398.6370
61135 411.9344 455.9135 513.1303
61136 517.4093 550.8675 580.5619
61137 610.7258 657.5071 721.9628
61138 859.4426 941.2603 957.9680
61139 1008.3047 1022.4373 1051.3320
61140 1096.9202 1126.9074 1148.4176
61141 1162.7902 1191.4911 1251.4122
61142 1297.2888 1337.1726 1376.5023
61143 1406.0188 1412.1341 1416.6141
61144 1448.6014 1450.4096 1481.2708
61145 1496.8679 1502.9773 1984.8491
61146 3077.6530 3089.2917 3094.2253
61147 3143.1467 3158.3722 3169.2167
61148 3719.8607 3756.9429 3790.5146
61149 Zero-point correction (Hartree): 0.157024
61150
61151 triHPacyl.ptppmtpmu
61152 -----
61153 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17823460
61154 Electronic state : 2-A
61155 Cartesian coordinates (Angs):
61156 O 2.138150 1.182054 -1.061810
61157 O 1.901117 0.770776 0.276220
61158 C 0.509296 0.594903 0.444372
61159 C 0.002223 -0.550793 -0.486704
61160 C -1.112100 -1.410186 0.101052
61161 O -2.245157 -0.652670 0.454017
61162 O -2.884527 -0.251866 -0.750879
61163 H 2.228340 0.329212 -1.515988
61164 C 0.304428 0.381851 1.937692
61165 H 0.739270 1.218987 2.479582
61166 H 0.791641 -0.540475 2.247876
61167 H -0.757925 0.317294 2.162536
61168 C -0.189111 1.925399 0.086789
61169 O -1.281292 2.077792 -0.311720
61170 H -2.685821 0.696596 -0.761701
61171 H -0.347867 -0.119118 -1.426405
61172 O 1.082432 -1.366353 -0.906095
61173 O 1.637652 -2.021139 0.227745

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61174      H      2.323892      -1.390507      0.494101
61175      H      -1.378941      -2.180647      -0.623361
61176      H      -0.787992      -1.887137      1.024336
61177      Rotational constants (GHz):      1.2183800      0.8503700      0.6572900
61178      Vibrational harmonic frequencies (cm-1):
61179      83.1551      96.8043      122.0636
61180      155.4712      169.3698      183.3072
61181      202.1076      233.4693      254.2132
61182      262.0789      284.2983      332.5249
61183      365.8771      395.7620      443.0498
61184      454.2778      467.1816      479.5432
61185      517.0436      526.2776      561.5602
61186      605.3518      655.8165      780.6361
61187      849.4782      940.0236      954.3644
61188      976.6903      1022.3824      1056.2848
61189      1097.9023      1122.3356      1132.4504
61190      1156.7257      1190.5356      1242.9162
61191      1286.7002      1344.1197      1376.8226
61192      1402.9134      1413.0154      1430.8937
61193      1443.0370      1443.8722      1486.6261
61194      1495.9667      1506.1751      1978.5976
61195      3083.4597      3089.4152      3098.6572
61196      3153.5974      3165.7781      3171.9032
61197      3739.0765      3758.6383      3762.6010
61198      Zero-point correction (Hartree): 0.157205
61199
61200      triHPacyl.ptppppmpmu
61201      -----
61202      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17635499
61203      Electronic state : 2-A
61204      Cartesian coordinates (Angs):
61205      O      2.117578      0.713946      -0.984239
61206      O      1.770949      0.548193      0.384606
61207      C      0.359285      0.431666      0.502292
61208      C      -0.141005      -0.842350      -0.213021
61209      C      -1.561022      -1.262078      0.174586
61210      O      -2.496963      -0.214625      0.221349
61211      O      -2.721399      0.209883      -1.117104
61212      H      2.225197      1.674448      -1.040551
61213      C      0.095768      0.416759      2.000037
61214      H      0.591640      1.264442      2.468102
61215      H      0.492828      -0.508598      2.414313
61216      H      -0.973537      0.475516      2.190226
61217      C      -0.298151      1.697784      -0.082710
61218      O      0.240024      2.705939      -0.341676
61219      H      -2.360001      1.108026      -1.088725
61220      H      -0.043160      -0.725919      -1.291606
61221      O      0.642143      -1.941923      0.208319
61222      O      1.746477      -2.114875      -0.660125
61223      H      2.390030      -1.482421      -0.309116
61224      H      -1.894424      -2.044175      -0.507436
61225      H      -1.548291      -1.664319      1.188645
61226      Rotational constants (GHz):      1.0791400      0.8784000      0.6330400
61227      Vibrational harmonic frequencies (cm-1):
61228      64.7362      88.9676      95.9689
61229      137.6791      166.9140      171.2400
61230      193.8635      218.7045      237.7625
61231      267.2699      286.2969      309.6557
61232      328.8651      357.0511      388.0632
61233      395.8885      415.1590      433.6905
61234      441.3675      505.4894      545.7719
61235      617.1758      697.6357      756.1445
61236      852.6770      932.6543      958.2579
61237      1006.3830      1025.8866      1044.8792
61238      1102.6081      1126.6117      1145.7228
61239      1157.0572      1189.6664      1237.8771
61240      1292.6454      1337.9443      1384.4235
61241      1401.7649      1410.2815      1417.4898
61242      1425.4382      1433.0586      1481.5280
61243      1497.5325      1502.4858      1979.0543
61244      3081.2265      3085.3034      3117.6748
61245      3139.2441      3163.5219      3171.7952

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61246          3749.4697          3785.1770          3788.7677
61247 Zero-point correction (Hartree): 0.156163
61248
61249 triHPacyl.ptppptpmu
61250 -----
61251 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17584534
61252 Electronic state : 2-A
61253 Cartesian coordinates (Angs):
61254 O      2.184219      1.104994      -1.076067
61255 O      1.929273      0.708857      0.264065
61256 C      0.532826      0.549606      0.418554
61257 C     -0.000367     -0.579121     -0.520769
61258 C     -1.156786     -1.388068      0.063443
61259 O     -2.261048     -0.599777      0.440703
61260 O     -2.897702     -0.157549     -0.751391
61261 H      2.335728      2.054234     -0.967226
61262 C      0.317923      0.335115      1.911379
61263 H      0.755194      1.165470      2.462379
61264 H      0.799678     -0.592004      2.214134
61265 H     -0.745994      0.276991      2.128626
61266 C     -0.132437      1.894051      0.058872
61267 O     -1.254906      2.111049     -0.197661
61268 H     -2.699801      0.789913     -0.726509
61269 H     -0.313001     -0.136734     -1.468117
61270 O      1.032395     -1.451622     -0.914816
61271 O      1.573491     -2.074932      0.244329
61272 H      2.357102     -1.525553      0.389843
61273 H     -1.458012     -2.135917     -0.670766
61274 H     -0.843631     -1.894062      0.975463
61275 Rotational constants (GHz):      1.2130800      0.8498600      0.6497200
61276 Vibrational harmonic frequencies (cm-1):
61277      75.0033      98.4454      123.8750
61278      157.0583      166.3947      184.4503
61279      187.0853      227.8153      253.0629
61280      267.8471      280.9051      312.2864
61281      333.2349      354.5215      382.3606
61282      433.7054      439.2447      452.1728
61283      468.1870      518.3144      555.7820
61284      605.0961      657.5746      779.0298
61285      840.2489      940.2502      954.7351
61286      977.4129      1017.9799      1054.4967
61287      1097.0892      1124.4885      1133.8834
61288      1148.8398      1188.7294      1237.5044
61289      1286.2918      1339.1903      1381.4161
61290      1400.2469      1414.3070      1416.2900
61291      1427.3364      1438.5322      1486.7964
61292      1496.1384      1507.2730      1985.3479
61293      3084.6960      3090.5733      3102.3852
61294      3151.4815      3165.7948      3176.5697
61295      3774.6978      3783.0571      3791.8563
61296 Zero-point correction (Hartree): 0.156577
61297
61298 triHPacyl.pttpmtpmu
61299 -----
61300 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17524711
61301 Electronic state : 2-A
61302 Cartesian coordinates (Angs):
61303 O      -2.203296      1.144991     -1.022873
61304 O     -1.919351      0.863087      0.338137
61305 C     -1.084197     -0.276348      0.391102
61306 C      0.297939      0.035714     -0.222669
61307 C      1.346415     -1.039944      0.039922
61308 O      2.535542     -0.763986     -0.664319
61309 O      3.374129      0.041185      0.150000
61310 H     -1.487993      1.760088     -1.252544
61311 C     -1.021942     -0.657336      1.861579
61312 H     -2.031486     -0.714338      2.261950
61313 H     -0.458090      0.097755      2.407324
61314 H     -0.537158     -1.624029      1.983763
61315 C     -1.786641     -1.424589     -0.368231
61316 O     -1.289217     -2.375134     -0.837663
61317 H      2.982598      0.920059      0.045111

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61318	H	0.210348	0.177480	-1.301477		
61319	O	0.837102	1.225130	0.348311		
61320	O	0.243565	2.367838	-0.256578		
61321	H	-0.366985	2.653459	0.438238		
61322	H	1.570598	-1.125804	1.103577		
61323	H	0.980927	-1.994549	-0.336289		
61324	Rotational constants (GHz):			1.2188700	0.7511400	0.5763200
61325	Vibrational harmonic frequencies (cm-1):					
61326		51.7210		74.7217		105.8846
61327		134.3771		161.6016		181.9573
61328		204.3162		223.6841		243.6885
61329		252.3745		277.8960		300.8269
61330		342.6164		352.2423		388.9810
61331		391.8726		417.7276		510.1845
61332		512.9962		552.1121		573.5689
61333		587.4608		646.3099		786.1270
61334		878.3427		890.9764		957.7289
61335		976.7690		1043.7796		1052.4348
61336		1104.9742		1119.2558		1133.3632
61337		1163.2909		1178.7078		1246.8768
61338		1311.2338		1332.9208		1377.9590
61339		1406.2120		1409.9304		1420.8237
61340		1444.1565		1449.7193		1472.0144
61341		1492.4169		1498.4599		1984.5195
61342		3079.3144		3088.1871		3097.7416
61343		3152.1680		3160.4473		3168.8830
61344		3727.9238		3784.5796		3787.1204
61345	Zero-point correction (Hartree): 0.156438					
61346	triHPacyl.pttpmtppmu					
61347	-----					
61348	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17641335					
61349	Electronic state : 2-A					
61350	Cartesian coordinates (Angs):					
61351	O	1.916565	-1.429207	-1.273679		
61352	O	1.830498	-1.183373	0.120660		
61353	C	1.191789	0.048052	0.315678		
61354	C	-0.199379	0.072608	-0.374244		
61355	C	-1.160592	1.076398	0.243076		
61356	O	-2.367716	1.171089	-0.485920		
61357	O	-3.180366	0.049448	-0.147907		
61358	H	1.148405	-2.004662	-1.404817		
61359	C	1.200643	0.259880	1.823635		
61360	H	2.225367	0.190870	2.183562		
61361	H	0.599078	-0.511492	2.297781		
61362	H	0.808149	1.243514	2.074271		
61363	C	2.041059	1.188591	-0.305501		
61364	O	1.677524	2.285803	-0.500305		
61365	H	-3.121460	-0.480045	-0.954506		
61366	H	-0.064024	0.332335	-1.426254		
61367	O	-0.759429	-1.227647	-0.464696		
61368	O	-1.105689	-1.689100	0.831954		
61369	H	-2.022726	-1.376651	0.900598		
61370	H	-1.382358	0.843417	1.284722		
61371	H	-0.722652	2.073429	0.187928		
61372	Rotational constants (GHz):			1.2941800	0.7460900	0.6032100
61373	Vibrational harmonic frequencies (cm-1):					
61374		64.5003		84.1178		111.2335
61375		137.9867		167.2280		174.0304
61376		206.2881		222.2497		244.4400
61377		262.2436		289.7450		319.5563
61378		335.2540		368.1821		383.8394
61379		399.9086		460.7174		485.4179
61380		508.0664		557.7571		571.7276
61381		620.4111		669.8844		807.6507
61382		851.2148		911.6911		952.1325
61383		971.1550		1006.9586		1056.0540
61384		1092.8330		1112.1959		1138.7837
61385		1161.3817		1187.8482		1257.9583
61386		1304.8991		1324.3498		1395.8881
61387		1403.8951		1408.2512		1418.8392
61388		1430.2060		1452.4342		1479.0984

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61390      1493.5868          1502.6238          1974.3520
61391      3083.4978          3088.9476          3096.5328
61392      3145.9952          3161.8939          3177.5322
61393      3719.8551          3774.9704          3805.2204
61394 Zero-point correction (Hartree): 0.156728
61395
61396 triHPacyl.pttppmmpmu
61397 -----
61398 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17609974
61399 Electronic state : 2-A
61400 Cartesian coordinates (Angs):
61401 O      -2.005765          1.285502          -0.909128
61402 O      -1.767219          0.857758          0.423519
61403 C      -0.949635          -0.305135          0.412156
61404 C      0.417789          -0.007987          -0.231901
61405 C      1.386228          -1.181589          -0.153464
61406 O      2.573419          -0.897198          -0.855652
61407 O      3.477456          -0.248248          0.025867
61408 H      -2.850968          0.853803          -1.103095
61409 C      -0.847536          -0.714860          1.873964
61410 H      -1.843135          -0.755455          2.311018
61411 H      -0.244746          0.017533          2.407026
61412 H      -0.385378          -1.695638          1.960342
61413 C      -1.654972          -1.442429          -0.349862
61414 O      -2.741166          -1.422548          -0.787964
61415 H      3.116685          0.649779          0.067299
61416 H      0.284243          0.280623          -1.275032
61417 O      1.029316          1.073446          0.454736
61418 O      0.620244          2.301639          -0.124412
61419 H      -0.251912          2.442708          0.272812
61420 H      1.631689          -1.433065          0.879136
61421 H      0.942002          -2.051096          -0.640585
61422 Rotational constants (GHz): 1.4017700      0.6593100      0.5532100
61423 Vibrational harmonic frequencies (cm-1):
61424      63.7410          65.7101          94.3279
61425      125.3129          152.7529          182.6072
61426      185.8213          216.8110          234.8824
61427      260.3468          285.1969          306.8939
61428      328.0163          367.6620          396.3534
61429      406.6408          415.7612          442.8703
61430      451.4944          519.8227          533.8427
61431      584.3864          709.1862          777.6604
61432      877.5855          884.9855          956.5386
61433      976.3636          1044.2917          1052.8358
61434      1104.0015          1128.2833          1134.1464
61435      1158.5920          1177.9368          1235.7194
61436      1307.4788          1325.5562          1380.7581
61437      1408.1771          1410.9665          1421.3208
61438      1436.4210          1451.5038          1470.2877
61439      1491.2264          1498.3393          1984.0387
61440      3076.4168          3083.9687          3107.9733
61441      3133.6218          3165.9723          3170.9056
61442      3769.4586          3775.4602          3777.8585
61443 Zero-point correction (Hartree): 0.156025
61444
61445 triHPacyl.pttptmpmu
61446 -----
61447 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17554164
61448 Electronic state : 2-A
61449 Cartesian coordinates (Angs):
61450 O      -2.116437          1.307106          -0.995886
61451 O      -1.877078          0.932587          0.353974
61452 C      -1.077267          -0.240598          0.365746
61453 C      0.316145          0.057432          -0.232574
61454 C      1.318218          -1.075438          -0.045921
61455 O      2.523902          -0.784192          -0.714897
61456 O      3.370578          -0.059141          0.164255
61457 H      -2.989484          0.920587          -1.153437
61458 C      -1.031363          -0.666570          1.824973
61459 H      -2.041383          -0.723707          2.224812
61460 H      -0.460181          0.068196          2.389865
61461 H      -0.558331          -1.641950          1.915542

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61462	C	-1.811743	-1.330675	-0.438182	
61463	O	-1.423109	-2.398647	-0.715931	
61464	H	2.975122	0.824876	0.149901	
61465	H	0.225703	0.292171	-1.293475	
61466	O	0.865775	1.188424	0.429230	
61467	O	0.471257	2.376739	-0.235214	
61468	H	-0.413930	2.533374	0.125186	
61469	H	1.528753	-1.252690	1.009453	
61470	H	0.930695	-1.988781	-0.496344	
61471	Rotational constants (GHz):		1.2152200	0.7483200	0.5690300
61472	Vibrational harmonic frequencies (cm-1):				
61473		55.6953	69.5233		98.8098
61474		130.5448	154.4106		170.8350
61475		186.9787	215.0541		240.1068
61476		254.4848	283.1137		285.8529
61477		304.3992	342.5396		371.3104
61478		393.2519	416.6297		442.6661
61479		501.4803	513.8684		552.0809
61480		576.6740	649.1284		784.1247
61481		880.1088	886.0436		953.4491
61482		974.1961	1043.5779		1052.9795
61483		1104.7141	1122.0594		1131.7286
61484		1152.4086	1175.7403		1232.3184
61485		1307.7372	1329.5468		1378.0374
61486		1404.9304	1408.2094		1412.5652
61487		1431.1522	1449.7141		1471.5190
61488		1490.3398	1498.3150		1993.9310
61489		3081.0746	3085.5720		3112.7490
61490		3145.8769	3165.0307		3169.3909
61491		3772.0532	3777.9651		3787.6738
61492	Zero-point correction (Hartree): 0.155773				
61493					
61494	triHPacyl.tmmmmmpmpu				
61495	-----				
61496	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17405004				
61497	Electronic state : 2-A				
61498	Cartesian coordinates (Angs):				
61499	O	-2.807501	-0.898332	-0.480114	
61500	O	-1.513910	-0.574601	-0.950151	
61501	C	-0.925479	0.399061	-0.111761	
61502	C	0.367567	0.797681	-0.854545	
61503	C	1.191180	-0.399622	-1.311922	
61504	O	1.384319	-1.352808	-0.283661	
61505	O	2.726912	-1.309748	0.165477	
61506	H	-2.618301	-1.625891	0.131852	
61507	C	-1.821948	1.607011	0.123800	
61508	H	-2.692095	1.336120	0.714978	
61509	H	-2.155484	1.978721	-0.844282	
61510	H	-1.261218	2.386215	0.635171	
61511	C	-0.620279	-0.207289	1.278032	
61512	O	-1.119578	-1.151692	1.757005	
61513	H	2.738420	-0.481878	0.672785	
61514	H	0.050869	1.343022	-1.747659	
61515	O	1.085460	1.788238	-0.140330	
61516	O	1.844801	1.215989	0.915672	
61517	H	1.189630	1.114787	1.626053	
61518	H	0.642468	-0.902007	-2.108489	
61519	H	2.155449	-0.066504	-1.693228	
61520	Rotational constants (GHz):		1.3323600	0.7642900	0.6777600
61521	Vibrational harmonic frequencies (cm-1):				
61522		50.5379	71.1206		121.2098
61523		138.1855	164.7003		197.9858
61524		207.6809	216.9951		225.0251
61525		249.3744	287.6121		303.5572
61526		332.1536	358.3543		388.1343
61527		400.0789	450.5760		491.9573
61528		504.7606	538.7988		571.4958
61529		606.9915	704.4655		808.4392
61530		836.4522	911.1310		954.0367
61531		962.7904	1022.7735		1051.0625
61532		1055.9039	1130.8355		1136.7449
61533		1155.8256	1191.3099		1240.2347

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61534      1300.0094      1347.0186      1373.2714
61535      1399.9260      1405.8133      1438.3322
61536      1443.2172      1459.1525      1470.2455
61537      1484.3917      1499.3770      1982.3130
61538      3081.3616      3082.8834      3092.3857
61539      3145.2277      3162.8392      3179.0257
61540      3695.9494      3716.0193      3762.6948
61541 Zero-point correction (Hartree): 0.156193
61542
61543 triHPacyl.tmmmmppmu
61544 -----
61545 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17343674
61546 Electronic state : 2-A
61547 Cartesian coordinates (Angs):
61548 O      3.045535      -0.524499      0.401494
61549 O      1.776243      -0.282425      0.974997
61550 C      0.931255      0.379720      0.035923
61551 C     -0.353436      0.581066      0.870308
61552 C     -1.094499     -0.713211      1.192235
61553 O     -1.687158     -1.355486      0.079538
61554 O     -2.938651     -0.705787     -0.159476
61555 H      2.900764     -1.371819     -0.046407
61556 C      1.513185      1.695822     -0.444026
61557 H      2.480068      1.522451     -0.909322
61558 H      1.642375      2.356473      0.412057
61559 H      0.837930      2.157834     -1.158173
61560 C      0.695312     -0.545999     -1.177590
61561 O      1.175005     -1.607249     -1.335931
61562 H     -3.469515     -1.449427     -0.468491
61563 H      0.000943      0.972544      1.828980
61564 O     -1.178167      1.617620      0.392827
61565 O     -1.454096      1.428399     -0.987428
61566 H     -2.218589      0.829263     -0.966753
61567 H     -0.375033     -1.439853      1.572775
61568 H     -1.859534     -0.526448      1.946067
61569 Rotational constants (GHz): 1.4343800      0.7406700      0.6408600
61570 Vibrational harmonic frequencies (cm-1):
61571 47.9369      79.3881      96.0146
61572 141.2411      166.1440      184.4732
61573 194.2754      213.1766      228.5071
61574 251.1060      259.8767      294.7467
61575 315.6625      330.7611      364.6742
61576 412.5736      447.8470      470.4191
61577 505.8712      531.4688      563.9978
61578 620.1113      728.6614      817.4467
61579 848.4869      909.3891      950.6811
61580 959.6928      1009.6040      1043.8065
61581 1055.7739      1122.0691      1147.6008
61582 1158.4566      1201.2352      1232.0261
61583 1308.2005      1352.1901      1384.6640
61584 1398.0369      1410.1632      1420.3776
61585 1441.1128      1458.9517      1475.3313
61586 1487.3002      1501.7579      1957.8825
61587 3069.8950      3082.5273      3087.4874
61588 3137.6477      3166.7233      3189.5135
61589 3705.5481      3760.5097      3842.7517
61590 Zero-point correction (Hartree): 0.156154
61591
61592 triHPacyl.tmmmmpppu
61593 -----
61594 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17368528
61595 Electronic state : 2-A
61596 Cartesian coordinates (Angs):
61597 O      2.944499      -0.346042      0.497542
61598 O      1.645714      -0.150072      1.017691
61599 C      0.788129      0.412417      0.032434
61600 C     -0.470488      0.742705      0.858645
61601 C     -1.228285     -0.482914      1.378669
61602 O     -1.325979     -1.589492      0.510311
61603 O     -2.307977     -1.321227     -0.483016
61604 H      2.861273     -1.207509      0.060610
61605 C      1.360975      1.650589     -0.637329

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61606	H	2.298886	1.407895	-1.128458			
61607	H	1.538696	2.408435	0.124300			
61608	H	0.650423	2.035248	-1.364230			
61609	C	0.543277	-0.640129	-1.076130			
61610	O	1.280352	-1.500264	-1.385484			
61611	H	-1.752213	-1.251353	-1.276301			
61612	H	-0.096032	1.262184	1.745068			
61613	O	-1.283801	1.740495	0.281116			
61614	O	-1.714269	1.357567	-1.015073			
61615	H	-2.473907	0.787271	-0.822657			
61616	H	-0.675275	-0.889718	2.225634			
61617	H	-2.221810	-0.176178	1.713597			
61618	Rotational constants (GHz):				1.2786200	0.8100800	0.6906200
61619	Vibrational harmonic frequencies (cm-1):						
61620		64.8722		106.0827		120.1766	
61621		140.4933		171.1402		181.2671	
61622		201.7174		223.8622		226.0565	
61623		236.9506		252.2600		296.7411	
61624		318.5306		356.2081		374.3496	
61625		404.5575		421.6622		453.6693	
61626		524.5497		549.7979		568.0739	
61627		616.3696		709.6688		789.8747	
61628		834.5318		904.2339		949.9092	
61629		981.1702		1022.3662		1052.5710	
61630		1060.1002		1129.6232		1136.4984	
61631		1157.9229		1199.1659		1243.9435	
61632		1305.3173		1358.2294		1387.2658	
61633		1402.0704		1410.3841		1436.1730	
61634		1448.4896		1457.3062		1471.2833	
61635		1485.4754		1497.8505		1962.1135	
61636		3070.3081		3080.2724		3087.5959	
61637		3133.5042		3168.8495		3186.8257	
61638		3723.2596		3753.9514		3757.7217	
61639	Zero-point correction (Hartree):				0.156203		
61640							
61641	triHPacyl.tmmmmmtmmu						
61642	-----						
61643	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17468198						
61644	Electronic state : 2-A						
61645	Cartesian coordinates (Angs):						
61646	O	3.033618	-0.187423	0.704395			
61647	O	1.675996	-0.019956	1.060347			
61648	C	0.934083	0.450393	-0.054892			
61649	C	-0.456718	0.729372	0.535914			
61650	C	-1.079930	-0.486112	1.208905			
61651	O	-1.309054	-1.554202	0.311189			
61652	O	-2.497148	-1.262263	-0.423659			
61653	H	3.024838	-1.071194	0.305065			
61654	C	1.536960	1.695857	-0.686717			
61655	H	2.526364	1.479216	-1.079630			
61656	H	1.619663	2.466908	0.078303			
61657	H	0.893058	2.047901	-1.487894			
61658	C	0.862789	-0.640744	-1.147923			
61659	O	1.558427	-1.584641	-1.216270			
61660	H	-3.019373	-2.053139	-0.243201			
61661	H	-0.336586	1.512248	1.293286			
61662	O	-1.221227	1.218053	-0.545719			
61663	O	-2.502884	1.571266	-0.059716			
61664	H	-3.004602	0.775307	-0.293579			
61665	H	-0.379775	-0.884138	1.942617			
61666	H	-2.008535	-0.212377	1.708773			
61667	Rotational constants (GHz):				1.4285000	0.7202800	0.6095000
61668	Vibrational harmonic frequencies (cm-1):						
61669		39.6904		67.3235		111.0677	
61670		158.0203		164.8647		177.9145	
61671		194.1699		212.6380		222.3694	
61672		238.3547		250.2756		288.8544	
61673		312.7267		346.7370		381.5181	
61674		398.6353		440.7173		449.8899	
61675		489.3643		510.4897		557.7076	
61676		658.6610		715.5091		778.0853	
61677		871.4632		900.5265		926.3508	

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61678          982.9400          1037.2957          1051.3456
61679          1064.4977          1115.7163          1147.4951
61680          1162.0428          1206.0085          1245.2887
61681          1295.1882          1368.5630          1378.0061
61682          1395.1262          1404.9802          1420.4836
61683          1447.6582          1452.6119          1470.7626
61684          1487.1204          1498.7254          1965.2529
61685          3048.6462          3085.1938          3095.3247
61686          3149.1310          3166.5650          3184.6194
61687          3748.0161          3763.2780          3833.3310
61688 Zero-point correction (Hartree): 0.156135
61689
61690 triHPacyl.tmmmmmtmpu
61691 -----
61692 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17889956
61693 Electronic state : 2-A
61694 Cartesian coordinates (Angs):
61695 O          3.002804          -0.033125          0.707298
61696 O          1.641553          0.075833          1.070153
61697 C          0.865619          0.471225          -0.046324
61698 C          -0.522266          0.739139          0.552227
61699 C          -1.100973          -0.467032          1.278712
61700 O          -1.188144          -1.621623          0.469373
61701 O          -2.233271          -1.426900          -0.478650
61702 H          3.044802          -0.934912          0.353399
61703 C          1.420476          1.690622          -0.767227
61704 H          2.409207          1.477975          -1.162975
61705 H          1.490594          2.510280          -0.053186
61706 H          0.753368          1.975276          -1.576341
61707 C          0.800603          -0.686399          -1.077566
61708 O          1.609937          -1.523471          -1.218172
61709 H          -1.730360          -1.185391          -1.272626
61710 H          -0.424556          1.559798          1.270629
61711 O          -1.309372          1.161094          -0.550013
61712 O          -2.619801          1.432706          -0.093444
61713 H          -3.049481          0.573592          -0.235651
61714 H          -0.426774          -0.750999          2.085828
61715 H          -2.077202          -0.227048          1.699639
61716 Rotational constants (GHz):          1.4154400          0.7396400          0.6329500
61717 Vibrational harmonic frequencies (cm-1):
61718          57.9096          90.9178          124.0962
61719          152.2674          161.5417          170.8689
61720          209.4655          229.4758          231.5950
61721          254.6016          298.9025          322.3421
61722          346.4184          378.9676          394.5774
61723          421.8280          429.4487          458.1855
61724          480.4725          548.2852          556.2235
61725          657.0244          702.6349          787.2861
61726          868.5727          899.7495          934.3953
61727          977.1476          1038.7172          1050.7246
61728          1065.3092          1119.4505          1142.4349
61729          1162.9652          1205.1486          1244.5346
61730          1292.3914          1365.1339          1379.4867
61731          1402.9335          1408.4752          1430.3742
61732          1447.5063          1451.1716          1479.7855
61733          1486.8526          1498.5764          1971.4402
61734          3055.6519          3086.6807          3095.8784
61735          3149.0160          3168.2047          3186.4359
61736          3733.1585          3743.4599          3756.8396
61737 Zero-point correction (Hartree): 0.156656
61738
61739 triHPacyl.tmmmmmtmpu
61740 -----
61741 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17459318
61742 Electronic state : 2-A
61743 Cartesian coordinates (Angs):
61744 O          -2.903825          -0.930500          -0.333207
61745 O          -1.689211          -0.540545          -0.944121
61746 C          -0.904564          0.184477          -0.015059
61747 C          0.370662          0.513214          -0.824085
61748 C          1.074424          -0.737537          -1.339438
61749 O          1.289371          -1.718875          -0.351755

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61750	O	2.405528	-1.327043	0.429803		
61751	H	-2.658449	-1.775329	0.071685		
61752	C	-1.617154	1.417202	0.518626		
61753	H	-2.532230	1.122838	1.025607		
61754	H	-1.863923	2.071425	-0.316221		
61755	H	-0.968799	1.947552	1.210951		
61756	C	-0.581736	-0.719726	1.192826		
61757	O	0.143011	-0.479844	2.084898		
61758	H	1.988267	-0.907155	1.199509		
61759	H	0.060233	1.109359	-1.686692		
61760	O	1.293948	1.256495	-0.057401		
61761	O	0.927674	2.633927	-0.123065		
61762	H	1.742323	3.017174	-0.470873		
61763	H	0.428619	-1.220648	-2.071338		
61764	H	2.022216	-0.459921	-1.801075		
61765	Rotational constants (GHz):			1.1106700	0.8621600	0.6918100
61766	Vibrational harmonic frequencies (cm-1):					
61767		59.8887	100.6685			126.6738
61768		134.3151	172.9711			180.0753
61769		192.1954	208.9511			220.6379
61770		239.3347	269.9268			286.5019
61771		298.0133	327.1451			371.3592
61772		385.9080	407.9915			437.4619
61773		462.8773	477.6518			498.3831
61774		630.3137	678.6819			783.9581
61775		874.7808	915.7539			930.2318
61776		991.0576	1023.9763			1050.2263
61777		1064.6712	1125.4060			1141.6223
61778		1167.6436	1198.1017			1224.5114
61779		1304.1775	1340.3221			1364.7140
61780		1401.4922	1406.7253			1415.3413
61781		1427.3459	1460.4092			1464.6658
61782		1481.9075	1500.0058			1966.9473
61783		3068.0430	3084.7441			3091.1497
61784		3151.3491	3166.2701			3182.9423
61785		3732.9759	3772.7698			3827.6767
61786	Zero-point correction (Hartree):			0.155535		
61787	triHPacyl.tmmmtmpu					
61788	-----					
61790	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.17388372		
61791	Electronic state : 2-A					
61792	Cartesian coordinates (Angs):					
61793	O	-2.688093	-1.270291	0.218407		
61794	O	-1.532345	-1.038986	-0.563836		
61795	C	-0.921314	0.172773	-0.153236		
61796	C	0.357611	0.249736	-1.039120		
61797	C	1.033195	-1.113862	-1.145549		
61798	O	1.219618	-1.687506	0.134302		
61799	O	2.453413	-1.238588	0.672023		
61800	H	-2.329576	-1.815014	0.933841		
61801	C	-1.888281	1.339357	-0.321264		
61802	H	-2.809610	1.122969	0.212456		
61803	H	-2.111609	1.448711	-1.381756		
61804	H	-1.462831	2.266545	0.045606		
61805	C	-0.523312	0.069596	1.328987		
61806	O	0.130447	0.833802	1.937117		
61807	H	2.235167	-0.357284	1.011684		
61808	H	0.059302	0.610523	-2.028274		
61809	O	1.369359	1.079713	-0.508971		
61810	O	0.908412	2.415212	-0.393785		
61811	H	0.797455	2.486913	0.566477		
61812	H	0.393808	-1.801972	-1.692294		
61813	H	1.994003	-1.013838	-1.648710		
61814	Rotational constants (GHz):			1.1443700	0.8979400	0.7079700
61815	Vibrational harmonic frequencies (cm-1):					
61816		31.5761	80.5557			112.5775
61817		127.9996	155.2417			172.8406
61818		188.0115	210.7688			230.3621
61819		261.2360	286.0464			316.2160
61820		330.4058	342.7224			357.4310
61821		396.0298	442.7261			455.5395

61822	472.5619	492.8456	513.4008			
61823	647.9920	678.5492	779.9170			
61824	874.2244	907.6201	936.5238			
61825	988.4980	1013.7246	1049.9858			
61826	1072.5050	1118.3028	1137.5697			
61827	1160.4503	1186.5719	1205.1156			
61828	1299.9867	1334.1462	1358.6273			
61829	1392.0218	1408.1669	1425.1755			
61830	1440.0258	1454.3668	1468.9148			
61831	1482.0972	1499.4287	1964.3062			
61832	3060.7215	3091.9250	3106.0492			
61833	3169.2567	3169.4479	3205.0725			
61834	3757.7370	3759.8959	3779.0226			
61835	Zero-point correction (Hartree): 0.155738					
61836						
61837	triHPacyl.tmmmtpppu					
61838	-----					
61839	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17369095					
61840	Electronic state : 2-A					
61841	Cartesian coordinates (Angs):					
61842	O	-2.831885	-1.160823	0.247334		
61843	O	-1.682141	-0.989166	-0.559444		
61844	C	-1.016097	0.196558	-0.169881		
61845	C	0.194081	0.234561	-1.134322		
61846	C	1.038549	-1.033688	-1.071297		
61847	O	1.291608	-1.456127	0.255970		
61848	O	2.632444	-1.173820	0.612803		
61849	H	-2.489392	-1.721653	0.958264		
61850	C	-1.895807	1.429780	-0.316500		
61851	H	-2.747081	1.371039	0.356292		
61852	H	-2.257904	1.479520	-1.342772		
61853	H	-1.319154	2.324577	-0.093796		
61854	C	-0.622358	0.082786	1.317027		
61855	O	-0.081044	0.886076	1.981031		
61856	H	2.622666	-0.205312	0.684282		
61857	H	-0.238690	0.295001	-2.137174		
61858	O	0.914002	1.448421	-1.054133		
61859	O	1.818665	1.434762	0.042218		
61860	H	1.290755	1.805604	0.765943		
61861	H	0.476045	-1.836198	-1.547491		
61862	H	1.979362	-0.887135	-1.599934		
61863	Rotational constants (GHz):			1.2981000	0.7855700	0.7064000
61864	Vibrational harmonic frequencies (cm-1):					
61865		39.9696	57.6377			109.2410
61866		139.3815	179.2656			189.8575
61867		195.3699	215.7619			237.9516
61868		244.9787	281.4588			301.8566
61869		319.5580	353.1288			383.1484
61870		428.7216	448.1077			481.7401
61871		497.6182	525.0060			561.7214
61872		623.7964	682.1281			795.3436
61873		839.0161	923.5646			956.2733
61874		956.7303	1023.8004			1049.5128
61875		1054.0965	1126.4783			1137.7601
61876		1159.1781	1195.7600			1224.1443
61877		1299.4142	1333.3386			1373.2817
61878		1398.0522	1404.9541			1424.1439
61879		1443.2833	1465.5243			1469.8754
61880		1479.5556	1498.7290			1970.0003
61881		3074.4021	3082.4407			3093.0305
61882		3148.1056	3162.8507			3178.3657
61883		3712.3422	3749.5233			3778.0385
61884	Zero-point correction (Hartree): 0.156005					
61885						
61886	triHPacyl.tmmmtpppu					
61887	-----					
61888	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17366847					
61889	Electronic state : 2-A					
61890	Cartesian coordinates (Angs):					
61891	O	-2.967923	-0.875350	-0.093445		
61892	O	-1.844240	-0.499389	-0.864692		
61893	C	-0.944080	0.250238	-0.055335		

61894	C	0.204191	0.516299	-1.057587	
61895	C	1.048123	-0.716671	-1.392887	
61896	O	1.360259	-1.586954	-0.327451	
61897	O	2.418112	-1.027931	0.440094	
61898	H	-2.682162	-1.723109	0.276856	
61899	C	-1.564617	1.533714	0.468983	
61900	H	-2.447728	1.301545	1.058467	
61901	H	-1.851765	2.154639	-0.378425	
61902	H	-0.841286	2.066954	1.080069	
61903	C	-0.563794	-0.637155	1.150545	
61904	O	0.125429	-0.401070	2.070200	
61905	H	1.989186	-0.936697	1.307135	
61906	H	-0.304553	0.790408	-1.987232	
61907	O	0.939491	1.684473	-0.788244	
61908	O	1.511152	1.625494	0.507683	
61909	H	2.291623	1.066598	0.370698	
61910	H	0.467911	-1.352395	-2.061954	
61911	H	1.961606	-0.400668	-1.901096	
61912	Rotational constants (GHz):		1.2760900	0.8037800	0.7396800
61913	Vibrational harmonic frequencies (cm-1):				
61914		78.8735	120.2892		134.5588
61915		151.8676	173.5245		185.3648
61916		212.7797	217.9370		234.0228
61917		238.8485	257.1272		275.9316
61918		308.0519	319.3262		364.9431
61919		398.9094	419.4999		473.3140
61920		496.9404	564.8781		568.6250
61921		612.5927	668.3561		779.0509
61922		838.9956	918.7593		951.4858
61923		975.1061	1024.0700		1048.1658
61924		1060.1462	1126.1372		1138.8657
61925		1163.1882	1200.6292		1223.9689
61926		1302.5430	1349.6870		1389.5818
61927		1401.5936	1408.8160		1424.7761
61928		1447.7367	1458.3594		1478.8964
61929		1484.3033	1497.9035		1973.4849
61930		3068.3395	3076.9825		3084.8289
61931		3135.7852	3166.3821		3184.8159
61932		3724.7533	3748.5639		3773.3613
61933	Zero-point correction (Hartree):		0.156070		
61934	triHPacyl.tmmmtttmpu				
61935	-----				
61936	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.20370532				
61938	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.08679453				
61939	T1 diagnostic: 0.015633				
61940	E(MP2/Aug-CC-pVTZ) (Hartree): -721.05287312				
61941	E(MP3/Aug-CC-pVTZ) (Hartree): -721.06846688				
61942	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.05519009				
61943	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.06970056				
61944	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.52073401				
61945	E(UHF/Aug-CC-pVTZ) (Hartree): -718.51693468				
61946	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17926125				
61947	Electronic state : 2-A				
61948	Cartesian coordinates (Angs):				
61949	O	-3.088937	-0.554124	-0.518175	
61950	O	-1.824923	-0.196297	-1.041663	
61951	C	-1.024726	0.330501	-0.000473	
61952	C	0.303695	0.659243	-0.705823	
61953	C	0.958485	-0.557045	-1.344386	
61954	O	1.200743	-1.611432	-0.436195	
61955	O	2.275161	-1.231826	0.416249	
61956	H	-2.940302	-1.473045	-0.251658	
61957	C	-1.649842	1.549236	0.660665	
61958	H	-2.606742	1.285623	1.102617	
61959	H	-1.807994	2.312127	-0.101014	
61960	H	-0.983529	1.934782	1.427562	
61961	C	-0.828921	-0.757294	1.083475	
61962	O	-0.155937	-0.697356	2.042386	
61963	H	1.805284	-1.017185	1.239012	
61964	H	0.081068	1.382631	-1.499029	
61965	O	1.098850	1.273123	0.292554	

61966	O	2.354293	1.601763	-0.268785	
61967	H	2.869477	0.809392	-0.046513	
61968	H	0.273510	-0.981353	-2.077399	
61969	H	1.883075	-0.271630	-1.845289	
61970	Rotational constants (GHz):		1.3730600	0.7440000	0.6916200
61971	Vibrational harmonic frequencies (cm-1):				
61972		70.8518	113.4248		134.0989
61973		142.4229	162.4140		185.2900
61974		201.8769	210.8572		232.9182
61975		252.9813	284.9499		302.9375
61976		326.3296	362.0083		391.5972
61977		398.4286	443.7724		446.1190
61978		491.5360	530.5254		559.6772
61979		638.0243	695.2264		782.4413
61980		865.5707	913.3983		933.3374
61981		978.0884	1037.9955		1043.6731
61982		1062.7239	1122.0210		1136.4421
61983		1168.9183	1211.2276		1230.8886
61984		1291.5382	1358.2817		1371.9859
61985		1400.9966	1405.8274		1427.3796
61986		1443.5084	1454.1313		1478.5516
61987		1484.5721	1498.0086		1973.3852
61988		3038.9357	3083.0473		3098.3208
61989		3150.7307	3164.7908		3185.6552
61990		3722.9463	3733.1236		3776.4894
61991	Zero-point correction (Hartree): 0.156299				
61992					
61993	triHPacyl.tmmmpptmpu				
61994	-----				
61995	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17586823				
61996	Electronic state : 2-A				
61997	Cartesian coordinates (Angs):				
61998	O	-3.065520	-0.653883	-0.493426	
61999	O	-1.840275	-0.187137	-1.032856	
62000	C	-1.028977	0.286143	0.025368	
62001	C	0.283103	0.660895	-0.688895	
62002	C	0.963818	-0.526266	-1.356909	
62003	O	1.265270	-1.585717	-0.474273	
62004	O	2.325937	-1.174296	0.380693	
62005	H	-3.687497	0.008040	-0.821143	
62006	C	-1.648972	1.468137	0.755168	
62007	H	-2.586115	1.171983	1.220724	
62008	H	-1.833184	2.269164	0.038736	
62009	H	-0.968294	1.825320	1.522886	
62010	C	-0.793371	-0.846516	1.052337	
62011	O	-0.128466	-0.779310	2.018437	
62012	H	1.850882	-1.011982	1.212658	
62013	H	0.034233	1.389405	-1.470084	
62014	O	1.071861	1.284268	0.308452	
62015	O	2.315216	1.646167	-0.259017	
62016	H	2.845542	0.858246	-0.055723	
62017	H	0.274227	-0.964784	-2.077422	
62018	H	1.864410	-0.200471	-1.877122	
62019	Rotational constants (GHz):		1.3810800	0.7382400	0.6887100
62020	Vibrational harmonic frequencies (cm-1):				
62021		71.3027	109.8944		127.5017
62022		154.3649	173.6773		177.6148
62023		204.3533	215.7344		234.5578
62024		248.6055	255.1301		290.4113
62025		325.0506	349.0187		389.4595
62026		394.5667	435.3673		446.1879
62027		485.1799	535.7531		570.0195
62028		636.9091	703.1024		785.1887
62029		863.7698	915.2051		931.4027
62030		977.3473	1037.8547		1043.5739
62031		1062.9953	1123.5957		1136.2046
62032		1171.8605	1210.0859		1229.6635
62033		1294.5143	1360.4474		1371.1143
62034		1398.8188	1405.2134		1411.2610
62035		1445.1170	1456.1349		1477.4096
62036		1486.8060	1501.0719		1963.1881
62037		3034.2704	3076.5380		3094.8622

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62038          3148.7278          3157.1906          3181.0733
62039          3720.4514          3734.9019          3817.0166
62040 Zero-point correction (Hartree): 0.156188
62041
62042 triHPacyl.tmpmmppmu
62043 -----
62044 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17473398
62045 Electronic state : 2-A
62046 Cartesian coordinates (Angs):
62047 O          2.535473          -0.809254          -0.688519
62048 O          1.353032          -0.052215          -0.845056
62049 C          0.249015          -0.685593          -0.193925
62050 C          -0.945453          0.219116          -0.582466
62051 C          -1.130720          1.433580          0.325452
62052 O          0.086894          2.077988          0.607577
62053 O          0.561355          2.651909          -0.603885
62054 H          2.822052          -0.558580          0.204262
62055 C          0.059625          -2.122296          -0.650310
62056 H          0.963367          -2.693035          -0.455870
62057 H          -0.146691          -2.125034          -1.719323
62058 H          -0.780058          -2.569923          -0.125583
62059 C          0.487374          -0.695341          1.329781
62060 O          1.522130          -0.614588          1.877441
62061 H          1.222752          1.996214          -0.874382
62062 H          -0.745120          0.547719          -1.604362
62063 O          -2.153804          -0.493118          -0.725821
62064 O          -2.518696          -1.020245          0.550842
62065 H          -3.407228          -0.659148          0.655923
62066 H          -1.838522          2.127414          -0.132016
62067 H          -1.500676          1.113765          1.299532
62068 Rotational constants (GHz): 1.0533600          0.9189300          0.6760900
62069 Vibrational harmonic frequencies (cm-1):
62070 66.4699          96.9616          101.3728
62071 137.9400          155.7611          181.4413
62072 195.2454          198.7959          228.3225
62073 232.9504          255.9597          298.6989
62074 317.8331          355.6189          368.4942
62075 409.1658          444.8447          450.1756
62076 497.7270          513.5214          575.8657
62077 603.5333          698.3185          740.5436
62078 879.3334          897.4033          956.9352
62079 975.4289          1037.0967          1053.2992
62080 1113.7849          1124.7252          1139.4363
62081 1160.2221          1183.7916          1235.6333
62082 1287.3568          1340.1863          1368.5606
62083 1395.4320          1404.1264          1426.6843
62084 1441.7445          1456.3703          1484.8587
62085 1490.3998          1496.8028          1973.4169
62086 3074.4321          3088.7681          3098.5787
62087 3140.3758          3170.0688          3185.9288
62088 3738.1085          3743.9587          3833.2113
62089 Zero-point correction (Hartree): 0.156105
62090
62091 triHPacyl.tmpmtpmu
62092 -----
62093 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17387988
62094 Electronic state : 2-A
62095 Cartesian coordinates (Angs):
62096 O          2.190253          -1.803979          -0.203402
62097 O          1.445621          -0.696657          -0.667109
62098 C          0.100675          -0.773279          -0.188648
62099 C          -0.521597          0.538947          -0.736901
62100 C          -0.338360          1.746235          0.180844
62101 O          0.964982          1.811878          0.707805
62102 O          1.852252          2.092843          -0.367218
62103 H          2.384427          -1.550542          0.712952
62104 C          -0.604280          -2.020272          -0.690106
62105 H          -0.053120          -2.903978          -0.379911
62106 H          -0.644830          -1.985097          -1.777697
62107 H          -1.616019          -2.057054          -0.294891
62108 C          0.161811          -0.825998          1.353755
62109 O          -0.715035          -0.722226          2.119253

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62110	H	2.177521	1.203964	-0.580868	
62111	H	-0.014625	0.720383	-1.687845	
62112	O	-1.863097	0.393470	-1.135881	
62113	O	-2.646594	0.104680	0.021728	
62114	H	-3.287718	0.825562	0.003203	
62115	H	-0.579612	2.660251	-0.364296	
62116	H	-0.982570	1.652637	1.054269	
62117	Rotational constants (GHz):		1.0458500	0.9278400	0.7015200
62118	Vibrational harmonic frequencies (cm-1):				
62119		61.1584	103.8493		116.1392
62120		143.3395	145.0446		182.0420
62121		190.6136	200.1935		220.3980
62122		230.4230	261.8499		280.7171
62123		318.8659	330.2495		364.3192
62124		405.6069	425.8039		469.6553
62125		500.8532	520.3002		549.4151
62126		627.9643	661.5051		724.0276
62127		874.7446	918.1781		958.3413
62128		976.1810	1032.4536		1052.1787
62129		1111.5408	1124.2729		1140.6900
62130		1169.3794	1180.3580		1216.5236
62131		1285.2298	1337.6165		1363.6740
62132		1393.7600	1404.4898		1425.3918
62133		1436.2094	1446.9215		1484.3049
62134		1492.4263	1497.6639		2000.3574
62135		3078.8710	3086.7251		3087.7904
62136		3147.9394	3167.9221		3184.5400
62137		3736.5346	3741.5109		3831.3081
62138	Zero-point correction (Hartree):		0.155873		
62139	triHPacyl.tmtmmmtmpu				
62140	-----				
62142	E(UM062X/Aug-CC-pVTZ) (Hartree):		-722.17498333		
62143	Electronic state :		2-A		
62144	Cartesian coordinates (Angs):				
62145	O	-2.877184	-0.830759	-0.998125	
62146	O	-1.469905	-0.844845	-0.862722	
62147	C	-1.043474	0.327207	-0.191114	
62148	C	0.489525	0.220652	-0.231066	
62149	C	0.997031	-1.071560	0.398827	
62150	O	2.405307	-1.075584	0.526200	
62151	O	2.958096	-1.139524	-0.780053	
62152	H	-3.158269	-1.266345	-0.179302	
62153	C	-1.549933	1.607322	-0.832610	
62154	H	-2.634264	1.652473	-0.783438	
62155	H	-1.242152	1.615417	-1.877405	
62156	H	-1.123334	2.465899	-0.321369	
62157	C	-1.519872	0.298299	1.281744	
62158	O	-2.317811	-0.433813	1.732744	
62159	H	3.071361	-0.200945	-0.995447	
62160	H	0.785649	0.283965	-1.280561	
62161	O	0.979300	1.358179	0.458456	
62162	O	2.314580	1.597264	0.032545	
62163	H	2.816194	1.198925	0.758634	
62164	H	0.639598	-1.151955	1.428136	
62165	H	0.666502	-1.936312	-0.176287	
62166	Rotational constants (GHz):		1.5020200	0.5993000	0.5537100
62167	Vibrational harmonic frequencies (cm-1):				
62168		45.5494	71.6029		96.3764
62169		137.6745	156.3432		166.1827
62170		182.7021	202.9233		224.8119
62171		250.6286	292.8341		314.5817
62172		346.0968	374.8773		390.4258
62173		408.4788	420.2651		435.4386
62174		475.9917	509.3415		556.0961
62175		572.6279	712.0877		758.9540
62176		894.3982	902.4785		963.9883
62177		992.8389	1034.3705		1057.7434
62178		1083.2804	1136.3422		1147.0550
62179		1161.4359	1204.6972		1244.9521
62180		1306.9309	1333.8757		1373.1733
62181		1404.4331	1420.9938		1429.6086

62182	1441.3794	1441.7050	1470.9214			
62183	1486.6390	1497.7486	1974.1769			
62184	3073.9082	3086.7989	3088.1839			
62185	3137.1234	3168.6113	3185.2552			
62186	3748.8928	3764.3815	3782.8791			
62187	Zero-point correction (Hartree): 0.156155					
62188						
62189	triHPacyl.tmtmmppppu					
62190	-----					
62191	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17493364					
62192	Electronic state : 2-A					
62193	Cartesian coordinates (Angs):					
62194	O	-2.887449	-1.223540	-0.062251		
62195	O	-1.476094	-1.227999	-0.164451		
62196	C	-1.017205	0.088865	-0.424928		
62197	C	0.506278	-0.116539	-0.541968		
62198	C	1.104865	-0.864586	0.653870		
62199	O	2.490379	-0.601964	0.762447		
62200	O	3.119939	-1.100069	-0.409120		
62201	H	-3.012031	-1.087262	0.888823		
62202	C	-1.606505	0.689335	-1.685553		
62203	H	-2.675598	0.848597	-1.570582		
62204	H	-1.437565	0.006567	-2.517159		
62205	H	-1.121356	1.641737	-1.888491		
62206	C	-1.350675	1.007356	0.772390		
62207	O	-1.834333	0.662701	1.785422		
62208	H	3.162957	-0.306744	-0.962475		
62209	H	0.665248	-0.695647	-1.454072		
62210	O	1.203422	1.082888	-0.804052		
62211	O	1.250257	1.867947	0.379754		
62212	H	2.057563	1.531798	0.799928		
62213	H	0.689847	-0.511559	1.598497		
62214	H	0.921415	-1.933775	0.560668		
62215	Rotational constants (GHz):			1.4804400	0.6386100	0.6030600
62216	Vibrational harmonic frequencies (cm-1):					
62217		38.9827	59.2956			99.0719
62218		132.9011	161.7555			166.1507
62219		190.7201	212.8885			243.7344
62220		278.9553	282.7131			316.2861
62221		350.2254	360.8706			397.1430
62222		412.2796	425.7549			440.1244
62223		483.8665	494.8325			584.8242
62224		663.1404	727.4440			750.3346
62225		871.8895	907.4478			957.7595
62226		982.3283	1014.9355			1048.2592
62227		1079.9754	1128.5835			1145.2388
62228		1167.6438	1205.1706			1235.2917
62229		1296.1983	1330.8487			1381.4636
62230		1405.7822	1408.3644			1426.1894
62231		1433.8803	1440.5665			1483.8184
62232		1487.3781	1499.6207			1966.4630
62233		3081.7330	3092.5058			3095.1982
62234		3148.7886	3163.3034			3173.8884
62235		3747.5099	3768.0673			3778.1361
62236	Zero-point correction (Hartree): 0.156347					
62237						
62238	triHPacyl.tmtpmppmu					
62239	-----					
62240	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17644898					
62241	Electronic state : 2-A					
62242	Cartesian coordinates (Angs):					
62243	O	-3.080245	-0.630020	-0.697597		
62244	O	-1.689769	-0.682992	-0.949063		
62245	C	-1.020673	0.310150	-0.182127		
62246	C	0.449792	0.115645	-0.620904		
62247	C	1.092700	-1.113776	0.005480		
62248	O	2.382840	-1.362126	-0.510421		
62249	O	3.288838	-0.452632	0.108852		
62250	H	-3.168720	-1.237083	0.052309		
62251	C	-1.520264	1.714906	-0.456141		
62252	H	-2.581875	1.779821	-0.232509		
62253	H	-1.358410	1.949983	-1.506863		

62254	H	-0.971594	2.424187	0.158395	
62255	C	-1.189471	0.000578	1.321792	
62256	O	-1.818274	-0.877255	1.783017	
62257	H	3.441580	0.182546	-0.604125	
62258	H	0.421497	-0.014475	-1.705616	
62259	O	1.231617	1.279804	-0.467932	
62260	O	1.375384	1.565415	0.915472	
62261	H	2.175577	1.061306	1.135457	
62262	H	1.140653	-1.038682	1.093804	
62263	H	0.505664	-1.994166	-0.258086	
62264	Rotational constants (GHz):		1.5426300	0.6226200	0.5759300
62265	Vibrational harmonic frequencies (cm-1):				
62266		51.6878	66.0535		90.3792
62267		134.7552	161.1282		181.3557
62268		196.6422	220.8466		235.1584
62269		251.6990	296.5494		312.0125
62270		336.3516	361.6553		377.8402
62271		411.6585	426.1510		432.0985
62272		501.0671	534.2870		575.8927
62273		634.4452	708.7359		755.4237
62274		886.8759	904.4853		946.2573
62275		983.7372	1004.1174		1050.1779
62276		1102.4207	1121.9523		1150.9440
62277		1161.5026	1195.1397		1228.5204
62278		1304.3779	1316.8145		1386.2530
62279		1407.1182	1409.9675		1422.0671
62280		1436.7990	1442.0755		1476.7580
62281		1483.0709	1497.5804		1966.3265
62282		3074.6165	3086.8241		3092.1968
62283		3135.9952	3168.2141		3180.7946
62284		3719.7170	3768.5215		3799.4662
62285	Zero-point correction (Hartree): 0.156204				
62286	triHPacyl.tmtpmpppu				
62287	-----				
62288	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17475912				
62289	Electronic state : 2-A				
62290	Cartesian coordinates (Angs):				
62291	O	-3.083303	-0.700220	-0.637257	
62292	O	-1.698523	-0.706323	-0.925564	
62293	C	-1.043463	0.311385	-0.178967	
62294	C	0.423863	0.170075	-0.653414	
62295	C	1.096067	-1.070171	-0.079649	
62296	O	2.389764	-1.267983	-0.611730	
62297	O	3.288745	-0.411521	0.089444	
62298	H	-3.129423	-1.302596	0.120127	
62299	C	-1.595250	1.697966	-0.444124	
62300	H	-2.651514	1.732572	-0.190240	
62301	H	-1.470148	1.932963	-1.499889	
62302	H	-1.049695	2.426063	0.150884	
62303	C	-1.163074	0.002556	1.328359	
62304	O	-1.737121	-0.902907	1.808933	
62305	H	3.879755	-1.057176	0.495581	
62306	H	0.375502	0.072245	-1.740589	
62307	O	1.172851	1.345227	-0.480596	
62308	O	1.391335	1.560544	0.906164	
62309	H	2.275615	1.175334	1.006158	
62310	H	1.146335	-1.035749	1.009986	
62311	H	0.524742	-1.949049	-0.380404	
62312	Rotational constants (GHz):		1.5358600	0.6200600	0.5745200
62313	Vibrational harmonic frequencies (cm-1):				
62314		38.7796	65.8540		84.8735
62315		126.9261	159.8566		178.6230
62316		184.3819	221.3252		234.9226
62317		246.7259	272.5410		301.3024
62318		325.2614	332.3983		364.5662
62319		406.8931	421.1740		436.5550
62320		473.3202	505.3950		576.5614
62321		635.5176	704.5652		752.4720
62322		885.1878	903.4027		946.0707
62323		982.3823	1003.6774		1049.6359
62324		1097.2993	1121.6794		1157.5816

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62326      1161.4700      1198.4080      1225.6360
62327      1305.6148      1318.6026      1384.9495
62328      1397.7644      1408.1057      1429.8083
62329      1438.3507      1442.9134      1470.5580
62330      1482.7220      1498.0579      1963.1226
62331      3077.6057      3086.2552      3093.0294
62332      3137.4418      3167.7328      3179.7620
62333      3742.4830      3766.9938      3826.6618
62334      Zero-point correction (Hartree): 0.155831
62335
62336      triHPacyl.tmtpmmtmpu
62337      -----
62338      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17398169
62339      Electronic state : 2-A
62340      Cartesian coordinates (Angs):
62341      O      -3.049035      -0.494371      -0.926502
62342      O      -1.638277      -0.528319      -1.019189
62343      C      -1.072813      0.357686      -0.067536
62344      C      0.438391      0.297983      -0.360028
62345      C      0.971899      -1.126609      -0.276080
62346      O      2.313810      -1.238157      -0.711213
62347      O      3.156016      -0.762915      0.337221
62348      H      -3.218097      -1.168188      -0.250735
62349      C      -1.614865      1.772455      -0.169105
62350      H      -2.678196      1.789274      0.053287
62351      H      -1.459112      2.128314      -1.186686
62352      H      -1.082496      2.415934      0.525474
62353      C      -1.334260      -0.169182      1.362400
62354      O      -2.069110      -1.036708      1.654964
62355      H      3.747408      -1.514015      0.462432
62356      H      0.594203      0.694465      -1.365337
62357      O      1.060230      1.158441      0.573580
62358      O      2.174409      1.776341      -0.047540
62359      H      2.884092      1.145079      0.151407
62360      H      0.881870      -1.513023      0.742420
62361      H      0.415860      -1.766341      -0.960741
62362      Rotational constants (GHz): 1.5249500      0.5990400      0.5402400
62363      Vibrational harmonic frequencies (cm-1):
62364      44.1906      51.7540      77.1549
62365      115.4946      124.0772      154.4397
62366      170.5276      194.2677      201.6478
62367      233.4953      249.9535      309.9398
62368      329.5748      341.8501      371.0285
62369      396.8404      425.9068      440.7352
62370      457.0053      519.5885      539.2800
62371      572.0351      709.9286      749.8112
62372      886.6711      911.6273      966.9955
62373      985.2075      1035.9196      1061.4107
62374      1088.7390      1118.8095      1150.8040
62375      1158.9760      1200.7395      1235.1822
62376      1311.6316      1314.2727      1369.8524
62377      1389.7736      1402.3398      1432.7128
62378      1439.3764      1459.2923      1469.3540
62379      1487.0236      1496.6803      1969.4882
62380      3065.0211      3087.3744      3094.3602
62381      3142.3068      3168.3838      3186.5389
62382      3741.3895      3763.5041      3842.6398
62383      Zero-point correction (Hartree): 0.155405
62384
62385      triHPacyl.tmtpmtpmpu
62386      -----
62387      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17539347
62388      Electronic state : 2-A
62389      Cartesian coordinates (Angs):
62390      O      -2.988190      -1.254252      0.049506
62391      O      -1.630952      -1.337240      -0.353424
62392      C      -1.061575      -0.039806      -0.280572
62393      C      0.424994      -0.327032      -0.579360
62394      C      1.154704      -0.995493      0.578818
62395      O      2.471400      -1.364870      0.225632
62396      O      3.284057      -0.194448      0.266440
62397      H      -2.944767      -1.595161      0.953372

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62398	C	-1.683286	0.928623	-1.264702	
62399	H	-2.754246	0.988520	-1.088772	
62400	H	-1.498902	0.578432	-2.279609	
62401	H	-1.240649	1.913414	-1.136520	
62402	C	-1.259128	0.458345	1.181565	
62403	O	-1.501971	1.539525	1.546492	
62404	H	3.391063	-0.001152	-0.674974	
62405	H	0.434648	-1.005064	-1.437410	
62406	O	1.104885	0.808505	-1.066688	
62407	O	1.175230	1.769955	-0.024014	
62408	H	2.015299	1.532062	0.401555	
62409	H	1.176195	-0.366335	1.469966	
62410	H	0.651428	-1.929942	0.826334	
62411	Rotational constants (GHz):			1.4731300	0.6520300 0.5744000
62412	Vibrational harmonic frequencies (cm-1):				
62413		33.2658	84.2703		90.7142
62414		121.3649	158.1474		183.9419
62415		207.4864	215.2750		236.2595
62416		250.8599	279.7400		295.4221
62417		309.8057	332.5952		359.5415
62418		379.2232	423.6472		475.5617
62419		506.2073	546.8592		569.2363
62420		627.1998	682.3510		740.2916
62421		888.6741	926.0817		944.8983
62422		982.4840	1003.6944		1045.1241
62423		1091.7233	1118.6884		1149.1582
62424		1158.5018	1191.1740		1242.2600
62425		1300.0921	1311.4535		1383.2532
62426		1405.8364	1408.4786		1412.0492
62427		1418.3061	1441.7167		1475.5537
62428		1480.2808	1494.4165		2006.5540
62429		3080.0968	3082.8225		3088.1273
62430		3143.5409	3164.6971		3180.9088
62431		3739.8360	3797.6992		3801.0326
62432	Zero-point correction (Hartree):			0.155983	
62433	-----				
62434	triHPacyl.tpmmmmppu				
62435	-----				
62436	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.17609094	
62437	Electronic state : 2-A				
62438	Cartesian coordinates (Angs):				
62439	O	1.226326	-1.736070	-1.219060	
62440	O	0.414841	-0.623579	-0.897324	
62441	C	0.555638	-0.298662	0.478040	
62442	C	-0.510990	0.773302	0.761114	
62443	C	-1.923647	0.223083	0.955935	
62444	O	-2.281210	-0.836616	0.104845	
62445	O	-2.444197	-0.326134	-1.207116	
62446	H	2.080013	-1.313097	-1.401168	
62447	C	0.431382	-1.497233	1.411176	
62448	H	1.295819	-2.148733	1.317577	
62449	H	-0.465858	-2.054704	1.154856	
62450	H	0.370951	-1.145521	2.440812	
62451	C	1.970580	0.284935	0.715571	
62452	O	2.886259	0.188293	-0.013167	
62453	H	-1.553694	-0.447490	-1.571953	
62454	H	-0.213205	1.285997	1.682264	
62455	O	-0.594607	1.719874	-0.285523	
62456	O	0.668178	2.364408	-0.373898	
62457	H	0.980226	2.060429	-1.237197	
62458	H	-2.005854	-0.199206	1.957639	
62459	H	-2.630902	1.048384	0.856108	
62460	Rotational constants (GHz):			1.2726000	0.8295000 0.6890200
62461	Vibrational harmonic frequencies (cm-1):				
62462		65.5006	101.2182		122.4520
62463		135.0165	170.6995		176.5027
62464		212.9688	221.1539		251.7278
62465		263.6625	281.5032		304.2168
62466		332.1382	366.4043		382.5144
62467		421.2500	440.5629		450.9924
62468		465.4391	479.0583		581.4875
62469		611.2175	706.3316		809.0423

62470	857.4415	888.7566	942.0968		
62471	984.6553	1028.9006	1059.2533		
62472	1072.3810	1124.8724	1150.3996		
62473	1165.5061	1186.8038	1243.2725		
62474	1314.8499	1357.1502	1380.6051		
62475	1399.3547	1410.0217	1413.9824		
62476	1444.8994	1456.2453	1464.1486		
62477	1486.9377	1509.3606	1962.0406		
62478	3051.1821	3079.4443	3084.0255		
62479	3134.3634	3162.1110	3181.8603		
62480	3748.1128	3753.7867	3798.2715		
62481	Zero-point correction (Hartree): 0.156397				
62482					
62483	triHPacyl.tpmmmtmpu				
62484	-----				
62485	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17600393				
62486	Electronic state : 2-A				
62487	Cartesian coordinates (Angs):				
62488	O	1.981846	-1.249313	-1.159278	
62489	O	0.770993	-0.597607	-0.834014	
62490	C	0.859110	-0.045470	0.468596	
62491	C	-0.523958	0.535585	0.781018	
62492	C	-1.609854	-0.502291	1.038632	
62493	O	-1.721501	-1.519889	0.073252	
62494	O	-2.088607	-0.912287	-1.158411	
62495	H	2.493308	-0.524775	-1.551306	
62496	C	1.315867	-1.053970	1.511867	
62497	H	2.362519	-1.306134	1.368001	
62498	H	0.720549	-1.958825	1.404250	
62499	H	1.185955	-0.639198	2.510470	
62500	C	1.872342	1.131729	0.463584	
62501	O	2.652003	1.366490	-0.378082	
62502	H	-1.219225	-0.805031	-1.577453	
62503	H	-0.429028	1.132972	1.695439	
62504	O	-0.777013	1.398888	-0.317152	
62505	O	-2.076593	1.940162	-0.203061	
62506	H	-2.581347	1.318274	-0.751138	
62507	H	-1.378411	-1.030988	1.963933	
62508	H	-2.564381	0.008647	1.169588	
62509	Rotational constants (GHz): 1.3176300			0.7741700	0.6595800
62510	Vibrational harmonic frequencies (cm-1):				
62511	60.6686	91.0717	100.9376		
62512	106.6162	163.5503	185.0521		
62513	208.3735	234.4375	243.0389		
62514	271.9414	279.8974	330.4420		
62515	357.9065	363.3718	409.1841		
62516	418.2662	435.6502	470.9148		
62517	478.9419	520.8388	568.1755		
62518	644.4211	697.5338	811.5714		
62519	846.0543	894.6768	943.1654		
62520	977.5946	1032.0611	1049.3269		
62521	1072.6141	1125.9739	1133.5997		
62522	1169.4300	1200.1436	1244.4431		
62523	1303.3739	1370.6923	1383.8647		
62524	1400.6748	1415.9322	1434.8123		
62525	1443.5713	1448.4729	1477.4760		
62526	1488.8027	1509.3445	1982.2512		
62527	3041.9238	3082.4177	3089.3122		
62528	3132.6884	3162.6604	3177.2226		
62529	3735.7067	3743.3426	3756.7853		
62530	Zero-point correction (Hartree): 0.156563				
62531					
62532	triHPacyl.tpmmmtmpu				
62533	-----				
62534	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17575358				
62535	Electronic state : 2-A				
62536	Cartesian coordinates (Angs):				
62537	O	0.828383	-1.956482	-1.443623	
62538	O	0.132869	-0.795366	-1.032405	
62539	C	0.610281	-0.389934	0.238884	
62540	C	-0.244455	0.833398	0.629135	
62541	C	-1.622060	0.482607	1.194266	

62542	O	-2.274675	-0.592912	0.568148
62543	O	-2.680750	-0.185391	-0.727193
62544	H	1.624241	-1.581142	-1.849745
62545	C	0.573870	-1.493781	1.287140
62546	H	1.318792	-2.253704	1.067764
62547	H	-0.412482	-1.951028	1.291984
62548	H	0.794748	-1.063508	2.263559
62549	C	2.094875	0.032016	0.090729
62550	O	2.779447	0.473696	0.928785
62551	H	-1.916323	-0.452471	-1.261286
62552	H	0.311615	1.383202	1.396446
62553	O	-0.478218	1.681309	-0.476242
62554	O	0.784114	2.116507	-0.958727
62555	H	0.829075	1.661665	-1.811164
62556	H	-1.509749	0.161343	2.229840
62557	H	-2.244338	1.378926	1.161729
62558	Rotational constants (GHz): 1.2029600 0.8153700 0.7080200			
62559	Vibrational harmonic frequencies (cm-1):			
62560	72.1013	101.5131	115.0237	
62561	131.4153	138.6343	165.6309	
62562	214.2840	225.4843	232.1673	
62563	255.3826	279.2845	292.0457	
62564	313.7095	320.3501	373.5434	
62565	405.5344	416.4324	441.8533	
62566	464.3345	485.9804	588.7503	
62567	615.4201	665.0424	805.5651	
62568	856.5043	895.7820	942.7100	
62569	985.3259	1029.0407	1056.7956	
62570	1070.8531	1117.8546	1149.0478	
62571	1172.2126	1186.2192	1231.5376	
62572	1315.1807	1355.8583	1379.6277	
62573	1398.1367	1408.8011	1413.0110	
62574	1427.0768	1456.5200	1463.6750	
62575	1486.1152	1507.9870	1991.8321	
62576	3053.0796	3079.5021	3083.4580	
62577	3136.1427	3162.8920	3179.5361	
62578	3740.5095	3760.2890	3796.2160	
62579	Zero-point correction (Hartree): 0.155847			
62580				
62581	triHPacyl.tpmmmttmpu			
62582	-----			
62583	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17556748			
62584	Electronic state : 2-A			
62585	Cartesian coordinates (Angs):			
62586	O	1.729172	-1.763966	-1.173944
62587	O	0.585188	-1.012843	-0.819076
62588	C	0.935947	-0.101207	0.204291
62589	C	-0.327023	0.715937	0.507938
62590	C	-1.412375	-0.051148	1.255387
62591	O	-1.757367	-1.300750	0.708712
62592	O	-2.310640	-1.073662	-0.581138
62593	H	2.109272	-1.220706	-1.880011
62594	C	1.505129	-0.791950	1.433274
62595	H	2.482891	-1.211251	1.212588
62596	H	0.835971	-1.600655	1.722720
62597	H	1.603529	-0.074991	2.247227
62598	C	2.011493	0.878362	-0.345442
62599	O	2.433466	1.812329	0.216035
62600	H	-1.530213	-1.206412	-1.142974
62601	H	-0.029257	1.555482	1.147018
62602	O	-0.722132	1.209780	-0.763769
62603	O	-1.936235	1.920354	-0.634753
62604	H	-2.577078	1.228656	-0.863541
62605	H	-1.051385	-0.283461	2.257730
62606	H	-2.294364	0.583432	1.350014
62607	Rotational constants (GHz): 1.2169700 0.8059100 0.6536500			
62608	Vibrational harmonic frequencies (cm-1):			
62609	62.0715	87.8365	97.7210	
62610	106.1976	126.4369	179.7147	
62611	202.7198	224.9178	241.6914	
62612	249.2452	272.7089	307.6360	
62613	329.9329	355.5428	391.2674	

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62614      396.2072          466.2819          483.8706
62615      493.3325          523.5580          557.0279
62616      623.1371          686.2870          809.8287
62617      845.4529          900.1720          950.0214
62618      976.0685          1033.7681         1048.4729
62619      1070.6778          1121.1758         1131.2814
62620      1173.3209          1192.7508         1244.2022
62621      1300.1150          1366.4429         1376.6611
62622      1399.6660          1411.9019         1424.0204
62623      1438.6533          1447.2757         1476.2703
62624      1487.7392          1509.2110         1995.7603
62625      3040.6834          3079.1274         3087.7221
62626      3133.1885          3160.2671         3173.0255
62627      3736.2184          3742.8069         3770.9811
62628      Zero-point correction (Hartree): 0.156101
62629
62630      triHPacyl.tppmpmpmpu
62631      -----
62632      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17489724
62633      Electronic state : 2-A
62634      Cartesian coordinates (Angs):
62635      O      -2.327814      -0.772460      1.378216
62636      O      -1.236440      0.046990      1.004087
62637      C      -0.601337      -0.483317      -0.151185
62638      C      0.596596      0.434553      -0.433594
62639      C      1.684385      0.414052      0.637748
62640      O      2.487142      -0.746525      0.548106
62641      O      3.168969      -0.707924      -0.700025
62642      H      -3.037797      -0.428114      0.814192
62643      C      -0.218602      -1.947517      -0.000042
62644      H      -1.107097      -2.572217      0.029205
62645      H      0.338959      -2.075747      0.924465
62646      H      0.411798      -2.250881      -0.833943
62647      C      -1.557987      -0.354995      -1.362701
62648      O      -2.697809      -0.083262      -1.316720
62649      H      4.074643      -0.525753      -0.420963
62650      H      1.034081      0.101159      -1.375990
62651      O      0.163999      1.753778      -0.709359
62652      O      -0.031804      2.453129      0.513730
62653      H      -0.899276      2.133444      0.802224
62654      H      2.289525      1.315592      0.532646
62655      H      1.266876      0.376050      1.642528
62656      Rotational constants (GHz):      1.3093800      0.6895600      0.5977700
62657      Vibrational harmonic frequencies (cm-1):
62658      43.4834          58.1958          90.9568
62659      154.5534          164.9823          174.5996
62660      194.6411          206.4604          221.5963
62661      236.9440          241.3037          292.5419
62662      312.6772          344.6334          358.2315
62663      402.4072          429.3880          439.8180
62664      447.6514          532.4040          553.8756
62665      610.6703          715.9249          744.4694
62666      872.0956          905.5068          944.5164
62667      975.1213          1029.3441         1063.6746
62668      1103.6306          1114.1946         1125.6049
62669      1165.5888          1183.9827         1240.3854
62670      1290.2829          1334.7196         1385.7360
62671      1394.5294          1411.4342         1422.1411
62672      1439.5138          1445.4070         1475.5223
62673      1479.4132          1500.5088         1976.0732
62674      3086.0790          3088.9731         3109.0803
62675      3153.1196          3169.2820         3178.6204
62676      3751.2958          3770.4995         3825.2256
62677      Zero-point correction (Hartree): 0.155789
62678
62679      triHPacyl.tppmpmpmpu
62680      -----
62681      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17489723
62682      Electronic state : 2-A
62683      Cartesian coordinates (Angs):
62684      O      -2.327649      -0.772655      1.378452
62685      O      -1.236263      0.046770      1.004233

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62686	C	-0.601375	-0.483316	-0.151177	
62687	C	0.596582	0.434527	-0.433587	
62688	C	1.684369	0.413994	0.637752	
62689	O	2.487117	-0.746590	0.548094	
62690	O	3.168979	-0.707878	-0.699973	
62691	H	-3.037850	-0.427799	0.815012	
62692	C	-0.218699	-1.947555	-0.000570	
62693	H	-1.107308	-2.572156	0.029236	
62694	H	0.339684	-2.076204	0.923407	
62695	H	0.410856	-2.250840	-0.835188	
62696	C	-1.558137	-0.354542	-1.362789	
62697	O	-2.697970	-0.083046	-1.316648	
62698	H	4.074638	-0.525636	-0.420848	
62699	H	1.034082	0.101145	-1.376022	
62700	O	0.164014	1.753802	-0.709300	
62701	O	-0.031693	2.453080	0.513791	
62702	H	-0.899162	2.133395	0.802305	
62703	H	2.289502	1.315569	0.532579	
62704	H	1.266852	0.376012	1.642560	
62705	Rotational constants (GHz):		1.3093300	0.6895500	0.5977700
62706	Vibrational harmonic frequencies (cm-1):				
62707		43.4847	58.1761		90.8397
62708		154.5855	165.0561		174.5463
62709		194.6475	206.6927		221.7916
62710		237.1856	241.9423		292.5651
62711		312.6661	344.6284		358.2096
62712		402.4942	429.3450		439.6977
62713		447.6743	532.4149		553.8629
62714		610.6467	715.7347		744.3355
62715		872.0917	905.6076		944.5797
62716		975.2111	1029.3983		1063.6540
62717		1103.6671	1114.2095		1125.5879
62718		1165.6609	1183.9952		1240.4347
62719		1290.3392	1334.7833		1385.8013
62720		1394.6315	1411.5057		1422.2080
62721		1439.5063	1445.4246		1475.5898
62722		1479.4488	1500.6188		1976.2599
62723		3085.7983	3088.6724		3108.7740
62724		3152.8604	3168.9316		3178.3002
62725		3751.3048	3770.4559		3824.9758
62726	Zero-point correction (Hartree): 0.155789				
62727					
62728	triHPacyl.tpppmtmpmpu				
62729	-----				
62730	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17395153				
62731	Electronic state : 2-A				
62732	Cartesian coordinates (Angs):				
62733	O	2.535052	-0.128951	-1.498233	
62734	O	1.362687	0.479366	-0.989568	
62735	C	0.723283	-0.412016	-0.090539	
62736	C	-0.500984	0.337331	0.458704	
62737	C	-1.594060	0.613941	-0.573596	
62738	O	-2.351939	-0.543525	-0.860642	
62739	O	-3.026899	-0.926789	0.331714	
62740	H	3.174217	0.040148	-0.789068	
62741	C	0.390256	-1.752656	-0.724424	
62742	H	1.300065	-2.308543	-0.935288	
62743	H	-0.148397	-1.585645	-1.654651	
62744	H	-0.240076	-2.328966	-0.049679	
62745	C	1.682804	-0.666967	1.104974	
62746	O	1.427775	-1.253165	2.082694	
62747	H	-3.941584	-0.707523	0.115850	
62748	H	-0.922885	-0.285623	1.249311	
62749	O	-0.110904	1.522657	1.125898	
62750	O	0.047651	2.570210	0.176573	
62751	H	0.915427	2.375060	-0.206895	
62752	H	-2.231284	1.413265	-0.191987	
62753	H	-1.180661	0.911609	-1.535798	
62754	Rotational constants (GHz):		1.1134000	0.7192800	0.6524600
62755	Vibrational harmonic frequencies (cm-1):				
62756		44.6692	65.0798		104.6533
62757		125.4949	155.9901		174.7080

62758	185.0633	203.5755	213.7535
62759	235.7449	254.1357	294.0970
62760	302.2581	315.7786	353.0326
62761	388.0940	411.5043	417.3904
62762	490.8562	497.2423	561.0379
62763	614.5680	668.9702	749.3491
62764	871.1528	916.5622	946.7679
62765	974.4303	1031.7111	1063.2808
62766	1099.6341	1114.4257	1119.4219
62767	1159.9861	1186.8866	1234.3159
62768	1294.3986	1333.3103	1387.2292
62769	1393.4550	1409.1952	1419.5181
62770	1428.6540	1441.5305	1475.5583
62771	1479.1755	1501.2931	1999.1396
62772	3083.3199	3086.5771	3109.9528
62773	3151.2084	3168.7453	3173.5624
62774	3754.3704	3767.5464	3822.2120

62775 Zero-point correction (Hartree): 0.155429

62776 triHPacyl.ttpmmmpmu

62777 -----
 62779 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.17552424

62780 Electronic state : 2-A

62781 Cartesian coordinates (Angs):

62782	O	-2.792068	-0.684361	0.232357
62783	O	-1.754110	0.146292	-0.247591
62784	C	-0.496085	-0.264698	0.274471
62785	C	0.483354	0.821762	-0.233091
62786	C	1.862147	0.773563	0.430205
62787	O	2.431718	-0.506727	0.522740
62788	O	2.771711	-0.914295	-0.796379
62789	H	-2.803220	-1.390227	-0.431895
62790	C	-0.502891	-0.408789	1.786249
62791	H	-1.300699	-1.076196	2.097639
62792	H	-0.667403	0.575391	2.223553
62793	H	0.450972	-0.807362	2.125022
62794	C	-0.129668	-1.622730	-0.367021
62795	O	-0.871211	-2.365214	-0.890634
62796	H	2.166171	-1.660269	-0.920693
62797	H	0.568595	0.758372	-1.318581
62798	O	0.004344	2.102697	0.117463
62799	O	-0.832686	2.605472	-0.908782
62800	H	-1.675583	2.170418	-0.710732
62801	H	2.525661	1.452215	-0.105697
62802	H	1.772774	1.112102	1.463113

62803 Rotational constants (GHz): 1.0873000 0.8443800 0.5929100

62804 Vibrational harmonic frequencies (cm-1):

62805	57.1800	86.1800	96.6480
62806	150.3037	168.9954	183.0199
62807	190.6042	224.3863	239.7405
62808	254.7163	286.5260	319.3398
62809	346.1965	363.5978	383.1602
62810	399.1910	431.7490	435.7169
62811	442.9533	505.1994	513.8063
62812	608.1253	692.5057	743.2762
62813	874.7667	919.3734	956.3589
62814	1013.7045	1027.4251	1047.4796
62815	1106.7541	1128.5602	1145.9055
62816	1155.3964	1194.6280	1230.1032
62817	1291.5588	1336.5317	1384.7623
62818	1403.5920	1411.5038	1426.9500
62819	1440.5942	1455.5689	1480.6140
62820	1499.7656	1504.4730	1973.6443
62821	3083.1171	3086.7665	3099.3192
62822	3140.3598	3163.6098	3182.7092
62823	3754.8847	3760.8044	3768.0142

62824 Zero-point correction (Hartree): 0.156220

62825
 62826
 62827
 62828 CO elimination from (2R,3S)-2-Me-2,3,4-triOOH-1-oxo-butyl (D', R,S-di-HPALD-I)
 62829 =====

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62830
62831 TS.triHPacyl.COelim.mpmmppppmpu
62832 -----
62833 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16023090
62834 Electronic state : 2-A
62835 Cartesian coordinates (Angs):
62836 O -0.030834 1.640125 -1.517548
62837 O -0.757578 0.476279 -1.071603
62838 C -0.884930 0.462243 0.298333
62839 C 0.081616 -0.452650 1.023143
62840 C 1.451368 0.174669 1.277073
62841 O 2.056933 0.726083 0.116899
62842 O 3.028294 -0.168239 -0.396569
62843 H 0.872415 1.434119 -1.208768
62844 C -1.258408 1.751709 0.952839
62845 H -2.058308 2.231264 0.391086
62846 H -0.414370 2.442580 0.986006
62847 H -1.597976 1.558769 1.970174
62848 C -2.588078 -0.624553 0.472295
62849 O -3.162276 -0.866786 -0.479705
62850 H 2.466823 -0.876473 -0.763226
62851 H -0.355567 -0.665772 2.003550
62852 O 0.131120 -1.743822 0.434345
62853 O 0.816235 -1.708796 -0.812447
62854 H 0.169559 -1.282099 -1.398074
62855 H 1.323431 1.005921 1.973016
62856 H 2.129428 -0.555580 1.717157
62857 Rotational constants (GHz): 1.3623300 0.7319700 0.6488400
62858 Vibrational harmonic frequencies (cm-1):
62859 i390.8216 22.7131 62.0145
62860 63.1736 131.8685 147.5584
62861 167.4375 198.0056 220.5804
62862 235.1134 238.5259 268.7046
62863 280.0970 295.5512 324.7466
62864 372.9867 452.2875 471.8289
62865 482.2534 504.7463 586.8858
62866 601.9149 678.1948 718.2709
62867 820.0725 897.2688 923.2141
62868 947.6037 962.4660 1017.3342
62869 1031.8059 1054.2704 1126.8221
62870 1148.4430 1212.5299 1264.3387
62871 1294.2740 1327.8282 1382.2257
62872 1397.2582 1410.5760 1455.7010
62873 1463.1994 1466.9263 1472.6563
62874 1490.5927 1491.7566 2097.2531
62875 3062.1062 3070.8281 3080.3643
62876 3128.8544 3137.6533 3154.5536
62877 3618.6756 3644.4551 3725.4319
62878 Zero-point correction (Hartree): 0.153332
62879
62880 TS.triHPacyl.COelim.mpmmptppmpu
62881 -----
62882 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16018214
62883 Electronic state : 2-A
62884 Cartesian coordinates (Angs):
62885 O 0.278740 2.137836 -1.007534
62886 O -0.403941 0.880475 -1.126629
62887 C -0.872845 0.494206 0.110699
62888 C 0.012449 -0.433399 0.922677
62889 C 1.372486 0.169798 1.294417
62890 O 2.173197 0.587779 0.207996
62891 O 2.959571 -0.495107 -0.252550
62892 H 1.187844 1.824703 -0.850536
62893 C -1.659652 1.518386 0.860896
62894 H -2.269240 2.093516 0.166749
62895 H -0.999528 2.215762 1.381520
62896 H -2.304882 1.034996 1.593575
62897 C -2.266307 -0.837082 -0.572253
62898 O -3.224684 -0.903660 0.040042
62899 H 2.313956 -1.005591 -0.774178
62900 H -0.501877 -0.617694 1.870966
62901 O 0.101885 -1.750230 0.390488

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62902	O	0.623540	-1.719093	-0.927061	
62903	H	-0.141659	-1.448117	-1.460591	
62904	H	1.196295	1.073250	1.882438	
62905	H	1.935855	-0.546285	1.893429	
62906	Rotational constants (GHz):		1.3280500	0.7671400	0.6259800
62907	Vibrational harmonic frequencies (cm-1):				
62908	i386.0517		38.5063		57.3814
62909	78.7668		145.4336		163.8970
62910	169.6987		196.2123		221.9951
62911	234.8902		253.0097		257.2814
62912	270.2966		320.1300		340.0771
62913	346.8976		410.8153		452.8376
62914	471.0305		517.6342		603.2519
62915	626.3455		636.6137		714.6155
62916	825.5145		922.9072		946.2515
62917	962.2678		970.3586		1008.0391
62918	1035.8807		1048.4599		1127.3082
62919	1153.8115		1193.9404		1257.2776
62920	1312.0037		1332.5474		1382.8477
62921	1402.2142		1410.1229		1435.7304
62922	1446.9184		1456.5224		1474.0371
62923	1485.2335		1490.5577		2089.4639
62924	3057.3499		3067.3275		3076.2659
62925	3124.5242		3128.5314		3160.4915
62926	3643.6075		3669.0322		3725.2672
62927	Zero-point correction (Hartree): 0.153435				
62928					
62929	TS.triHPacyl.COelim.pmmmpmtmpu				
62930	-----				
62931	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16162539				
62932	Electronic state : 2-A				
62933	Cartesian coordinates (Angs):				
62934	O	-1.799547	-0.866494	-1.417920	
62935	O	-1.900636	0.468778	-0.939441	
62936	C	-0.852708	0.816019	-0.134077	
62937	C	0.558468	0.686662	-0.675205	
62938	C	1.002450	-0.680358	-1.180670	
62939	O	0.839591	-1.725919	-0.245952	
62940	O	1.795433	-1.541451	0.793438	
62941	H	-2.299191	-1.348620	-0.742822	
62942	C	-1.198533	2.099009	0.554437	
62943	H	-2.219217	2.049614	0.928883	
62944	H	-1.123585	2.936498	-0.145134	
62945	H	-0.511448	2.280161	1.376128	
62946	C	-0.995877	-0.552636	1.504230	
62947	O	-2.044321	-1.002399	1.538288	
62948	H	1.261743	-1.078242	1.460531	
62949	H	0.661692	1.390352	-1.515968	
62950	O	1.356676	1.153143	0.411146	
62951	O	2.718346	1.127458	0.036419	
62952	H	2.980887	0.245293	0.345642	
62953	H	0.396709	-0.968249	-2.034365	
62954	H	2.045274	-0.623930	-1.493011	
62955	Rotational constants (GHz):		1.1914200	0.7981100	0.6951500
62956	Vibrational harmonic frequencies (cm-1):				
62957	i315.3535		48.9120		99.1904
62958	117.4600		127.0284		137.6373
62959	163.8245		182.5105		204.6953
62960	229.0830		233.7008		261.8593
62961	271.9326		291.0700		332.4833
62962	353.0577		378.0552		437.6341
62963	477.7898		496.5698		515.0456
62964	559.8441		582.4370		718.4843
62965	830.6884		889.5730		950.8671
62966	968.5116		1027.3869		1033.1871
62967	1055.5107		1092.0252		1117.4922
62968	1155.9676		1223.6896		1264.6344
62969	1297.2754		1351.4163		1377.2586
62970	1407.6080		1411.4450		1418.4809
62971	1437.0014		1453.2436		1480.0619
62972	1486.8524		1491.4622		2073.4694
62973	2981.3763		3049.1345		3101.9241

```

62974          3131.8864          3177.9161          3178.7719
62975          3710.6067          3725.0438          3780.6318
62976 Zero-point correction (Hartree): 0.153441
62977
62978 TS.triHPacyl.COelim.pmmpttmpu
62979 -----
62980 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16205921
62981 Electronic state : 2-A
62982 Cartesian coordinates (Angs):
62983 O      -1.933512      -1.520895      -0.863606
62984 O      -2.204067      -0.130682      -0.743763
62985 C      -1.162166       0.546063      -0.173683
62986 C       0.177453       0.531713      -0.891209
62987 C       0.795496      -0.822330      -1.207112
62988 O       1.009743      -1.623654      -0.060824
62989 O       2.151898      -1.120211       0.625250
62990 H      -1.961977      -1.799315       0.066588
62991 C      -1.649263       1.876657       0.305930
62992 H      -2.596095       1.754799       0.827928
62993 H      -1.803206       2.551344      -0.541392
62994 H      -0.915885       2.329153       0.968340
62995 C      -0.931197      -0.507950       1.662591
62996 O      -0.127615      -0.101919       2.363432
62997 H       1.744858      -0.634293       1.359202
62998 H       0.044469       1.064476      -1.845922
62999 O       1.015894       1.311350      -0.042962
63000 O       2.272302       1.478969      -0.669066
63001 H       2.765059       0.722528      -0.311288
63002 H       0.124526      -1.397592      -1.837149
63003 H       1.739163      -0.679678      -1.733089
63004 Rotational constants (GHz): 1.1382400      0.8121600      0.7556800
63005 Vibrational harmonic frequencies (cm-1):
63006 i310.1633          52.7497          113.6961
63007 122.5726          136.2226          155.0733
63008 165.8051          183.6436          199.8901
63009 214.8239          225.2940          260.0999
63010 264.2324          312.1438          332.6169
63011 348.0504          376.7865          409.6823
63012 441.3776          500.7680          509.8736
63013 567.0999          585.5650          715.5212
63014 830.3677          888.8232          948.1720
63015 969.4104          1026.1814          1032.5404
63016 1054.2006          1092.0276          1114.2297
63017 1154.1400          1224.1559          1266.0530
63018 1292.8160          1352.7764          1374.7019
63019 1406.8417          1408.2475          1432.1076
63020 1435.7396          1455.1851          1478.3368
63021 1484.4880          1490.4141          2073.9505
63022 2983.4136          3046.8789          3104.9811
63023 3130.0125          3174.2404          3182.9589
63024 3725.8359          3730.7572          3756.7627
63025 Zero-point correction (Hartree): 0.153356
63026
63027 TS.triHPacyl.COelim.pmtmptpppu
63028 -----
63029 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16143354
63030 Electronic state : 2-A
63031 Cartesian coordinates (Angs):
63032 O      -1.132448       2.323192      -0.281595
63033 O      -1.709654       1.411548       0.639866
63034 C      -1.080122       0.196368       0.547057
63035 C       0.440892       0.242772       0.571438
63036 C       1.156148       0.745131      -0.700132
63037 O       2.408604       0.107068      -0.852961
63038 O       3.234700       0.504362       0.231298
63039 H      -1.549906       2.043465      -1.112320
63040 C      -1.746303      -0.780037       1.459223
63041 H      -2.826126      -0.663024       1.395615
63042 H      -1.430304      -0.614849       2.492122
63043 H      -1.474300      -1.793374       1.173261
63044 C      -1.763211      -0.369206      -1.334997
63045 O      -2.185392      -1.425374      -1.406523

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63046	H	3.056806	-0.196033	0.876495	
63047	H	0.722182	0.879237	1.418838	
63048	O	0.958957	-1.021074	0.948637	
63049	O	0.686253	-1.940745	-0.101029	
63050	H	1.475668	-1.834486	-0.654937	
63051	H	0.609346	0.473095	-1.601580	
63052	H	1.284045	1.824003	-0.664573	
63053	Rotational constants (GHz):		1.2372000	0.7170700	0.6115700
63054	Vibrational harmonic frequencies (cm-1):				
63055	i315.7908		42.9782		75.4130
63056	89.9094		137.6503		149.2866
63057	174.9446		194.6754		208.1430
63058	212.5624		226.7902		243.7447
63059	302.6260		324.5706		353.3213
63060	369.8777		384.5344		428.9368
63061	438.7363		469.1654		503.0980
63062	548.1370		587.6835		744.4156
63063	814.0510		940.2589		956.0565
63064	974.9143		1001.1132		1032.7406
63065	1053.9720		1095.7524		1121.1766
63066	1160.0703		1254.2130		1254.8536
63067	1294.9024		1327.7537		1359.6605
63068	1391.0871		1409.8885		1423.6480
63069	1426.9364		1434.8622		1479.8866
63070	1484.3690		1488.6320		2085.4816
63071	3040.2985		3057.5260		3109.0679
63072	3136.8110		3166.6040		3173.3104
63073	3737.2959		3747.7449		3768.3402
63074	Zero-point correction (Hartree): 0.153581				
63075					
63076	TS.triHPacyl.COelim.pmtpppppmu				
63077	-----				
63078	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16153020				
63079	Electronic state : 2-A				
63080	Cartesian coordinates (Angs):				
63081	O	-1.784141	-1.428548	-1.187589	
63082	O	-2.017854	-0.033108	-1.063870	
63083	C	-1.035218	0.554256	-0.306627	
63084	C	0.385827	0.096901	-0.612095	
63085	C	0.907663	-1.037403	0.263436	
63086	O	2.168539	-1.505883	-0.171620	
63087	O	3.170947	-0.596884	0.275966	
63088	H	-2.406109	-1.777057	-0.532309	
63089	C	-1.324496	2.015159	-0.203033	
63090	H	-2.380934	2.161191	0.016266	
63091	H	-1.084976	2.519610	-1.141568	
63092	H	-0.722270	2.452984	0.587453	
63093	C	-1.562832	-0.108503	1.648521	
63094	O	-2.420977	-0.862798	1.598217	
63095	H	3.379556	-0.123564	-0.541133	
63096	H	0.399613	-0.246782	-1.651428	
63097	O	1.290692	1.191642	-0.634664	
63098	O	1.486492	1.662928	0.691576	
63099	H	2.234216	1.114870	0.980297	
63100	H	0.959581	-0.746551	1.312424	
63101	H	0.246077	-1.895953	0.164655	
63102	Rotational constants (GHz):		1.2979300	0.6664600	0.5886400
63103	Vibrational harmonic frequencies (cm-1):				
63104	i300.6523		43.0620		47.1454
63105	100.3437		142.5959		155.6136
63106	180.5367		184.9173		208.9545
63107	221.8067		232.5092		250.5790
63108	276.5421		286.2536		329.0171
63109	351.9746		361.4602		394.4210
63110	424.3142		488.1917		551.9997
63111	576.1034		583.2980		669.6550
63112	855.8437		911.7870		955.1358
63113	971.1912		998.9361		1041.2057
63114	1053.7012		1113.2528		1125.9982
63115	1139.6016		1230.5237		1267.5465
63116	1295.2059		1316.5545		1375.1134
63117	1396.5768		1409.6452		1410.1106

63118	1415.3817	1445.9025	1480.0986			
63119	1482.8234	1486.9167	2052.1016			
63120	3062.1493	3065.1764	3100.6967			
63121	3134.7939	3160.7042	3182.7847			
63122	3722.8802	3784.1028	3797.8751			
63123	Zero-point correction (Hartree): 0.153329					
63124						
63125	TS.triHPacyl.COelim.pmtpptmmpu					
63126	-----					
63127	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16075867					
63128	Electronic state : 2-A					
63129	Cartesian coordinates (Angs):					
63130	O	-0.760145	-1.066668	1.904647		
63131	O	-1.325407	-1.523185	0.688127		
63132	C	-1.137718	-0.587537	-0.291326		
63133	C	0.234035	0.038627	-0.418021		
63134	C	1.306452	-1.046685	-0.335180		
63135	O	2.579057	-0.628755	-0.800171		
63136	O	3.176353	0.194861	0.191250		
63137	H	-1.288993	-0.269068	2.082748		
63138	C	-1.824115	-1.021506	-1.544386		
63139	H	-2.803325	-1.435630	-1.311120		
63140	H	-1.245209	-1.787189	-2.069517		
63141	H	-1.947769	-0.167224	-2.208171		
63142	C	-2.310441	0.996770	0.411741		
63143	O	-2.635196	1.732012	-0.396183		
63144	H	3.810695	-0.402902	0.605193		
63145	H	0.284506	0.529068	-1.392024		
63146	O	0.411715	1.043250	0.574094		
63147	O	1.187027	2.092616	0.020966		
63148	H	2.089084	1.792870	0.214853		
63149	H	1.376562	-1.422902	0.685716		
63150	H	1.047942	-1.868090	-1.006485		
63151	Rotational constants (GHz):			1.2889900	0.6672600	0.5784900
63152	Vibrational harmonic frequencies (cm-1):					
63153	i301.3243		46.0622			63.9432
63154	68.9607		133.9812			149.3396
63155	150.6854		170.3612			183.7445
63156	200.6144		210.2882			233.7450
63157	238.8028		272.2901			312.3819
63158	334.1028		381.9457			423.5668
63159	429.4447		471.1743			511.4168
63160	531.6356		548.7486			610.9453
63161	875.3048		930.9844			963.9587
63162	979.3423		1026.3213			1056.1553
63163	1063.1448		1091.3113			1107.9983
63164	1129.7498		1206.0128			1305.9580
63165	1311.9704		1332.2415			1381.1950
63166	1387.2418		1409.6720			1418.5011
63167	1449.9322		1455.1626			1458.7298
63168	1478.6564		1491.1564			2087.7334
63169	3041.8768		3077.7389			3092.8905
63170	3119.2355		3138.7207			3158.5208
63171	3698.5629		3740.2898			3822.2499
63172	Zero-point correction (Hartree): 0.152561					
63173						
63174	TS.triHPacyl.COelim.pmtpptppmu					
63175	-----					
63176	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16197453					
63177	Electronic state : 2-A					
63178	Cartesian coordinates (Angs):					
63179	O	1.653793	2.162542	-0.126501		
63180	O	2.050783	0.966056	-0.775872		
63181	C	1.171070	-0.046254	-0.481648		
63182	C	-0.304838	0.308435	-0.629185		
63183	C	-0.992164	0.852423	0.620496		
63184	O	-2.319657	1.259923	0.355818		
63185	O	-3.153403	0.104908	0.311477		
63186	H	2.002093	2.012101	0.766911		
63187	C	1.671123	-1.313542	-1.091888		
63188	H	2.741500	-1.402752	-0.916523		
63189	H	1.486806	-1.314979	-2.168438		

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63190      H      1.156251      -2.164941      -0.655190
63191      C      1.606902      -0.288072      1.556676
63192      O      1.529987      -1.358357      1.941501
63193      H     -3.299995      0.010944      -0.639802
63194      H     -0.374576      1.072759      -1.410848
63195      O     -1.035209      -0.777322      -1.180760
63196      O     -1.126766      -1.809388      -0.207372
63197      H     -1.949097      -1.567550      0.250118
63198      H     -0.984771      0.130074      1.437365
63199      H     -0.486988      1.759504      0.943365
63200      Rotational constants (GHz):      1.1976900      0.7018400      0.6204400
63201      Vibrational harmonic frequencies (cm-1):
63202      i300.5371      41.0806      61.7556
63203      109.3703      129.5530      163.1552
63204      178.0678      192.2040      198.4296
63205      225.2222      234.2380      266.7898
63206      278.6625      308.5360      330.4570
63207      360.1056      395.5175      417.5699
63208      441.5734      480.6571      554.8545
63209      571.3729      593.2874      668.5030
63210      855.0232      912.8806      956.2970
63211      972.6387      998.6365      1038.2128
63212      1053.7916      1114.7153      1124.0042
63213      1137.6516      1235.9801      1264.7174
63214      1297.2066      1319.6998      1369.5724
63215      1399.2734      1408.9872      1411.3905
63216      1428.1082      1445.4502      1476.7072
63217      1479.3776      1486.3247      2082.7606
63218      3059.1825      3061.0748      3096.7330
63219      3137.2332      3170.4808      3179.2876
63220      3716.0055      3740.4808      3799.6814
63221      Zero-point correction (Hartree): 0.153618
63222
63223      TS.triHPacyl.COelim.ppmmmmpmpu
63224      -----
63225      IRC pathway available
63226      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18805922
63227      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.06957720
63228      T1 diagnostic: 0.017128
63229      E(MP2/Aug-CC-pVTZ) (Hartree): -721.03102741
63230      E(MP3/Aug-CC-pVTZ) (Hartree): -721.04844550
63231      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03686691
63232      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05224551
63233      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.50697098
63234      E(UHF/Aug-CC-pVTZ) (Hartree): -718.49932757
63235      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16364686
63236      Electronic state : 2-A
63237      Cartesian coordinates (Angs):
63238      O      0.059685      -0.145586      1.910281
63239      O      -0.647663      -1.094497      1.127877
63240      C      -0.963494      -0.618260      -0.115535
63241      C      0.149352      -0.158685      -1.058519
63242      C      1.459254      -0.938346      -0.904776
63243      O      2.155924      -0.757481      0.313922
63244      O      3.056246      0.330632      0.184770
63245      H      0.982003      -0.351661      1.661284
63246      C      -1.970227      -1.550055      -0.719338
63247      H      -2.743787      -1.788786      0.006632
63248      H      -1.491618      -2.481583      -1.035942
63249      H      -2.432847      -1.085641      -1.588528
63250      C      -2.058955      1.082969      0.304212
63251      O      -3.173188      0.986996      0.083237
63252      H      2.456078      1.096813      0.255955
63253      H      -0.205238      -0.399627      -2.065002
63254      O      0.304908      1.247608      -1.175996
63255      O      0.791575      1.808377      0.029645
63256      H      0.006999      1.788574      0.607657
63257      H      1.222134      -2.004052      -0.942387
63258      H      2.130789      -0.688159      -1.725822
63259      Rotational constants (GHz):      1.4451200      0.7079000      0.6569500
63260      Vibrational harmonic frequencies (cm-1):
63261      i321.8545      33.6399      87.2889

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63262	99.0342	157.3734	175.4494			
63263	198.0846	207.2494	227.7120			
63264	232.7120	254.4286	267.3102			
63265	279.0335	302.1402	337.9573			
63266	373.8006	426.4893	498.4243			
63267	498.9231	547.3746	557.7805			
63268	592.6391	672.7555	724.5748			
63269	825.7728	917.4248	948.5917			
63270	963.7123	1010.3014	1046.6228			
63271	1055.2275	1059.2372	1128.9693			
63272	1157.4516	1188.8064	1281.2431			
63273	1327.6115	1341.6417	1387.7185			
63274	1402.3899	1410.6482	1450.1214			
63275	1458.1548	1477.8135	1487.0534			
63276	1491.1672	1505.2875	2084.3650			
63277	3045.1039	3068.3590	3076.8145			
63278	3126.0215	3132.0163	3166.8172			
63279	3581.4212	3628.8298	3651.0098			
63280	Zero-point correction (Hartree): 0.154086					
63281						
63282	TS.triHPacyl.COelim.ppmmpmpmu					
63283	-----					
63284	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16165605					
63285	Electronic state : 2-A					
63286	Cartesian coordinates (Angs):					
63287	O	0.449665	-0.748013	1.671465		
63288	O	0.332600	0.610214	1.274827		
63289	C	0.455630	0.772293	-0.076615		
63290	C	-0.330668	-0.105924	-1.033006		
63291	C	-1.807415	0.288876	-1.109744		
63292	O	-2.389661	0.651743	0.126916		
63293	O	-2.335414	-0.462762	1.002842		
63294	H	-0.479362	-1.030736	1.616621		
63295	C	0.402679	2.239985	-0.374556		
63296	H	1.148020	2.767701	0.218287		
63297	H	-0.581239	2.646898	-0.131273		
63298	H	0.616608	2.406944	-1.429291		
63299	C	2.451196	0.436452	-0.544594		
63300	O	3.089037	0.101913	0.340543		
63301	H	-3.208831	-0.860845	0.897204		
63302	H	0.116255	0.050520	-2.021581		
63303	O	-0.337571	-1.493590	-0.754333		
63304	O	0.988540	-1.981419	-0.806007		
63305	H	1.267052	-1.863941	0.118219		
63306	H	-1.916496	1.192812	-1.708617		
63307	H	-2.368103	-0.524134	-1.578495		
63308	Rotational constants (GHz):			1.3356700	0.7777600	0.7047700
63309	Vibrational harmonic frequencies (cm-1):					
63310	i317.3308		75.1753			89.0043
63311	100.3279		128.6027			150.9747
63312	179.1825		197.8635			201.1703
63313	228.1041		237.4121			254.5253
63314	265.5446		270.8944			296.5495
63315	338.4488		370.5571			400.3648
63316	455.8752		511.9821			518.5710
63317	595.6370		619.7575			724.7224
63318	839.9090		892.4112			952.4478
63319	972.3953		1018.8831			1050.8473
63320	1060.5825		1072.7314			1132.4460
63321	1164.9992		1213.6171			1291.2395
63322	1318.2005		1341.6567			1379.4635
63323	1390.6147		1406.7369			1418.5141
63324	1441.7024		1465.3598			1471.2959
63325	1479.1337		1504.5338			2073.8392
63326	3041.5112		3057.4100			3061.5611
63327	3129.0075		3135.7175			3153.5311
63328	3706.9545		3718.3259			3814.3159
63329	Zero-point correction (Hartree): 0.153510					
63330						
63331	TS.triHPacyl.COelim.ppmmpmpmu					
63332	-----					
63333	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16098160					

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63334 Electronic state : 2-A
63335 Cartesian coordinates (Angs):
63336 O 0.510621 -0.626847 1.711980
63337 O 0.254516 0.682300 1.217927
63338 C 0.387534 0.763162 -0.144954
63339 C -0.331527 -0.240772 -1.026205
63340 C -1.837700 0.036627 -1.130568
63341 O -2.427975 0.581175 0.024959
63342 O -2.342359 -0.402752 1.058350
63343 H -0.321735 -1.082353 1.491817
63344 C 0.240423 2.196763 -0.553378
63345 H 0.932316 2.819300 0.011693
63346 H -0.775877 2.550226 -0.368708
63347 H 0.471414 2.296047 -1.613074
63348 C 2.409565 0.534793 -0.565210
63349 O 3.057907 0.307863 0.345436
63350 H -2.178258 0.173205 1.817294
63351 H 0.109312 -0.149242 -2.024337
63352 O -0.234958 -1.595233 -0.617429
63353 O 1.116906 -2.005270 -0.700894
63354 H 1.441376 -1.798206 0.191329
63355 H -2.019310 0.802491 -1.883930
63356 H -2.346261 -0.884807 -1.422825
63357 Rotational constants (GHz): 1.3259500 0.7805300 0.7082900
63358 Vibrational harmonic frequencies (cm-1):
63359 1323.4060 65.2931 77.7806
63360 89.4657 129.8851 172.7456
63361 178.7646 200.2067 212.9085
63362 220.8798 241.0638 264.3271
63363 273.4978 285.4470 324.9122
63364 337.2345 366.9716 404.2704
63365 445.6402 511.6623 551.3332
63366 616.7621 621.6728 722.8416
63367 835.1618 894.6810 950.2412
63368 969.4079 1018.7160 1040.7141
63369 1059.5692 1068.4563 1140.1288
63370 1158.0584 1208.9530 1290.0581
63371 1308.4893 1335.1074 1373.7718
63372 1407.4885 1413.1263 1441.9492
63373 1446.8482 1466.9670 1471.8277
63374 1479.3623 1503.5385 2076.4655
63375 3051.5744 3061.5671 3074.5431
63376 3132.4389 3138.0332 3153.8550
63377 3679.5376 3729.9182 3808.7763
63378 Zero-point correction (Hartree): 0.153787
63379
63380 TS.triHPacyl.COelim.ppmmpmpu
63381 -----
63382 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16146033
63383 Electronic state : 2-A
63384 Cartesian coordinates (Angs):
63385 O 0.146590 -0.333631 1.788085
63386 O 0.809867 0.818381 1.296226
63387 C 1.044038 0.759591 -0.051154
63388 C -0.094138 0.437693 -1.017002
63389 C -1.420564 1.118185 -0.662212
63390 O -2.036298 0.690173 0.539491
63391 O -2.972610 -0.335984 0.253199
63392 H -0.785655 -0.057194 1.693869
63393 C 1.870115 1.956266 -0.413755
63394 H 2.674383 2.083336 0.307893
63395 H 1.264875 2.867150 -0.418185
63396 H 2.305016 1.813757 -1.400697
63397 C 2.390977 -0.806335 -0.350986
63398 O 2.173890 -1.750329 0.253888
63399 H -2.387468 -1.097180 0.078028
63400 H 0.212322 0.888530 -1.965222
63401 O -0.207012 -0.921033 -1.420938
63402 O -0.748034 -1.742563 -0.402176
63403 H -0.004945 -1.863802 0.213524
63404 H -1.221368 2.182980 -0.522149
63405 H -2.130877 0.989896 -1.478617

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63406	Rotational constants (GHz):	1.2966300	0.8016000	0.7047600
63407	Vibrational harmonic frequencies (cm-1):			
63408	i314.0495	79.2130		89.4150
63409	98.6654	132.5539		168.4617
63410	180.1952	190.6444		199.2173
63411	235.0477	243.7304		264.2175
63412	271.2264	296.6116		334.4099
63413	363.8179	396.9759		445.1996
63414	498.4902	543.0021		563.8290
63415	602.0919	691.0341		724.6843
63416	822.5701	914.2525		945.7375
63417	962.5660	1010.9991		1045.1576
63418	1056.9229	1063.1671		1128.5767
63419	1156.8602	1189.1743		1284.6490
63420	1326.1968	1335.1422		1391.9420
63421	1400.4768	1411.5024		1459.3459
63422	1461.0211	1477.0211		1488.8016
63423	1492.2422	1507.5074		2064.1778
63424	3049.6688	3070.2254		3079.2763
63425	3130.0020	3132.2926		3165.5824
63426	3594.7784	3621.2436		3711.2770
63427	Zero-point correction (Hartree):	0.153920		
63428				
63429	TS.triHPacyl.COelim.ppmmtmpmu			
63430	-----			
63431	E(UM062X/Aug-CC-pVTZ) (Hartree):	-722.16200844		
63432	Electronic state : 2-A			
63433	Cartesian coordinates (Angs):			
63434	O	-0.106285	-1.001970	1.789271
63435	O	0.001524	0.389025	1.526461
63436	C	0.514055	0.639771	0.287267
63437	C	-0.076972	-0.039534	-0.935915
63438	C	-1.426685	0.561306	-1.340565
63439	O	-2.273804	0.898019	-0.260635
63440	O	-2.579087	-0.282559	0.464696
63441	H	-1.006500	-1.175994	1.465496
63442	C	0.727243	2.116551	0.155331
63443	H	1.344881	2.479958	0.974948
63444	H	-0.229195	2.643985	0.187636
63445	H	1.229441	2.336423	-0.786015
63446	C	2.512616	0.022172	0.341094
63447	O	3.122343	0.388170	-0.552090
63448	H	-3.440487	-0.533968	0.108057
63449	H	0.627527	0.132537	-1.758570
63450	O	-0.312388	-1.430201	-0.825001
63451	O	0.920494	-2.088651	-0.608828
63452	H	0.986199	-2.050016	0.360995
63453	H	-1.268645	1.517256	-1.839398
63454	H	-1.927136	-0.126453	-2.027419
63455	Rotational constants (GHz):	1.2933300	0.7693200	0.7015800
63456	Vibrational harmonic frequencies (cm-1):			
63457	i314.2819	68.4728		85.2460
63458	115.0186	120.7782		129.0149
63459	174.2846	185.6492		202.2405
63460	225.2145	231.0951		240.5142
63461	266.0664	276.3502		292.2986
63462	347.2826	390.2321		393.5687
63463	450.1643	472.7576		493.4725
63464	587.7306	618.9858		715.6119
63465	842.2841	894.8373		953.7869
63466	973.6342	1018.4590		1048.9561
63467	1056.9766	1071.3098		1132.4319
63468	1166.2416	1214.1743		1291.1953
63469	1323.7804	1339.8641		1379.1245
63470	1390.6117	1406.0016		1418.9693
63471	1448.6164	1464.6327		1469.2697
63472	1477.4737	1503.9047		2069.7435
63473	3035.0815	3053.4604		3062.5976
63474	3124.8278	3135.3827		3153.2589
63475	3694.4617	3706.2716		3815.7780
63476	Zero-point correction (Hartree):	0.153137		
63477				

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63478 TS.triHPacyl.COelim.ppmmtmpu
63479 -----
63480 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16165985
63481 Electronic state : 2-A
63482 Cartesian coordinates (Angs):
63483 O -0.028885 -1.012660 1.800337
63484 O -0.078848 0.375126 1.489461
63485 C 0.445649 0.648853 0.253041
63486 C -0.084181 -0.103240 -0.953951
63487 C -1.473633 0.387430 -1.389767
63488 O -2.306743 0.833874 -0.348270
63489 O -2.601515 -0.286528 0.486005
63490 H -0.777567 -1.358029 1.282156
63491 C 0.561259 2.132475 0.092348
63492 H 1.125080 2.557246 0.921162
63493 H -0.428332 2.594435 0.072961
63494 H 1.080700 2.361038 -0.837571
63495 C 2.479220 0.165766 0.372348
63496 O 3.097582 0.590009 -0.487142
63497 H -2.464414 0.115668 1.354798
63498 H 0.615890 0.074189 -1.777532
63499 O -0.220892 -1.503584 -0.778144
63500 O 1.065664 -2.071513 -0.615495
63501 H 1.198811 -1.994157 0.344565
63502 H -1.368922 1.270513 -2.019438
63503 H -1.962032 -0.406399 -1.959223
63504 Rotational constants (GHz): 1.2782200 0.7724900 0.7029400
63505 Vibrational harmonic frequencies (cm-1):
63506 i319.7179 67.8205 85.0364
63507 112.0352 125.8905 177.1969
63508 181.8588 199.6714 220.3774
63509 227.7337 239.5060 257.1492
63510 267.8686 304.5947 319.0297
63511 362.0474 386.2580 398.2096
63512 447.7300 491.7626 541.7438
63513 611.5956 617.9638 713.4554
63514 836.9616 895.9764 949.7605
63515 970.9902 1018.3946 1036.3991
63516 1054.8314 1065.7263 1140.4162
63517 1158.8195 1209.9537 1286.8771
63518 1310.9920 1334.6262 1374.3496
63519 1405.7391 1412.3818 1440.1608
63520 1452.3242 1466.6537 1472.1957
63521 1478.3565 1502.3229 2077.7705
63522 3048.8827 3057.3827 3073.0865
63523 3127.5828 3138.1189 3153.3270
63524 3694.1144 3714.9174 3803.4704
63525 Zero-point correction (Hartree): 0.153823
63526
63527 TS.triHPacyl.COelim.ppmptmpu
63528 -----
63529 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16361997
63530 Electronic state : 2-A
63531 Cartesian coordinates (Angs):
63532 O -0.358526 -0.046673 1.813241
63533 O -0.982932 -0.999019 0.973128
63534 C -0.969823 -0.630117 -0.345685
63535 C 0.259617 -0.012299 -0.959500
63536 C 1.511330 -0.885951 -0.836411
63537 O 1.920797 -1.159929 0.480286
63538 O 2.401282 0.051016 1.052869
63539 H -1.045486 0.633436 1.896763
63540 C -1.667115 -1.691941 -1.134089
63541 H -2.597588 -1.970254 -0.642260
63542 H -1.049249 -2.589694 -1.220435
63543 H -1.893675 -1.318279 -2.130216
63544 C -2.357662 0.970213 -0.439190
63545 O -2.635253 1.333894 0.608546
63546 H 1.611827 0.328101 1.546746
63547 H 0.050781 0.093268 -2.030142
63548 O 0.419631 1.289520 -0.407849
63549 O 1.534200 1.902609 -1.026628

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63550      H      2.245060      1.653332      -0.413395
63551      H      1.297347      -1.866206      -1.265793
63552      H      2.329302      -0.434459      -1.400769
63553      Rotational constants (GHz): 1.2550900      0.7667700      0.7028100
63554      Vibrational harmonic frequencies (cm-1):
63555      i293.8682      67.3061      78.9857
63556      123.4846      147.4852      164.6564
63557      173.6235      190.0884      200.2821
63558      216.3821      243.3860      259.6910
63559      277.1479      303.2416      325.7722
63560      349.9902      363.7646      404.2420
63561      476.3682      520.7773      537.1544
63562      572.9497      583.5689      747.0311
63563      844.0710      878.8467      953.4034
63564      975.6237      1031.4025      1046.3956
63565      1059.5992      1066.9594      1125.1266
63566      1167.3504      1211.4916      1296.7792
63567      1322.1001      1345.6050      1387.0704
63568      1409.8495      1413.8279      1426.5526
63569      1446.7159      1464.5457      1475.4989
63570      1478.6740      1496.6322      2056.9953
63571      3043.5686      3051.9624      3074.4847
63572      3122.6435      3127.0111      3163.4043
63573      3717.5226      3730.3770      3751.2216
63574      Zero-point correction (Hartree): 0.153755
63575
63576      TS.triHPacyl.COelim.ppmptmpu
63577      -----
63578      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16097280
63579      Electronic state : 2-A
63580      Cartesian coordinates (Angs):
63581      O      0.485142      -1.097486      1.791607
63582      O      0.015007      0.223069      1.504260
63583      C      0.412098      0.652413      0.256643
63584      C      -0.187514      -0.042261      -0.950189
63585      C      -1.595326      0.499335      -1.251493
63586      O      -2.360287      0.789807      -0.107110
63587      O      -2.736593      -0.434186      0.501605
63588      H      1.305656      -0.892088      2.262416
63589      C      0.435867      2.147175      0.222829
63590      H      1.091951      2.536336      0.999748
63591      H      -0.568011      2.545965      0.385357
63592      H      0.798431      2.484966      -0.748050
63593      C      2.485334      0.280688      0.196684
63594      O      2.982018      0.647949      -0.759177
63595      H      -2.016394      -0.575021      1.135013
63596      H      0.452634      0.165593      -1.815200
63597      O      -0.329715      -1.435879      -0.804332
63598      O      0.963264      -2.017109      -0.819360
63599      H      1.107912      -2.142653      0.130078
63600      H      -1.508533      1.457353      -1.764547
63601      H      -2.117092      -0.213877      -1.891617
63602      Rotational constants (GHz): 1.2605900      0.7558300      0.6953700
63603      Vibrational harmonic frequencies (cm-1):
63604      i325.6438      69.6598      82.2829
63605      98.6789      114.7647      155.1432
63606      176.8065      187.6017      204.8382
63607      224.8027      241.2356      246.4637
63608      264.3674      271.5181      314.9244
63609      348.6453      374.8085      388.0660
63610      399.2170      459.4242      484.1540
63611      510.3731      604.8905      718.9344
63612      844.3525      889.8393      939.9992
63613      985.0417      993.0475      1014.8431
63614      1055.0153      1066.4653      1140.5700
63615      1169.7718      1204.8640      1276.0247
63616      1293.7276      1331.2356      1376.8493
63617      1405.0070      1407.3937      1408.3644
63618      1431.6722      1437.3711      1463.4595
63619      1476.0792      1501.5480      2098.8546
63620      3045.1545      3055.6307      3079.5194
63621      3125.3591      3137.6730      3149.0167

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63622          3759.3525          3766.9639          3786.5919
63623 Zero-point correction (Hartree): 0.152770
63624
63625 TS.triHPacyl.COelim.ppmpttmpu
63626 -----
63627 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16449149
63628 Electronic state : 2-A
63629 Cartesian coordinates (Angs):
63630 O          0.060736          -0.906500          1.775359
63631 O          -0.629254          -1.512479          0.697716
63632 C          -0.961391          -0.594063          -0.258769
63633 C          0.080052          0.373365          -0.770051
63634 C          1.348290          -0.314831          -1.285768
63635 O          2.051430          -1.073036          -0.334093
63636 O          2.598877          -0.179920          0.629162
63637 H          -0.603756          -0.277063          2.107187
63638 C          -1.837633          -1.247954          -1.278184
63639 H          -2.588857          -1.861742          -0.784971
63640 H          -1.255858          -1.892595          -1.942684
63641 H          -2.336635          -0.487994          -1.877097
63642 C          -2.262789          0.650053          0.783678
63643 O          -2.959676          1.258976          0.117374
63644 H          1.929783          -0.258900          1.330130
63645 H          -0.363995          0.896366          -1.625137
63646 O          0.329611          1.329336          0.254771
63647 O          1.278649          2.263216          -0.220580
63648 H          2.105857          1.852994          0.081972
63649 H          1.065656          -1.036949          -2.053743
63650 H          2.005637          0.429701          -1.738758
63651 Rotational constants (GHz): 1.2808200          0.7660800          0.6642100
63652 Vibrational harmonic frequencies (cm-1):
63653 i302.9661          68.9775          70.8554
63654 132.3499          149.4906          162.1123
63655 173.3734          188.5769          199.6471
63656 226.4028          238.3287          274.0077
63657 296.2671          303.2390          335.8400
63658 362.0002          412.7459          434.3224
63659 479.6891          524.3352          531.9284
63660 572.2869          591.2749          744.3809
63661 844.3929          878.1014          954.4495
63662 975.0390          1028.5033          1047.4911
63663 1058.8341          1064.0149          1125.8485
63664 1167.7015          1210.5830          1296.2168
63665 1324.5525          1349.3899          1385.1998
63666 1410.0259          1412.6672          1440.3622
63667 1450.3823          1469.8612          1475.1105
63668 1479.6649          1494.1543          2082.8210
63669 3038.9344          3049.3580          3074.8836
63670 3122.5583          3124.2010          3160.6189
63671 3689.6114          3714.9663          3732.3092
63672 Zero-point correction (Hartree): 0.154016
63673
63674 TS.triHPacyl.COelim.ppmppmpmu
63675 -----
63676 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16222932
63677 Electronic state : 2-A
63678 Cartesian coordinates (Angs):
63679 O          -0.320718          0.201865          1.811099
63680 O          -0.086210          -0.925166          0.980721
63681 C          -0.326161          -0.662848          -0.352274
63682 C          0.230993          0.610416          -0.956400
63683 C          1.759944          0.645659          -0.942039
63684 O          2.273648          0.475681          0.371632
63685 O          2.677533          -0.876486          0.539618
63686 H          0.496678          0.716790          1.684191
63687 C          -0.060928          -1.918934          -1.126997
63688 H          -0.616551          -2.748463          -0.692015
63689 H          1.001656          -2.172297          -1.121607
63690 H          -0.390537          -1.784571          -2.155498
63691 C          -2.385979          -0.621613          -0.587466
63692 O          -2.972760          -0.733515          0.383792
63693 H          1.920530          -1.254058          1.013993

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63694	H	-0.131789	0.649114	-1.988940		
63695	O	-0.099312	1.818066	-0.288760		
63696	O	-1.499543	1.938979	-0.150219		
63697	H	-1.639372	1.553830	0.730534		
63698	H	2.188603	-0.108159	-1.598996		
63699	H	2.082454	1.636350	-1.263672		
63700	Rotational constants (GHz):			1.3345000	0.7882800	0.6825800
63701	Vibrational harmonic frequencies (cm-1):					
63702		i339.0617	77.3157			94.4304
63703		104.1273	126.9493			162.4180
63704		195.9212	204.0480			221.1450
63705		236.4902	270.3507			277.8158
63706		283.2387	301.8000			319.5114
63707		350.0575	434.5096			460.3540
63708		490.3370	517.0533			535.4128
63709		570.0260	613.1311			713.5536
63710		823.6492	919.5209			932.9951
63711		962.1594	1006.9516			1052.6092
63712		1063.2361	1074.7682			1117.9604
63713		1153.7166	1197.6379			1280.4985
63714		1298.8141	1325.9104			1377.8052
63715		1403.9051	1411.1274			1437.9250
63716		1447.1582	1465.5947			1472.4958
63717		1480.2996	1504.2668			2080.6360
63718		3055.0945	3059.6726			3093.2837
63719		3129.9151	3154.0850			3158.2590
63720		3695.4592	3728.6058			3742.5716
63721	Zero-point correction (Hartree): 0.154160					
63722						
63723	TS.triHPacyl.COelim.pppmptmpmu					
63724	-----					
63725	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16275084					
63726	Electronic state : 2-A					
63727	Cartesian coordinates (Angs):					
63728	O	-0.111811	-0.613935	1.930035		
63729	O	-0.204189	0.659517	1.309781		
63730	C	0.367275	0.674159	0.056966		
63731	C	-0.017638	-0.414344	-0.926669		
63732	C	-1.500288	-0.367265	-1.305272		
63733	O	-2.338617	-0.449738	-0.163890		
63734	O	-2.756756	0.859875	0.196388		
63735	H	-0.854191	-1.091576	1.520102		
63736	C	0.317475	2.076680	-0.468656		
63737	H	0.753315	2.762764	0.255895		
63738	H	-0.712138	2.386999	-0.663245		
63739	H	0.885780	2.141023	-1.395070		
63740	C	2.425541	0.541769	0.375498		
63741	O	3.057621	0.815503	-0.532908		
63742	H	-2.150782	1.067283	0.924441		
63743	H	0.593456	-0.265189	-1.823763		
63744	O	0.132015	-1.746129	-0.463837		
63745	O	1.467271	-1.977013	-0.064127		
63746	H	1.433633	-1.732691	0.875743		
63747	H	-1.742557	0.530116	-1.871043		
63748	H	-1.724967	-1.249357	-1.905792		
63749	Rotational constants (GHz):			1.3034800	0.7678100	0.6737300
63750	Vibrational harmonic frequencies (cm-1):					
63751		i333.4842	66.3072			69.7812
63752		102.7155	123.6699			164.9767
63753		196.7421	208.1304			219.0871
63754		238.1261	249.3480			265.7591
63755		286.8818	301.4201			318.4181
63756		381.0698	427.5543			447.4247
63757		473.4036	515.0813			519.4238
63758		566.9677	611.6906			704.4266
63759		823.9146	922.7186			935.7039
63760		962.7269	1007.9280			1048.6945
63761		1060.4914	1072.9649			1120.4454
63762		1154.9496	1199.8205			1279.0854
63763		1302.4581	1322.4767			1376.6611
63764		1402.2369	1410.4469			1442.1644
63765		1449.0709	1464.9673			1468.6492

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63766      1478.9625          1503.8949          2082.2958
63767      3049.1784          3055.6507          3090.7991
63768      3126.4224          3151.3759          3156.7701
63769      3702.1139          3724.0175          3742.6587
63770      Zero-point correction (Hartree): 0.153893
63771
63772      TS.triHPacyl.COelim.pppptmpu
63773      -----
63774      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16151348
63775      Electronic state : 2-A
63776      Cartesian coordinates (Angs):
63777      O      -2.157840          1.012642          0.953500
63778      O      -1.199739          0.111536          1.498845
63779      C      -0.476738          -0.524305          0.521201
63780      C      0.345226          0.263725          -0.477781
63781      C      1.571752          0.940557          0.150075
63782      O      2.510515          -0.004584          0.618324
63783      O      2.986080          -0.741290          -0.503014
63784      H      -2.715031          0.409105          0.431477
63785      C      0.139383          -1.756431          1.101020
63786      H      -0.634808          -2.408764          1.503919
63787      H      0.831735          -1.499622          1.904993
63788      H      0.702317          -2.284569          0.333256
63789      C      -1.984467          -1.312060          -0.723546
63790      O      -1.591268          -2.048158          -1.498413
63791      H      3.895588          -0.425847          -0.569487
63792      H      0.706111          -0.465399          -1.206678
63793      O      -0.385800          1.185619          -1.262606
63794      O      -0.467480          2.434360          -0.589567
63795      H      -1.233606          2.286464          -0.009006
63796      H      2.018818          1.608828          -0.588462
63797      H      1.302201          1.509885          1.037639
63798      Rotational constants (GHz): 1.0744200 0.7604500 0.6260900
63799      Vibrational harmonic frequencies (cm-1):
63800      i295.0621          30.4177          62.8105
63801      71.8166          125.0913          167.1234
63802      170.5112          182.5089          191.9898
63803      225.1833          233.5408          241.4463
63804      252.0554          273.1558          308.3451
63805      337.7097          369.5790          415.5419
63806      442.2337          489.6405          544.1178
63807      584.4516          635.3136          674.7057
63808      796.4843          942.5986          944.0720
63809      977.7569          1021.8663          1031.8974
63810      1047.7861          1097.7039          1118.7430
63811      1151.6674          1202.7687          1275.3009
63812      1298.9247          1323.7555          1379.3824
63813      1400.2635          1412.5671          1419.1132
63814      1437.5328          1458.8041          1471.5857
63815      1475.2282          1489.3072          2093.9293
63816      3059.5275          3076.1122          3093.6718
63817      3124.3647          3152.1790          3155.4223
63818      3656.8436          3688.1593          3826.3606
63819      Zero-point correction (Hartree): 0.152936
63820
63821      TS.triHPacyl.COelim.pptmpptmpu
63822      -----
63823      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16220527
63824      Electronic state : 2-A
63825      Cartesian coordinates (Angs):
63826      O      -1.323434          -0.048449          1.853675
63827      O      -1.587711          -1.028261          0.865866
63828      C      -0.995536          -0.701927          -0.324927
63829      C      0.382019          -0.092870          -0.306059
63830      C      1.324270          -0.883205          0.599497
63831      O      2.612469          -0.305214          0.665275
63832      O      3.210140          -0.415397          -0.617728
63833      H      -1.987617          0.628737          1.650641
63834      C      -1.258935          -1.791150          -1.313762
63835      H      -2.302487          -2.097148          -1.261367
63836      H      -0.635319          -2.666538          -1.113344
63837      H      -1.047606          -1.430085          -2.317818

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63838	C	-2.191509	0.880286	-1.063721		
63839	O	-2.887393	1.283492	-0.251898		
63840	H	2.957088	0.426786	-1.026069		
63841	H	0.740343	-0.112039	-1.336976		
63842	O	0.308302	1.273528	0.095992		
63843	O	1.459495	1.938728	-0.411331		
63844	H	2.021029	1.966897	0.376297		
63845	H	0.960603	-0.852053	1.625454		
63846	H	1.397162	-1.918776	0.258193		
63847	Rotational constants (GHz):			1.4010700	0.6391500	0.5809400
63848	Vibrational harmonic frequencies (cm-1):					
63849		i299.7071	64.8815			73.7432
63850		101.0757	123.9676			159.6520
63851		168.0240	172.1227			188.8938
63852		197.7169	213.4987			225.9257
63853		253.3130	293.3120			324.8864
63854		350.0522	369.2457			398.3794
63855		435.9590	473.7121			517.2201
63856		523.9135	591.6577			608.2246
63857		889.9048	922.1149			960.7808
63858		989.2960	1018.8910			1057.3527
63859		1061.8915	1086.2220			1124.8736
63860		1139.2543	1213.4401			1302.5394
63861		1322.2848	1339.4807			1395.9149
63862		1410.2078	1416.5164			1422.4856
63863		1432.5609	1439.1614			1468.7374
63864		1479.0853	1492.3635			2060.7623
63865		3050.7751	3067.7792			3092.3574
63866		3126.6420	3153.3229			3163.5384
63867		3752.4179	3756.6765			3787.5246
63868	Zero-point correction (Hartree):			0.153153		
63869	-----					
63870	TS.triHPacyl.COelim.pptmpttmpu					
63871	-----					
63872	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.16290169		
63873	Electronic state : 2-A					
63874	Cartesian coordinates (Angs):					
63875	O	1.152785	-1.143123	-1.812614		
63876	O	1.485050	-1.507256	-0.484847		
63877	C	1.089102	-0.527667	0.382228		
63878	C	-0.302688	0.038731	0.229970		
63879	C	-1.321223	-1.078568	0.014760		
63880	O	-2.629143	-0.579978	-0.180073		
63881	O	-3.050759	0.033844	1.028754		
63882	H	1.722270	-0.366849	-1.952639		
63883	C	1.546452	-0.862898	1.764696		
63884	H	2.565556	-1.243999	1.739122		
63885	H	0.905440	-1.624873	2.216797		
63886	H	1.515390	0.029218	2.388099		
63887	C	2.317695	1.058425	-0.180499		
63888	O	2.457982	1.852476	0.625297		
63889	H	-2.784295	0.955190	0.885896		
63890	H	-0.523880	0.585422	1.148860		
63891	O	-0.334635	0.976435	-0.844515		
63892	O	-1.441248	1.845053	-0.633793		
63893	H	-2.098626	1.458898	-1.230016		
63894	H	-1.091264	-1.609037	-0.908216		
63895	H	-1.306866	-1.771705	0.859495		
63896	Rotational constants (GHz):			1.2607900	0.6600300	0.5973000
63897	Vibrational harmonic frequencies (cm-1):					
63898		i307.7214	53.9246			73.7952
63899		98.1427	142.7450			149.5262
63900		167.0023	170.9056			191.4953
63901		198.4529	221.0282			242.6674
63902		271.9057	297.2385			340.8059
63903		366.9945	415.8464			426.6146
63904		450.5636	474.0919			512.6094
63905		518.2770	585.6201			609.4681
63906		890.4058	923.5833			960.2156
63907		987.4772	1017.9270			1057.5915
63908		1059.4367	1085.4627			1124.8013
63909		1139.0395	1213.1930			1302.9863

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63910      1316.7364          1341.5498          1392.8077
63911      1408.8046          1418.1160          1422.9319
63912      1440.0171          1443.8614          1469.1390
63913      1479.5169          1490.6810          2085.9198
63914      3047.6358          3068.0393          3086.4049
63915      3123.6947          3148.9226          3161.1502
63916      3705.4551          3749.0874          3787.1296
63917      Zero-point correction (Hartree): 0.153388
63918
63919      TS.triHPacyl.COelim.pptpptomu
63920      -----
63921      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16060178
63922      Electronic state : 2-A
63923      Cartesian coordinates (Angs):
63924      O      -0.603378      -0.592708      2.055915
63925      O      -1.229123      -1.296938      0.998334
63926      C      -1.088561      -0.642731      -0.194697
63927      C      0.293260      -0.184409      -0.640165
63928      C      1.419409      -1.025332      -0.046142
63929      O      2.661877      -0.738655      -0.657732
63930      O      3.160188      0.474089      -0.099800
63931      H      -0.980648      0.300669      1.962737
63932      C      -1.922402      -1.339862      -1.223966
63933      H      -2.898519      -1.591577      -0.814717
63934      H      -1.437021      -2.262724      -1.554926
63935      H      -2.056481      -0.689886      -2.087422
63936      C      -2.129957      1.096559      0.170208
63937      O      -2.674620      1.539548      -0.728296
63938      H      2.977426      1.103411      -0.811244
63939      H      0.327451      -0.306622      -1.725967
63940      O      0.539912      1.215974      -0.532433
63941      O      0.681873      1.600313      0.824944
63942      H      1.616975      1.395778      0.990650
63943      H      1.491840      -0.910630      1.032820
63944      H      1.234644      -2.076746      -0.270812
63945      Rotational constants (GHz):      1.3551400      0.6704700      0.6178300
63946      Vibrational harmonic frequencies (cm-1):
63947      i323.1840          64.8625          75.2355
63948      86.5986          145.4498          168.2335
63949      182.0731          190.5147          205.1828
63950      210.7988          231.3239          242.2070
63951      259.9902          299.8453          318.6284
63952      344.3223          385.3276          423.8966
63953      450.0444          499.9776          542.4779
63954      567.2049          582.3391          657.0096
63955      839.8159          912.3493          946.8197
63956      984.8553          1002.3075          1050.0058
63957      1058.4136          1101.9625          1112.5343
63958      1130.8058          1203.8916          1298.5942
63959      1303.0539          1329.1568          1394.6479
63960      1404.4115          1408.5762          1415.5157
63961      1450.1591          1475.8621          1479.3443
63962      1483.6148          1490.7867          2083.3139
63963      3043.7003          3079.9647          3098.3302
63964      3122.1584          3161.1564          3161.6308
63965      3683.3819          3722.5620          3795.6219
63966      Zero-point correction (Hartree): 0.153464
63967
63968      TS.triHPacyl.COelim.pptpttmpu
63969      -----
63970      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16075868
63971      Electronic state : 2-A
63972      Cartesian coordinates (Angs):
63973      O      -0.760055      -1.066352      1.904758
63974      O      -1.325304      -1.523085      0.688314
63975      C      -1.137736      -0.587535      -0.291263
63976      C      0.233971      0.038709      -0.418143
63977      C      1.306399      -1.046584      -0.335260
63978      O      2.579089      -0.628755      -0.800141
63979      O      3.176508      0.194766      0.191241
63980      H      -1.288928      -0.268729      2.082685
63981      C      -1.824137      -1.021706      -1.544253

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63982	H	-2.803021	-1.436519	-1.310847	
63983	H	-1.244836	-1.786887	-2.069682	
63984	H	-1.948497	-0.167373	-2.207849	
63985	C	-2.310508	0.996742	0.411744	
63986	O	-2.635519	1.731804	-0.396243	
63987	H	3.809797	-0.403427	0.606183	
63988	H	0.284318	0.529026	-1.392222	
63989	O	0.411591	1.043445	0.573847	
63990	O	1.187396	2.092475	0.020791	
63991	H	2.089272	1.792583	0.215270	
63992	H	1.376377	-1.422882	0.685619	
63993	H	1.047930	-1.867943	-1.006641	
63994	Rotational constants (GHz):		1.2890800	0.6672200	0.5784700
63995	Vibrational harmonic frequencies (cm-1):				
63996	i	301.3224	46.1303		64.0005
63997		68.9845	133.9985		149.4600
63998		150.7449	170.4630		183.9899
63999		200.6132	210.3781		233.8575
64000		238.8413	272.3082		312.3740
64001		334.1129	381.9040		423.6258
64002		429.5011	471.2083		511.4440
64003		531.6775	548.7555		610.9564
64004		875.2974	930.9844		963.9846
64005		979.3589	1026.3457		1056.1647
64006		1063.1654	1091.3160		1108.0182
64007		1129.7884	1206.0155		1305.9884
64008		1311.9621	1332.2558		1381.1973
64009		1387.2543	1409.6962		1418.5297
64010		1449.9586	1455.1543		1458.7306
64011		1478.6808	1491.1569		2087.7271
64012		3041.8682	3077.7178		3092.8329
64013		3119.2109	3138.6962		3158.5085
64014		3698.5233	3740.3556		3822.0538
64015	Zero-point correction (Hartree):		0.152564		
64016	TS.triHPacyl.COelim.ptmmmmpppu				
64017	-----				
64018	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16108232				
64019	Electronic state : 2-A				
64020	Cartesian coordinates (Angs):				
64021	O	-2.133543	1.441232	-0.479307	
64022	O	-1.623428	0.809754	0.685931	
64023	C	-0.717334	-0.170548	0.357393	
64024	C	0.366689	0.228341	-0.611524	
64025	C	1.321021	-0.909300	-0.961284	
64026	O	2.152784	-1.288335	0.115903	
64027	O	3.327559	-0.492973	0.089204	
64028	H	-1.490175	2.156780	-0.609523	
64029	C	-0.397018	-0.956859	1.587143	
64030	H	-1.316042	-1.143752	2.139754	
64031	H	0.304035	-0.417951	2.229346	
64032	H	0.066597	-1.905221	1.323766	
64033	C	-1.849566	-1.487426	-0.762617	
64034	O	-2.861656	-1.708406	-0.288142	
64035	H	3.027456	0.339556	0.481758	
64036	H	-0.083079	0.592905	-1.536539	
64037	O	1.200703	1.264802	-0.068947	
64038	O	0.467524	2.479463	-0.003209	
64039	H	0.234563	2.525991	0.934597	
64040	H	0.731067	-1.788782	-1.219440	
64041	H	1.943283	-0.629058	-1.809846	
64042	Rotational constants (GHz):		1.2609400	0.7215800	0.5453700
64043	Vibrational harmonic frequencies (cm-1):				
64044	i	326.4535	50.2752		76.8188
64045		79.1734	115.4296		136.6508
64046		158.0682	169.8641		190.3314
64047		206.7843	225.4755		242.6688
64048		261.9949	271.5909		310.9873
64049		376.9598	380.5642		388.0859
64050		416.2401	500.3157		539.4210
64051		550.2287	616.1246		691.8049
64052		794.8525	899.0137		958.0967

64054	985.8688	1020.5620	1044.9764			
64055	1054.6746	1059.8361	1104.7611			
64056	1140.3331	1224.7204	1288.6758			
64057	1331.4729	1345.4571	1383.9602			
64058	1401.7553	1413.3963	1417.4758			
64059	1441.2990	1449.1804	1470.2171			
64060	1475.1910	1486.9082	2087.4487			
64061	3054.4702	3089.4074	3097.9185			
64062	3128.5963	3147.5428	3164.9487			
64063	3730.0482	3776.2686	3792.3018			
64064	Zero-point correction (Hartree): 0.153133					
64065	TS.triHPacyl.COelim.ptmmmpmpu					
64066	-----					
64067	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16185239					
64068	Electronic state : 2-A					
64069	Cartesian coordinates (Angs):					
64070	O	-1.940325	1.712493	-0.460295		
64071	O	-1.447825	1.016220	0.677842		
64072	C	-0.771394	-0.120005	0.294967		
64073	C	0.251858	0.119246	-0.792230		
64074	C	1.248874	-1.013218	-0.981635		
64075	O	2.075077	-1.280999	0.129141		
64076	O	3.227365	-0.458893	0.044106		
64077	H	-1.179928	2.263167	-0.704747		
64078	C	-0.493999	-0.950780	1.506288		
64079	H	-1.411242	-1.051450	2.084646		
64080	H	0.282435	-0.502032	2.129094		
64081	H	-0.142767	-1.938601	1.215201		
64082	C	-2.165238	-1.262804	-0.673741		
64083	O	-3.161419	-1.333186	-0.124469		
64084	H	2.937909	0.339533	0.511385		
64085	H	-0.272458	0.234623	-1.745174		
64086	O	0.844873	1.416842	-0.641680		
64087	O	1.419602	1.541245	0.651680		
64088	H	0.674913	1.851189	1.188151		
64089	H	0.679308	-1.929136	-1.158574		
64090	H	1.872450	-0.811699	-1.852484		
64091	Rotational constants (GHz):			1.4418600	0.6893000	0.5692400
64092	Vibrational harmonic frequencies (cm-1):					
64093	i339.7327	50.2740	77.2873			
64094	90.4877	112.5437	132.3217			
64095	168.9178	203.8648	214.7051			
64096	224.9725	234.8236	243.2323			
64097	270.7787	287.7195	340.3607			
64098	357.4265	396.0681	429.7406			
64099	452.9887	492.7914	520.8967			
64100	541.1318	620.0084	719.6620			
64101	815.6250	898.7390	948.4192			
64102	962.4420	1014.2133	1027.2491			
64103	1047.3719	1068.2119	1106.8688			
64104	1162.3070	1225.0260	1295.9557			
64105	1316.8519	1364.2526	1375.0561			
64106	1408.9691	1412.6114	1417.2142			
64107	1436.2479	1451.3784	1461.7225			
64108	1470.9833	1485.1429	2085.3692			
64109	3060.6155	3069.7024	3077.7910			
64110	3129.4470	3130.8170	3161.8039			
64111	3746.7367	3752.1751	3767.4226			
64112	Zero-point correction (Hartree): 0.153407					
64113	TS.triHPacyl.COelim.ptmmmpmpu					
64114	-----					
64115	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16202811					
64116	Electronic state : 2-A					
64117	Cartesian coordinates (Angs):					
64118	O	-1.911191	1.754391	-0.531706		
64119	O	-1.583114	1.014807	0.632887		
64120	C	-0.815862	-0.072634	0.326414		
64121	C	0.220979	0.148340	-0.749803		
64122	C	1.172938	-1.022497	-0.943793		
64123	O	2.061763	-1.269868	0.133154		

64126	O	3.149537	-0.356359	0.008954			
64127	H	-1.145356	2.346278	-0.602302			
64128	C	-0.532304	-0.828093	1.584838			
64129	H	-1.459834	-0.943312	2.144367			
64130	H	0.194695	-0.290626	2.194746			
64131	H	-0.131509	-1.814311	1.358669			
64132	C	-2.078041	-1.360940	-0.634873			
64133	O	-3.123728	-1.391081	-0.176913			
64134	H	3.905715	-0.954673	0.017263			
64135	H	-0.302124	0.266377	-1.702655			
64136	O	0.874648	1.408451	-0.614893			
64137	O	1.350984	1.568194	0.714631			
64138	H	2.242946	1.191229	0.655376			
64139	H	0.584398	-1.936972	-1.036481			
64140	H	1.753608	-0.877323	-1.854602			
64141	Rotational constants (GHz):				1.4244700	0.6927200	0.5703900
64142	Vibrational harmonic frequencies (cm-1):						
64143	i311.4280			47.3061		80.8067	
64144	85.2961			110.6600		130.4415	
64145	164.0676			175.0855		204.1677	
64146	227.7096			234.3336		244.4304	
64147	247.3963			261.5639		290.2596	
64148	324.6212			370.0601		399.9860	
64149	444.6632			486.7566		522.9867	
64150	542.4025			627.6188		716.5731	
64151	826.2524			901.9323		946.8538	
64152	969.9588			1011.9193		1029.6122	
64153	1056.5141			1073.7861		1104.8494	
64154	1157.0658			1249.9212		1303.0013	
64155	1327.0023			1373.0149		1377.8479	
64156	1390.8399			1410.7528		1419.0748	
64157	1443.2363			1463.8307		1464.7899	
64158	1478.8495			1495.2871		2070.7002	
64159	3066.1578			3075.2714		3085.0361	
64160	3137.2681			3138.4551		3156.4636	
64161	3740.6862			3745.7217		3839.3704	
64162	Zero-point correction (Hartree):				0.153254		
64163							
64164	TS.triHPacyl.COelim.ptmmmtmmu						
64165	-----						
64166	E(UM062X/Aug-CC-pVTZ) (Hartree):				-722.16235546		
64167	Electronic state : 2-A						
64168	Cartesian coordinates (Angs):						
64169	O	-1.769326	1.951997	0.019850			
64170	O	-1.652503	0.861432	0.915493			
64171	C	-0.911072	-0.152907	0.374540			
64172	C	0.247567	0.275402	-0.489616			
64173	C	1.129316	-0.881382	-0.937026			
64174	O	1.879315	-1.467533	0.112478			
64175	O	3.025332	-0.654144	0.348159			
64176	H	-0.965612	2.455056	0.227247			
64177	C	-0.778814	-1.237987	1.394112			
64178	H	-1.743928	-1.391717	1.874675			
64179	H	-0.038434	-0.968253	2.149550			
64180	H	-0.462447	-2.168470	0.926818			
64181	C	-2.139023	-1.034105	-1.029236			
64182	O	-3.236640	-1.031490	-0.718976			
64183	H	3.737635	-1.261015	0.112365			
64184	H	-0.135960	0.764999	-1.388600			
64185	O	0.952137	1.238687	0.288958			
64186	O	1.963772	1.816620	-0.523153			
64187	H	2.724690	1.270552	-0.270885			
64188	H	0.495152	-1.681384	-1.321242			
64189	H	1.804362	-0.558448	-1.729047			
64190	Rotational constants (GHz):				1.3760300	0.6700700	0.5441400
64191	Vibrational harmonic frequencies (cm-1):						
64192	i311.8839			40.5118		76.8760	
64193	89.6754			106.1466		130.6686	
64194	164.0900			194.5723		207.2980	
64195	223.1655			235.7801		250.1357	
64196	259.7648			274.0859		290.5567	
64197	321.2932			345.8766		444.8231	

64198	454.3193	486.4722	505.7238			
64199	547.6225	602.3771	731.4099			
64200	806.6799	884.9427	965.2027			
64201	970.0640	1027.0194	1032.6213			
64202	1059.2852	1078.2382	1100.6619			
64203	1161.4914	1249.7943	1297.0114			
64204	1319.8688	1373.1891	1385.6308			
64205	1397.9610	1414.8318	1417.5522			
64206	1444.1593	1452.2584	1474.2032			
64207	1480.4111	1491.1861	2079.2469			
64208	3061.5088	3068.6391	3089.2762			
64209	3133.3116	3140.1307	3158.9128			
64210	3746.5293	3753.7134	3825.7850			
64211	Zero-point correction (Hartree): 0.153377					
64212						
64213	TS.triHPacyl.COelim.ptmmmtmpu					
64214	-----					
64215	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16359406					
64216	Electronic state : 2-A					
64217	Cartesian coordinates (Angs):					
64218	O	-1.701260	1.975565	0.066979		
64219	O	-1.589573	0.870069	0.945204		
64220	C	-0.893746	-0.156459	0.366027		
64221	C	0.268206	0.255426	-0.501313		
64222	C	1.122130	-0.909178	-0.980135		
64223	O	1.859411	-1.541489	0.048481		
64224	O	2.984499	-0.723856	0.358404		
64225	H	-0.894132	2.470713	0.278164		
64226	C	-0.799102	-1.276122	1.352537		
64227	H	-1.777073	-1.429588	1.806662		
64228	H	-0.078303	-1.044269	2.139582		
64229	H	-0.484063	-2.195241	0.863548		
64230	C	-2.160382	-0.942168	-1.039084		
64231	O	-3.251064	-0.945236	-0.705025		
64232	H	2.711123	-0.333263	1.199948		
64233	H	-0.110138	0.782225	-1.380106		
64234	O	1.019462	1.185006	0.286175		
64235	O	1.979169	1.805111	-0.557362		
64236	H	2.726353	1.189162	-0.485886		
64237	H	0.473822	-1.685972	-1.387148		
64238	H	1.804624	-0.584131	-1.765809		
64239	Rotational constants (GHz):			1.3675200	0.6796200	0.5521800
64240	Vibrational harmonic frequencies (cm-1):					
64241	i326.7123		40.2946			75.6469
64242	91.5689		107.7839			131.7974
64243	174.6700		195.2398			203.1777
64244	221.2312		239.2268			252.9923
64245	262.2196		294.5115			324.5789
64246	345.1976		387.4128			425.4545
64247	454.1316		482.1664			549.3286
64248	562.3887		600.7416			732.1570
64249	813.3268		887.3175			963.1391
64250	965.8705		1027.7190			1029.6243
64251	1057.0652		1076.8044			1101.6482
64252	1155.2313		1246.2854			1293.4478
64253	1321.3868		1369.8954			1387.7016
64254	1405.2720		1411.8207			1415.9211
64255	1438.4620		1448.2800			1478.2440
64256	1480.6837		1491.7057			2078.9384
64257	3057.9035		3078.5003			3089.4631
64258	3129.5649		3138.1598			3162.8481
64259	3741.0710		3753.4688			3796.9416
64260	Zero-point correction (Hartree): 0.153657					
64261						
64262	TS.triHPacyl.COelim.ptmmmtmpu					
64263	-----					
64264	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16154023					
64265	Electronic state : 2-A					
64266	Cartesian coordinates (Angs):					
64267	O	-2.118863	1.572568	-0.518697		
64268	O	-1.438063	1.233038	0.682690		
64269	C	-0.803466	0.020088	0.546635		

64270	C	0.069563	-0.069186	-0.688740	
64271	C	1.092265	-1.196440	-0.666004	
64272	O	2.051884	-1.119835	0.363708	
64273	O	3.148985	-0.347994	-0.096150	
64274	H	-1.424675	2.025090	-1.023046	
64275	C	-0.356875	-0.452974	1.890758	
64276	H	-1.195567	-0.389971	2.581442	
64277	H	0.475623	0.144630	2.267844	
64278	H	-0.014360	-1.484353	1.836723	
64279	C	-2.347348	-1.295903	0.124014	
64280	O	-2.210178	-1.958646	-0.795216	
64281	H	2.876135	0.550338	0.146058	
64282	H	-0.562385	-0.243432	-1.565033	
64283	O	0.617656	1.220058	-1.000175	
64284	O	1.338594	1.725459	0.114472	
64285	H	0.644833	2.146433	0.644491	
64286	H	0.554273	-2.133959	-0.504981	
64287	H	1.601166	-1.245466	-1.628539	
64288	Rotational constants (GHz):		1.2750600	0.7550400	0.6123200
64289	Vibrational harmonic frequencies (cm-1):				
64290	i338.1453		44.1647		80.6627
64291	93.1842		119.3094		142.7955
64292	169.4953		213.6786		230.5853
64293	237.4025		242.6699		250.3490
64294	255.2000		317.5068		348.6509
64295	386.1021		402.4357		434.4779
64296	454.0895		489.0505		523.1160
64297	538.5214		615.4688		707.4560
64298	812.6504		897.9407		948.6526
64299	961.4583		1013.2700		1030.0832
64300	1046.9304		1067.1832		1106.9374
64301	1161.0507		1230.2732		1293.7671
64302	1320.5116		1356.8754		1376.3271
64303	1406.8705		1415.1661		1418.1729
64304	1437.0583		1451.8518		1462.8705
64305	1476.1271		1486.0334		2071.1329
64306	3062.2011		3068.3505		3075.8015
64307	3129.8778		3134.0198		3164.5454
64308	3739.4179		3749.8301		3762.7617
64309	Zero-point correction (Hartree):		0.153622		
64310	TS.triHPacyl.COelim.ptmmmtppmu				
64311	-----				
64312	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16098271				
64313	Electronic state : 2-A				
64314	Cartesian coordinates (Angs):				
64315	O	2.125731	-1.549871	-0.635668	
64316	O	1.609412	-1.193083	0.636228	
64317	C	0.861018	-0.054679	0.554713	
64318	C	-0.045816	0.031392	-0.654082	
64319	C	-1.044508	1.180196	-0.611152	
64320	O	-2.051457	1.074563	0.381594	
64321	O	-3.071283	0.220753	-0.133059	
64322	H	1.407565	-2.102207	-0.983011	
64323	C	0.411145	0.324722	1.927188	
64324	H	1.268496	0.295965	2.597233	
64325	H	-0.354007	-0.367540	2.280419	
64326	H	-0.004672	1.330505	1.932809	
64327	C	2.257847	1.410021	0.142892	
64328	O	2.086783	2.025129	-0.807679	
64329	H	-3.857454	0.765276	-0.009385	
64330	H	0.572297	0.209346	-1.538644	
64331	O	-0.639072	-1.228222	-0.964482	
64332	O	-1.246207	-1.780328	0.195829	
64333	H	-2.146841	-1.424016	0.140515	
64334	H	-0.515023	2.104145	-0.373361	
64335	H	-1.519721	1.287084	-1.586030	
64336	Rotational constants (GHz):		1.2656600	0.7590200	0.6145700
64337	Vibrational harmonic frequencies (cm-1):				
64338	i318.3985		45.5958		78.0517
64339	87.5738		123.7223		130.4400
64340	138.1917		164.2125		203.8628

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64342      229.5070      234.1059      245.6256
64343      251.8209      256.8476      311.9172
64344      323.4314      394.6596      410.3413
64345      443.4227      481.4371      518.7422
64346      536.1190      622.4956      704.2288
64347      823.3815      899.0450      947.6114
64348      967.2788      1010.7407     1028.6084
64349     1054.0030     1071.2186     1105.3040
64350     1155.6233     1253.2271     1303.1228
64351     1329.4148     1368.6219     1380.0726
64352     1390.1148     1409.8754     1417.7962
64353     1443.0252     1460.7448     1464.7791
64354     1477.7526     1492.7744     2044.7643
64355     3068.2204     3075.6422     3087.6188
64356     3139.5887     3141.9266     3159.0616
64357     3734.4981     3747.0246     3841.2813
64358 Zero-point correction (Hartree): 0.153161
64359
64360 TS.triHPacyl.COelim.ptmmttmpu
64361 -----
64362 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16250974
64363 Electronic state : 2-A
64364 Cartesian coordinates (Angs):
64365 O      -1.925092      1.859547      0.027163
64366 O      -1.636757      0.941675      1.067024
64367 C      -0.952932     -0.141828      0.587971
64368 C       0.108220      0.172681     -0.440352
64369 C       1.022071     -0.999415     -0.770676
64370 O       1.876173     -1.377045      0.291861
64371 O       2.950932     -0.443948      0.354387
64372 H      -1.138066      2.426321      0.048689
64373 C      -0.711796     -1.086056      1.720398
64374 H      -1.643468     -1.219815      2.266827
64375 H       0.047461     -0.695077      2.400858
64376 H      -0.373546     -2.052879      1.354300
64377 C      -2.357510     -1.148973     -0.539281
64378 O      -2.087713     -1.354868     -1.631123
64379 H       2.701824      0.083467      1.126008
64380 H      -0.367751      0.503134     -1.366407
64381 O       0.840543      1.279710      0.098574
64382 O       1.681933      1.792819     -0.924843
64383 H       2.481407      1.254654     -0.806150
64384 H       0.422947     -1.885409     -0.982754
64385 H       1.620738     -0.775962     -1.654078
64386 Rotational constants (GHz): 1.1988200 0.7307000 0.6224000
64387 Vibrational harmonic frequencies (cm-1):
64388 i331.8454      32.9796      68.3724
64389 89.2257      119.5182     120.7499
64390 167.2942     191.7488     212.0205
64391 220.7043     232.6459     249.6710
64392 270.9625     304.7437     316.6410
64393 345.0232     382.7433     414.4234
64394 468.2537     479.7978     529.2887
64395 562.5062     586.5604     725.9442
64396 809.7404     884.0692     961.9968
64397 964.8783     1026.7612    1028.6948
64398 1056.8458    1075.3192    1100.8003
64399 1153.8719    1249.6814    1294.6074
64400 1324.9692    1372.3842    1385.6854
64401 1404.0411    1413.2676    1417.6426
64402 1433.0316    1448.3901    1472.4892
64403 1479.7048    1491.9979    2056.1779
64404 3060.7670    3080.6078    3091.3344
64405 3134.4164    3140.5044    3164.3703
64406 3734.3629    3752.9240    3795.6308
64407 Zero-point correction (Hartree): 0.153443
64408
64409 TS.triHPacyl.COelim.ptmmpmpmpu
64410 -----
64411 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16182052
64412 Electronic state : 2-A
64413 Cartesian coordinates (Angs):

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64414	O	-2.015760	1.560950	-0.502450		
64415	O	-1.508551	0.961150	0.682918		
64416	C	-0.723201	-0.121526	0.381233		
64417	C	0.238192	0.071328	-0.769590		
64418	C	1.245557	-1.062341	-0.912725		
64419	O	2.146219	-1.196668	0.165445		
64420	O	3.254645	-0.340596	-0.059507		
64421	H	-2.923719	1.225145	-0.499007		
64422	C	-0.345748	-0.813257	1.650681		
64423	H	-1.228981	-0.916384	2.280208		
64424	H	0.420356	-0.253650	2.189582		
64425	H	0.058514	-1.799427	1.435177		
64426	C	-2.061453	-1.493393	-0.438037		
64427	O	-3.144326	-1.155978	-0.293916		
64428	H	2.963653	0.482836	0.361373		
64429	H	-0.328357	0.119098	-1.703264		
64430	O	0.835827	1.366667	-0.744113		
64431	O	1.393287	1.607483	0.541048		
64432	H	0.720401	2.170927	0.946704		
64433	H	0.696678	-2.005728	-0.960106		
64434	H	1.810644	-0.931751	-1.835437		
64435	Rotational constants (GHz):			1.5016300	0.6757600	0.5732500
64436	Vibrational harmonic frequencies (cm-1):					
64437	i308.4139		59.7013			69.9302
64438	92.6720		132.1063			142.8968
64439	182.7751		204.4778			219.6818
64440	223.8000		229.2661			248.2311
64441	254.5892		286.9104			295.3216
64442	334.6692		365.6582			379.4504
64443	433.0252		492.6659			506.6934
64444	548.5428		621.0013			716.9026
64445	824.0600		903.3938			950.0495
64446	965.8966		1009.0669			1029.9477
64447	1050.4995		1068.2520			1110.0134
64448	1159.5144		1232.7465			1296.3733
64449	1321.9772		1351.3120			1375.2363
64450	1398.2574		1408.2334			1415.6901
64451	1423.9805		1451.9937			1466.0835
64452	1478.9692		1488.5629			2057.2700
64453	3065.7513		3072.6987			3081.5570
64454	3131.1813		3134.3877			3164.7316
64455	3742.6443		3789.6729			3798.9471
64456	Zero-point correction (Hartree):			0.153229		
64457	-----					
64458	TS.triHPacyl.COelim.ptmmpmpu					
64459	-----					
64460	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.16168470		
64461	Electronic state : 2-A					
64462	Cartesian coordinates (Angs):					
64463	O	2.007998	-1.776535	-0.574290		
64464	O	1.493876	-1.249502	0.638870		
64465	C	0.826173	-0.074192	0.405058		
64466	C	-0.137686	-0.100766	-0.763410		
64467	C	-1.073799	1.101200	-0.816893		
64468	O	-1.966111	1.208173	0.270778		
64469	O	-3.126601	0.445041	-0.016520		
64470	H	2.825053	-1.261702	-0.665361		
64471	C	0.495624	0.577436	1.707237		
64472	H	1.368895	0.550416	2.357569		
64473	H	-0.337177	0.068557	2.195546		
64474	H	0.198148	1.611819	1.548357		
64475	C	2.353009	1.132511	-0.320244		
64476	O	2.121891	2.249971	-0.339998		
64477	H	-2.888449	-0.426309	0.335939		
64478	H	0.429728	-0.112503	-1.698749		
64479	O	-0.820348	-1.351415	-0.844151		
64480	O	-1.399263	-1.658970	0.416276		
64481	H	-0.748439	-2.269069	0.790253		
64482	H	-0.475094	2.015104	-0.796502		
64483	H	-1.644118	1.072443	-1.745277		
64484	Rotational constants (GHz):			1.2378700	0.7785200	0.5933200
64485	Vibrational harmonic frequencies (cm-1):					

64486	i307.4348	55.1540	73.7925			
64487	90.1976	133.3804	140.8702			
64488	179.7511	197.1386	212.8799			
64489	232.1800	234.0320	241.9651			
64490	256.1988	296.0822	315.0209			
64491	343.0299	356.3159	401.6436			
64492	416.5684	486.3038	512.4883			
64493	539.0017	624.1348	706.5227			
64494	821.2218	902.2982	949.6941			
64495	963.4369	1008.1934	1028.1916			
64496	1049.4923	1067.6999	1108.9020			
64497	1159.1985	1238.7268	1292.0973			
64498	1319.1621	1348.9883	1373.5763			
64499	1400.5445	1408.1176	1412.3003			
64500	1429.8015	1454.9942	1462.3420			
64501	1476.0962	1485.3062	2074.0405			
64502	3064.6718	3064.8176	3076.3920			
64503	3129.2596	3133.9929	3162.0804			
64504	3753.0172	3754.6764	3792.2451			
64505	Zero-point correction (Hartree): 0.153116					
64506						
64507	TS.triHPacyl.COelim.ptppmmmmmu					
64508	-----					
64509	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16374390					
64510	Electronic state : 2-A					
64511	Cartesian coordinates (Angs):					
64512	O	1.557172	1.415355	-1.162960		
64513	O	1.275064	1.401812	0.228418		
64514	C	0.232936	0.561074	0.505005		
64515	C	0.320457	-0.827047	-0.086332		
64516	C	-0.788343	-1.764447	0.394992		
64517	O	-2.077328	-1.235986	0.222432		
64518	O	-2.336072	-1.199140	-1.172706		
64519	H	2.240956	0.728602	-1.216782		
64520	C	-0.151871	0.723206	1.939881		
64521	H	-0.140025	1.779255	2.201171		
64522	H	0.552545	0.192930	2.586242		
64523	H	-1.152632	0.328326	2.107261		
64524	C	-1.302042	1.502151	-0.519674		
64525	O	-1.411917	2.587802	-0.189939		
64526	H	-2.188811	-0.256145	-1.361595		
64527	H	0.327765	-0.780288	-1.175035		
64528	O	1.505908	-1.492172	0.362687		
64529	O	2.615937	-1.058031	-0.413438		
64530	H	2.849679	-1.867455	-0.884495		
64531	H	-0.695386	-2.718841	-0.124240		
64532	H	-0.691014	-1.933114	1.468288		
64533	Rotational constants (GHz):			1.0083800	0.8754800	0.6140300
64534	Vibrational harmonic frequencies (cm-1):					
64535	i320.7131		46.8755			84.2641
64536	95.0662		134.1084			160.6209
64537	165.8077		199.9125			204.0005
64538	227.6784		236.8353			252.6729
64539	261.4151		282.0924			289.2291
64540	356.0037		379.5985			393.2395
64541	482.9100		503.4558			515.3456
64542	549.4088		607.9695			646.3281
64543	772.9745		945.6583			965.4167
64544	1003.4168		1009.9731			1053.1530
64545	1061.9842		1075.2147			1129.4022
64546	1161.4119		1241.0903			1294.8594
64547	1303.7377		1347.0237			1385.8372
64548	1394.7259		1407.3873			1413.1702
64549	1451.8259		1461.7921			1480.6986
64550	1488.3655		1500.8843			2086.5072
64551	3051.5577		3082.0819			3111.3742
64552	3128.9423		3136.8151			3163.3447
64553	3660.9808		3731.3318			3820.5332
64554	Zero-point correction (Hartree): 0.153545					
64555						
64556	TS.triHPacyl.COelim.ptppmmmpmu					
64557	-----					

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64558 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16452486
64559 Electronic state : 2-A
64560 Cartesian coordinates (Angs):
64561 O 1.575837 1.320318 -1.234187
64562 O 1.393103 1.260836 0.173288
64563 C 0.292503 0.503897 0.488947
64564 C 0.248522 -0.871885 -0.131877
64565 C -0.921332 -1.727846 0.355690
64566 O -2.163677 -1.084654 0.236182
64567 O -2.457356 -0.983920 -1.148884
64568 H 2.105115 0.520952 -1.393339
64569 C -0.008549 0.660861 1.944090
64570 H 0.106005 1.704492 2.229355
64571 H 0.669870 0.052679 2.548697
64572 H -1.031802 0.348814 2.147921
64573 C -1.198930 1.604132 -0.434748
64574 O -1.212240 2.679283 -0.057444
64575 H -2.237803 -0.051280 -1.316830
64576 H 0.231991 -0.805195 -1.219853
64577 O 1.382548 -1.644875 0.269194
64578 O 2.524532 -1.214050 -0.462941
64579 H 3.074291 -0.843512 0.240428
64580 H -0.922575 -2.670458 -0.191648
64581 H -0.810354 -1.934948 1.420989
64582 Rotational constants (GHz): 1.0187900 0.8762200 0.6173700
64583 Vibrational harmonic frequencies (cm-1):
64584 i328.1304 50.3616 90.8289
64585 97.8368 142.0667 153.7513
64586 172.1550 199.0774 201.4505
64587 227.6870 236.3736 251.6432
64588 269.4606 284.0172 356.0827
64589 359.3793 381.3574 394.8311
64590 498.6832 511.6413 543.7572
64591 561.4832 610.9339 652.6638
64592 769.6258 945.2074 963.4607
64593 1004.5886 1012.8448 1048.7828
64594 1060.3476 1078.6541 1130.4813
64595 1161.3491 1235.7555 1289.7102
64596 1304.6529 1341.3279 1389.5617
64597 1405.6582 1409.6806 1414.9998
64598 1450.8914 1453.1982 1480.8369
64599 1487.8315 1499.9950 2088.5890
64600 3049.4822 3083.4213 3108.0676
64601 3127.3847 3137.6578 3162.9372
64602 3658.2567 3713.7075 3805.1557
64603 Zero-point correction (Hartree): 0.153826
64604
64605 TS.triHPacyl.COelim.ptppmmpmmu
64606 -----
64607 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16447257
64608 Electronic state : 2-A
64609 Cartesian coordinates (Angs):
64610 O 1.875993 1.060659 -1.273100
64611 O 1.704310 0.882309 0.126573
64612 C 0.443200 0.416642 0.402028
64613 C 0.016968 -0.751646 -0.462171
64614 C -1.137775 -1.558443 0.116862
64615 O -2.263709 -0.750463 0.375076
64616 O -2.769085 -0.301503 -0.874129
64617 H 2.149316 0.173884 -1.556012
64618 C 0.231389 0.428266 1.881897
64619 H 0.560962 1.384131 2.285644
64620 H 0.795992 -0.373620 2.363882
64621 H -0.824551 0.291234 2.106168
64622 C -0.790709 1.948158 -0.205469
64623 O -0.409570 2.968798 0.128790
64624 H -2.431656 0.609492 -0.898824
64625 H -0.263296 -0.391330 -1.453615
64626 O 1.130472 -1.593953 -0.753065
64627 O 1.645704 -2.108430 0.469390
64628 H 2.380650 -1.504478 0.646990
64629 H -1.392243 -2.364410 -0.572749

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64630      H      -0.866534      -1.982103      1.083343
64631 Rotational constants (GHz):      0.9763300      0.9283400      0.6204900
64632 Vibrational harmonic frequencies (cm-1):
64633      i326.8232      54.4650      107.5298
64634      113.1452      125.8962      147.3441
64635      163.3702      176.9140      201.3088
64636      226.6545      243.7440      249.7330
64637      278.5647      288.7855      328.4660
64638      353.4290      377.8501      442.7658
64639      468.1757      478.5929      517.2657
64640      552.1038      598.5595      698.5443
64641      784.5220      945.7509      950.4828
64642      975.3062      1014.2054      1048.2602
64643      1066.3074      1088.2054      1123.6837
64644      1158.5131      1238.0246      1281.2846
64645      1305.8871      1351.1438      1374.5114
64646      1406.5003      1409.4560      1419.7667
64647      1441.8355      1450.2250      1483.5209
64648      1485.4579      1500.6341      2088.8560
64649      3054.6958      3084.0086      3098.2808
64650      3130.1084      3145.9795      3164.5262
64651      3702.8115      3754.4116      3782.2339
64652 Zero-point correction (Hartree): 0.153782
64653
64654 TS.triHPacyl.COelim.ptppmmpm
64655 -----
64656 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16359227
64657 Electronic state : 2-A
64658 Cartesian coordinates (Angs):
64659      O      1.367392      1.652657      -1.324155
64660      O      1.221202      1.529275      0.081660
64661      C      0.275281      0.593640      0.391805
64662      C      0.314470      -0.666220      -0.446466
64663      C      -0.484271      -1.822923      0.142235
64664      O      -1.833436      -1.488047      0.363488
64665      O      -2.442869      -1.290930      -0.903418
64666      H      2.050937      0.988522      -1.503268
64667      C      0.112810      0.545639      1.877249
64668      H      0.039493      1.561022      2.263044
64669      H      0.972785      0.053586      2.336355
64670      H      -0.793356      0.002214      2.137920
64671      C      -1.469560      1.487242      -0.200832
64672      O      -1.555476      2.559296      0.180713
64673      H      -2.454894      -0.319700      -0.955613
64674      H      -0.060572      -0.444326      -1.446609
64675      O      1.654837      -1.067127      -0.720647
64676      O      2.299005      -1.348624      0.522428
64677      H      2.579481      -2.261619      0.385233
64678      H      -0.409324      -2.682233      -0.527710
64679      H      -0.102165      -2.093730      1.126165
64680 Rotational constants (GHz):      0.9698900      0.9258700      0.6201100
64681 Vibrational harmonic frequencies (cm-1):
64682      i318.2070      50.0101      101.2363
64683      110.6907      125.8124      150.0218
64684      163.6332      169.0271      209.1282
64685      220.9149      228.3177      245.6718
64686      256.3423      275.2982      292.0335
64687      351.8498      357.0670      414.2785
64688      451.3278      481.5650      520.0035
64689      555.5162      598.1418      693.2916
64690      779.9836      948.9905      954.4527
64691      977.4685      1016.5659      1055.7569
64692      1070.9308      1089.2670      1127.6136
64693      1156.9847      1248.3358      1291.4747
64694      1310.6311      1351.9181      1375.5724
64695      1397.7537      1408.1474      1418.5688
64696      1436.8715      1451.3480      1484.2111
64697      1491.0745      1502.3826      2078.4523
64698      3061.2830      3069.9121      3105.8313
64699      3135.7206      3138.5428      3163.3760
64700      3672.3588      3759.3194      3831.5505
64701 Zero-point correction (Hartree): 0.153512

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64702
64703 TS.triHPacyl.COelim.ptppmpmpmu
64704 -----
64705 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16206419
64706 Electronic state : 2-A
64707 Cartesian coordinates (Angs):
64708 O 1.665626 1.417875 -1.065263
64709 O 1.673879 1.097581 0.318255
64710 C 0.516699 0.450622 0.682761
64711 C 0.140599 -0.740065 -0.168548
64712 C -1.081915 -1.494625 0.350932
64713 O -2.235938 -0.691942 0.395300
64714 O -2.723911 -0.585742 -0.934948
64715 H 2.026567 0.603715 -1.453479
64716 C 0.474581 0.330753 2.170119
64717 H 0.852907 1.248305 2.614790
64718 H 1.079556 -0.510797 2.517660
64719 H -0.552645 0.187197 2.501965
64720 C -0.895986 1.945932 0.288713
64721 O -1.378818 1.946989 -0.747816
64722 H -2.539880 0.342107 -1.142089
64723 H -0.023202 -0.444960 -1.206432
64724 O 1.164565 -1.740407 -0.124946
64725 O 2.267634 -1.323332 -0.919736
64726 H 2.940711 -1.158952 -0.245552
64727 H -1.253929 -2.369086 -0.275418
64728 H -0.918250 -1.821415 1.377920
64729 Rotational constants (GHz): 1.1297100 0.8068600 0.6537300
64730 Vibrational harmonic frequencies (cm-1):
64731 i322.0217 50.3290 84.7152
64732 103.9590 122.1292 145.9343
64733 178.8762 190.0194 198.9533
64734 223.4061 231.2883 233.6755
64735 256.5520 309.4678 323.0701
64736 345.6364 378.0648 387.5651
64737 400.8032 510.8514 535.1996
64738 554.9214 588.3917 644.4064
64739 760.5188 943.6991 961.7606
64740 997.6726 1020.3088 1050.4922
64741 1056.6892 1071.1328 1128.7209
64742 1155.2635 1233.8629 1289.4327
64743 1304.6631 1338.6751 1384.2603
64744 1404.1689 1411.8515 1414.6887
64745 1441.0812 1453.7321 1479.1362
64746 1486.0150 1500.4429 2052.1509
64747 3052.2346 3091.8561 3097.9868
64748 3129.7491 3146.1845 3163.9247
64749 3721.9514 3778.3044 3804.1161
64750 Zero-point correction (Hartree): 0.153378
64751
64752 TS.triHPacyl.COelim.ptppmppmu
64753 -----
64754 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16170684
64755 Electronic state : 2-A
64756 Cartesian coordinates (Angs):
64757 O 1.718927 1.540808 -1.134080
64758 O 1.730552 1.181064 0.238665
64759 C 0.583861 0.517597 0.574652
64760 C 0.124479 -0.522072 -0.427854
64761 C -0.879133 -1.515275 0.143214
64762 O -2.086792 -0.886924 0.509923
64763 O -2.806937 -0.622903 -0.686537
64764 H 2.128652 0.760370 -1.538026
64765 C 0.587785 0.246126 2.042134
64766 H 0.899032 1.146890 2.566901
64767 H 1.276226 -0.566543 2.283637
64768 H -0.413975 -0.018961 2.376389
64769 C -0.841914 2.030563 0.421749
64770 O -1.543230 1.988805 -0.483078
64771 H -2.728814 0.339194 -0.759790
64772 H -0.319665 -0.029816 -1.296474
64773 O 1.234668 -1.200092 -1.013743

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64774	O	1.926302	-1.889560	0.028518	
64775	H	1.898950	-2.797137	-0.298021	
64776	H	-1.071996	-2.295365	-0.595279	
64777	H	-0.506801	-1.969853	1.059943	
64778	Rotational constants (GHz):		1.0946400	0.8502100	0.6439900
64779	Vibrational harmonic frequencies (cm-1):				
64780	i	315.6754	64.3784		79.5095
64781		109.7120	118.2770		136.9781
64782		151.0785	170.7643		198.4899
64783		209.7135	230.6879		238.9414
64784		256.2927	271.1318		302.5606
64785		353.2523	374.3537		389.4201
64786		431.2566	456.2246		470.9606
64787		540.7548	588.5154		679.8720
64788		784.9147	944.8606		951.5987
64789		975.0742	1019.7251		1054.1854
64790		1066.9970	1081.4362		1125.0616
64791		1154.0599	1250.4897		1292.6940
64792		1309.6301	1350.2324		1369.7513
64793		1399.1880	1409.1675		1417.5116
64794		1436.4003	1438.9472		1480.5569
64795		1489.3100	1501.4602		2039.9572
64796		3060.0782	3078.4965		3091.2105
64797		3135.8484	3145.3593		3161.3554
64798		3760.9204	3779.9897		3830.7857
64799	Zero-point correction (Hartree): 0.153117				
64800					
64801	TS.triHPacyl.COelim.ptppmtpmmu				
64802	-----				
64803	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16317907				
64804	Electronic state : 2-A				
64805	Cartesian coordinates (Angs):				
64806	O	1.839420	1.462527	-1.067860	
64807	O	1.812320	0.987175	0.272233	
64808	C	0.576591	0.467376	0.567078	
64809	C	0.080506	-0.544552	-0.449921	
64810	C	-0.947347	-1.519730	0.108085	
64811	O	-2.125950	-0.851477	0.502853	
64812	O	-2.848756	-0.535135	-0.680199	
64813	H	2.064485	0.657437	-1.560481	
64814	C	0.476684	0.223867	2.035972	
64815	H	0.825293	1.106430	2.568027	
64816	H	1.079861	-0.637036	2.336757	
64817	H	-0.559193	0.033008	2.311685	
64818	C	-0.673889	2.138345	0.326395	
64819	O	-1.494829	2.057428	-0.464844	
64820	H	-2.756211	0.427029	-0.719731	
64821	H	-0.353529	-0.035331	-1.314569	
64822	O	1.181562	-1.241577	-1.031049	
64823	O	1.863599	-1.946508	-0.000826	
64824	H	2.557024	-1.317833	0.247408	
64825	H	-1.173544	-2.274937	-0.644643	
64826	H	-0.578384	-2.010067	1.007423	
64827	Rotational constants (GHz):		1.1133600	0.8417600	0.6401200
64828	Vibrational harmonic frequencies (cm-1):				
64829	i	316.9893	72.1498		75.4360
64830		112.7246	122.0565		143.6116
64831		163.5968	170.5120		204.1106
64832		222.3910	236.4316		248.3239
64833		273.8521	315.0073		366.4372
64834		369.6467	381.4465		405.4485
64835		446.9857	460.3065		476.2207
64836		542.0838	583.5287		685.1866
64837		789.5536	945.7849		946.0885
64838		973.1483	1015.6087		1045.0065
64839		1062.3370	1080.2161		1121.9164
64840		1154.8425	1239.7193		1280.0156
64841		1301.7642	1346.1526		1366.8051
64842		1407.4959	1409.7061		1422.6634
64843		1434.7201	1439.8577		1483.1413
64844		1484.0296	1500.8603		2058.1937
64845		3050.1497	3082.7190		3092.2267

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64846          3129.4519          3152.1278          3163.9994
64847          3749.4017          3772.9480          3791.9861
64848 Zero-point correction (Hartree): 0.153485
64849
64850 TS.triHPacyl.COelim.ptppmpmmu
64851 -----
64852 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16299971
64853 Electronic state : 2-A
64854 Cartesian coordinates (Angs):
64855 O          2.180241          0.175881          -1.169965
64856 O          1.902372          0.019029          0.216503
64857 C          0.556765          0.110599          0.445461
64858 C          -0.321783          -0.663378          -0.517548
64859 C          -1.738370          -0.885166          0.005366
64860 O          -2.385299          0.309544          0.379710
64861 O          -2.609272          1.067859          -0.800140
64862 H          2.598256          1.048576          -1.167998
64863 C          0.316615          0.100309          1.920710
64864 H          1.017954          0.774364          2.410385
64865 H          0.453414          -0.905800          2.323672
64866 H          -0.699531          0.425839          2.131750
64867 C          0.166981          2.102828          -0.044606
64868 O          1.115509          2.732332          0.052407
64869 H          -1.915928          1.742343          -0.720285
64870 H          -0.361737          -0.148923          -1.478616
64871 O          0.257694          -1.909768          -0.868131
64872 O          0.489363          -2.651315          0.325399
64873 H          1.450209          -2.578653          0.402614
64874 H          -2.314596          -1.409886          -0.757624
64875 H          -1.714155          -1.487504          0.913534
64876 Rotational constants (GHz):          0.9805200          0.9279300          0.6167400
64877 Vibrational harmonic frequencies (cm-1):
64878 i301.2368          53.2269          100.9004
64879 117.2283          123.4475          138.1058
64880 161.4968          167.3089          197.9221
64881 218.2941          233.3546          251.3467
64882 259.4490          284.1552          313.0360
64883 323.3609          354.4783          360.6042
64884 446.4432          462.9530          488.2524
64885 548.5026          603.3112          696.0856
64886 781.3515          949.0181          951.3393
64887 974.9909          1011.0135          1049.3379
64888 1063.8417          1096.1475          1121.8313
64889 1152.6648          1238.5984          1285.2681
64890 1300.2334          1341.9363          1375.1918
64891 1405.8548          1407.4433          1415.3649
64892 1423.5015          1440.7558          1485.2454
64893 1486.4470          1501.7673          2065.5322
64894 3058.7616          3084.6242          3105.7342
64895 3130.9344          3144.0601          3166.1580
64896 3710.8223          3794.8967          3801.0981
64897 Zero-point correction (Hartree): 0.153150
64898
64899 TS.triHPacyl.COelim.ptppptpmu
64900 -----
64901 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16119556
64902 Electronic state : 2-A
64903 Cartesian coordinates (Angs):
64904 O          1.791142          1.499128          -1.212118
64905 O          1.623935          1.268176          0.177346
64906 C          0.474276          0.557916          0.408473
64907 C          0.264796          -0.644049          -0.495164
64908 C          -0.713153          -1.668679          0.072048
64909 O          -1.982715          -1.133233          0.360994
64910 O          -2.591821          -0.827017          -0.893076
64911 H          1.186388          2.245886          -1.347636
64912 C          0.221123          0.487230          1.878651
64913 H          0.399909          1.461495          2.330473
64914 H          0.883983          -0.244950          2.346253
64915 H          -0.810160          0.192915          2.063965
64916 C          -0.927385          1.962686          -0.247313
64917 O          -1.977195          1.883847          0.196112

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64918	H	-2.938807	0.055534	-0.710620	
64919	H	-0.073655	-0.322275	-1.481328	
64920	O	1.493671	-1.290436	-0.790540	
64921	O	2.116308	-1.655083	0.436565	
64922	H	2.798944	-0.973462	0.505329	
64923	H	-0.800088	-2.495722	-0.633952	
64924	H	-0.351058	-2.053110	1.025093	
64925	Rotational constants (GHz):			1.1169300	0.8468600 0.6277000
64926	Vibrational harmonic frequencies (cm-1):				
64927		i293.4211	42.9007		95.2624
64928		118.7992	129.0433		146.4277
64929		149.7053	168.8041		197.7169
64930		200.2536	214.8679		240.1865
64931		264.2916	291.6366		304.8286
64932		338.0343	362.9770		370.1989
64933		388.6402	438.1194		462.3447
64934		546.7584	591.1808		685.0771
64935		783.0232	947.0287		949.1441
64936		973.2537	1011.0059		1051.0432
64937		1062.8367	1089.9960		1121.8278
64938		1149.9410	1240.4099		1283.8122
64939		1295.8925	1335.8130		1374.5057
64940		1404.0787	1404.6039		1414.0996
64941		1431.4551	1437.0111		1483.0376
64942		1484.8896	1500.7809		2065.1207
64943		3055.3897	3084.6318		3101.6383
64944		3129.8572	3145.9480		3162.7587
64945		3745.1031	3791.3022		3820.7445
64946	Zero-point correction (Hartree):			0.152820	
64947	TS.triHPacyl.COelim.pttmmpppu				
64948	-----				
64949	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16194693				
64950	Electronic state : 2-A				
64951	Cartesian coordinates (Angs):				
64952	O	-1.528199	1.282288	-1.543158	
64953	O	-1.727558	1.153208	-0.145654	
64954	C	-0.999213	0.111573	0.361760	
64955	C	0.380761	-0.056469	-0.222366	
64956	C	1.248249	-1.039316	0.558278	
64957	O	2.618575	-0.834894	0.279763	
64958	O	2.830300	-1.068653	-1.104046	
64959	H	-0.791354	1.911422	-1.571859	
64960	C	-1.262885	0.027903	1.832048	
64961	H	-2.327392	0.171184	2.010396	
64962	H	-0.704124	0.797446	2.368871	
64963	H	-0.980207	-0.950429	2.218234	
64964	C	-1.914084	-1.578631	-0.325992	
64965	O	-3.053457	-1.513113	-0.305071	
64966	H	2.792928	-0.170421	-1.462359	
64967	H	0.287395	-0.397637	-1.253785	
64968	O	1.052206	1.193979	-0.387613	
64969	O	1.382683	1.714560	0.892164	
64970	H	2.277386	1.362637	1.013598	
64971	H	1.185096	-0.870194	1.632071	
64972	H	0.946911	-2.063371	0.331384	
64973	Rotational constants (GHz):			1.3072000	0.6424700 0.5756700
64974	Vibrational harmonic frequencies (cm-1):				
64975		i334.0287	40.8353		62.8366
64976		63.7948	106.2718		122.0024
64977		137.2234	154.3655		209.7327
64978		213.1378	233.9788		255.4963
64979		267.3634	295.7727		343.7631
64980		366.5817	374.4407		397.4794
64981		428.6388	458.6062		474.8534
64982		565.0619	629.1509		709.6528
64983		812.0557	924.7753		960.2193
64984		979.9071	999.9804		1052.3415
64985		1057.0508	1093.3513		1113.1144
64986		1160.8436	1243.5745		1295.8402
64987		1324.3723	1340.3077		1388.3839
64988		1408.3210	1409.3243		1423.1282

64990	1430.7354	1435.1197	1481.7676			
64991	1492.7294	1496.7868	2073.4575			
64992	3057.6381	3084.6192	3110.6290			
64993	3130.4618	3148.6339	3154.3108			
64994	3765.3477	3766.6741	3782.2619			
64995	Zero-point correction (Hartree): 0.153341					
64996						
64997	TS.triHPacyl.COelim.pttmmmtmpu					
64998	-----					
64999	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16243587					
65000	Electronic state : 2-A					
65001	Cartesian coordinates (Angs):					
65002	O	-1.425001	1.748837	-1.024979		
65003	O	-1.816121	1.154053	0.198861		
65004	C	-1.094590	0.018578	0.449957		
65005	C	0.357875	0.067221	0.056008		
65006	C	1.137083	-1.128952	0.574139		
65007	O	2.520578	-1.013950	0.298208		
65008	O	2.701049	-1.096923	-1.106604		
65009	H	-0.718679	2.344799	-0.730241		
65010	C	-1.521965	-0.530587	1.774329		
65011	H	-2.607006	-0.481985	1.848616		
65012	H	-1.088520	0.047153	2.594479		
65013	H	-1.214394	-1.570477	1.875083		
65014	C	-1.821186	-1.375442	-0.852333		
65015	O	-2.951128	-1.310768	-0.994683		
65016	H	2.670826	-0.164507	-1.370147		
65017	H	0.427704	0.121066	-1.030948		
65018	O	0.874773	1.292114	0.590326		
65019	O	2.046822	1.644918	-0.140491		
65020	H	2.742592	1.273748	0.421095		
65021	H	1.097568	-1.167366	1.663377		
65022	H	0.738828	-2.053589	0.150981		
65023	Rotational constants (GHz):			1.2848700	0.6473600	0.5560800
65024	Vibrational harmonic frequencies (cm-1):					
65025	i336.6022		36.0901			70.4368
65026	82.5689		115.4325			122.9706
65027	150.2634		169.8944			202.0030
65028	219.7257		236.6782			242.2980
65029	273.6843		294.8436			321.5341
65030	365.2849		403.4674			417.7077
65031	446.4942		464.9588			497.0509
65032	561.1899		572.8999			617.6884
65033	886.5322		895.3626			963.6674
65034	979.6914		1020.1713			1054.4678
65035	1061.4879		1098.5056			1114.1214
65036	1156.6785		1240.9972			1306.1298
65037	1324.1929		1344.1431			1379.0643
65038	1411.3108		1415.8965			1425.8226
65039	1437.1960		1440.9430			1470.8762
65040	1486.9544		1492.8122			2077.9247
65041	3051.5584		3072.0759			3100.3603
65042	3125.5651		3135.4668			3155.5394
65043	3754.8965		3758.4080			3782.2832
65044	Zero-point correction (Hartree): 0.153335					
65045						
65046	TS.triHPacyl.COelim.pttpmmmpmu					
65047	-----					
65048	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16200630					
65049	Electronic state : 2-A					
65050	Cartesian coordinates (Angs):					
65051	O	-1.832505	1.406943	-1.038124		
65052	O	-1.740323	0.995668	0.317357		
65053	C	-0.910254	-0.090340	0.442439		
65054	C	0.441968	0.028022	-0.208844		
65055	C	1.294031	-1.219030	-0.022345		
65056	O	2.484353	-1.144568	-0.772268		
65057	O	3.477639	-0.503301	0.013433		
65058	H	-1.081024	2.018616	-1.106042		
65059	C	-1.013087	-0.620407	1.836624		
65060	H	-2.053632	-0.606040	2.154910		
65061	H	-0.421307	-0.018377	2.531413		

65062	H	-0.649495	-1.646379	1.880562		
65063	C	-1.854294	-1.539094	-0.690574		
65064	O	-2.979899	-1.565878	-0.517044		
65065	H	3.238083	0.430875	-0.070126		
65066	H	0.342207	0.221757	-1.277485		
65067	O	1.206252	1.098185	0.372983		
65068	O	0.675881	2.340682	-0.076643		
65069	H	0.265753	2.681760	0.729717		
65070	H	1.538418	-1.385795	1.027476		
65071	H	0.739625	-2.073158	-0.411783		
65072	Rotational constants (GHz):		1.2832500	0.6515200	0.5245800	
65073	Vibrational harmonic frequencies (cm-1):					
65074	i326.0657		52.7008		68.0986	
65075	80.2052		110.8303		131.0159	
65076	150.5866		167.2571		185.7452	
65077	205.1322		218.2745		227.6344	
65078	243.3675		282.0531		310.0129	
65079	346.0086		381.9876		391.2068	
65080	425.0701		507.1651		535.7691	
65081	544.4951		581.1421		642.1237	
65082	838.8020		871.4674		963.2588	
65083	974.3024		1039.1248		1044.2746	
65084	1054.0316		1094.8924		1128.0433	
65085	1145.9284		1223.5495		1303.0599	
65086	1317.1854		1338.1201		1368.0017	
65087	1402.3373		1411.0915		1420.7182	
65088	1443.4098		1448.6737		1466.0934	
65089	1483.7030		1490.7934		2089.5153	
65090	3049.6029		3081.4566		3105.9762	
65091	3123.0912		3142.4093		3158.8679	
65092	3723.6905		3777.8251		3803.5512	
65093	Zero-point correction (Hartree):		0.152899			
65094	TS.triHPacyl.COelim.pttpmppmu					
65095	-----					
65097	IRC pathway available					
65098	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18888084					
65099	E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07154751					
65100	T1 diagnostic: 0.016837					
65101	E(MP2/Aug-CC-pVTZ) (Hartree): -721.03221392					
65102	E(MP3/Aug-CC-pVTZ) (Hartree): -721.05005061					
65103	E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03802806					
65104	E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05380536					
65105	E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51187474					
65106	E(UHF/Aug-CC-pVTZ) (Hartree): -718.50422806					
65107	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16452610					
65108	Electronic state : 2-A					
65109	Cartesian coordinates (Angs):					
65110	O	-1.648580	1.538924	-1.236257		
65111	O	-1.702390	1.189226	0.136821		
65112	C	-0.986243	0.050944	0.378643		
65113	C	0.320281	-0.066229	-0.368045		
65114	C	1.183150	-1.203342	0.151436		
65115	O	2.361046	-1.369829	-0.610425		
65116	O	3.288877	-0.362418	-0.214632		
65117	H	-0.874266	2.122225	-1.252351		
65118	C	-1.101477	-0.284286	1.831677		
65119	H	-2.142286	-0.192578	2.138694		
65120	H	-0.491635	0.394244	2.431510		
65121	H	-0.776978	-1.307684	2.015476		
65122	C	-2.060642	-1.464106	-0.484502		
65123	O	-3.188257	-1.339709	-0.361567		
65124	H	3.249360	0.241609	-0.968541		
65125	H	0.119800	-0.241558	-1.426804		
65126	O	1.021096	1.179588	-0.403111		
65127	O	1.419720	1.526523	0.914898		
65128	H	2.292282	1.103103	0.964503		
65129	H	1.444521	-1.075466	1.202605		
65130	H	0.636687	-2.140219	0.033847		
65131	Rotational constants (GHz):		1.4186400	0.6310300	0.5480100	
65132	Vibrational harmonic frequencies (cm-1):					
65133	i323.4039		48.3486		73.2626	

65134	100.4506	110.2341	129.7821		
65135	180.7203	190.1353	196.6320		
65136	223.4293	231.3395	234.5082		
65137	276.6708	290.9189	316.4975		
65138	369.9064	392.3348	417.7403		
65139	431.7337	492.1812	547.1223		
65140	569.3400	601.8197	676.5909		
65141	834.4811	907.4399	950.5762		
65142	976.2991	1005.9915	1053.6812		
65143	1056.7208	1108.4918	1121.9076		
65144	1145.7862	1236.6762	1309.3477		
65145	1318.0789	1333.1169	1379.1896		
65146	1406.3374	1408.3399	1420.7412		
65147	1439.8482	1448.8298	1475.1946		
65148	1486.8725	1495.7779	2076.2454		
65149	3058.9641	3081.3562	3096.8024		
65150	3131.2604	3136.9695	3151.9133		
65151	3738.2298	3760.8730	3801.0108		
65152	Zero-point correction (Hartree): 0.153674				
65153	-----				
65154	TS.triHPacyl.COelim.pttpmmpu				
65155	-----				
65156	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16281551				
65157	Electronic state : 2-A				
65158	Cartesian coordinates (Angs):				
65159	O	-1.709560	1.536019	-1.207261	
65160	O	-1.740512	1.166233	0.160731	
65161	C	-0.992948	0.044940	0.383820	
65162	C	0.299551	-0.039355	-0.393083	
65163	C	1.188686	-1.166983	0.102515	
65164	O	2.363439	-1.292757	-0.674358	
65165	O	3.295415	-0.314086	-0.218085	
65166	H	-0.919169	2.098364	-1.233375	
65167	C	-1.066661	-0.292524	1.839089	
65168	H	-2.099088	-0.206949	2.174933	
65169	H	-0.444115	0.389087	2.422570	
65170	H	-0.731788	-1.314404	2.012963	
65171	C	-2.054241	-1.503137	-0.456655	
65172	O	-3.182663	-1.388432	-0.331508	
65173	H	4.026955	-0.875052	0.066611	
65174	H	0.079738	-0.216491	-1.447440	
65175	O	0.965881	1.218267	-0.438468	
65176	O	1.430731	1.548597	0.861970	
65177	H	2.346874	1.235587	0.801364	
65178	H	1.455577	-1.047760	1.152711	
65179	H	0.656852	-2.110749	-0.028614	
65180	Rotational constants (GHz): 1.4234400			0.6255700	0.5421200
65181	Vibrational harmonic frequencies (cm-1):				
65182	i315.6809	47.2053	68.9447		
65183	94.7513	104.4079	124.4536		
65184	170.8769	182.7768	190.7220		
65185	222.4673	226.2176	233.5672		
65186	240.0385	275.3567	302.3578		
65187	319.2159	374.9719	419.3741		
65188	435.4546	491.0577	500.1429		
65189	567.6018	599.2641	675.1085		
65190	830.2829	906.5028	952.2966		
65191	975.9914	1005.7684	1052.6340		
65192	1057.9113	1104.9553	1122.0548		
65193	1152.9462	1238.1221	1310.4673		
65194	1319.7281	1334.6369	1381.3769		
65195	1395.5452	1407.0383	1427.2604		
65196	1441.1052	1448.6056	1471.7202		
65197	1486.2445	1495.3137	2075.9293		
65198	3057.1808	3081.6247	3099.5863		
65199	3129.4804	3138.0022	3151.3906		
65200	3747.1126	3749.5581	3829.6461		
65201	Zero-point correction (Hartree): 0.153194				
65202	-----				
65203	TS.triHPacyl.COelim.pttpmmtmpu				
65204	-----				
65205	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16195296				

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65206 Electronic state : 2-A
65207 Cartesian coordinates (Angs):
65208 O -1.537742 1.883210 -0.617492
65209 O -1.794722 1.072089 0.513715
65210 C -1.076948 -0.088993 0.463433
65211 C 0.311742 0.028294 -0.112311
65212 C 1.094723 -1.262902 0.052621
65213 O 2.303548 -1.267971 -0.683948
65214 O 3.249063 -0.485779 0.046518
65215 H -0.751136 2.374628 -0.330023
65216 C -1.332098 -0.860422 1.719700
65217 H -2.395659 -0.830860 1.951126
65218 H -0.779812 -0.428917 2.558360
65219 H -1.032407 -1.900629 1.599705
65220 C -2.013800 -1.251856 -0.952081
65221 O -3.141708 -1.085737 -0.986255
65222 H 4.021699 -1.062129 0.029870
65223 H 0.251641 0.276481 -1.172655
65224 O 0.926897 1.131688 0.558565
65225 O 1.788175 1.808042 -0.346556
65226 H 2.607768 1.292924 -0.268260
65227 H 1.309386 -1.465743 1.103107
65228 H 0.518719 -2.084817 -0.375774
65229 Rotational constants (GHz): 1.3737800 0.6291600 0.5255200
65230 Vibrational harmonic frequencies (cm-1):
65231 i315.3926 41.6828 57.9637
65232 83.4755 103.8381 110.7356
65233 119.0159 160.2846 171.4829
65234 214.0090 230.4673 236.7863
65235 251.0192 266.8495 304.1170
65236 338.4150 385.5011 428.8415
65237 438.1591 461.3877 529.4473
65238 549.4846 572.8020 616.6406
65239 866.5642 897.1690 961.1449
65240 976.7291 1033.2345 1057.2134
65241 1063.3188 1098.6533 1115.5972
65242 1141.7245 1236.8435 1309.7175
65243 1317.1646 1337.5839 1376.4885
65244 1392.6905 1410.6542 1428.0822
65245 1437.7311 1460.8866 1466.8013
65246 1484.9669 1493.4401 2079.8305
65247 3050.8258 3074.0771 3102.1899
65248 3124.7629 3136.0721 3153.9588
65249 3739.6074 3743.7881 3843.6270
65250 Zero-point correction (Hartree): 0.152832
65251
65252 TS.triHPacyl.COelim.pttpmtppmu
65253 -----
65254 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16360227
65255 Electronic state : 2-A
65256 Cartesian coordinates (Angs):
65257 O 1.882944 -1.235796 -1.396995
65258 O 1.830280 -1.238761 0.020271
65259 C 1.097966 -0.180271 0.475704
65260 C -0.180803 0.091191 -0.286609
65261 C -1.118682 1.026670 0.459667
65262 O -2.274291 1.333457 -0.292345
65263 O -3.168496 0.227100 -0.201074
65264 H 1.119297 -1.792007 -1.614673
65265 C 1.140861 -0.175190 1.969326
65266 H 2.170203 -0.312736 2.294481
65267 H 0.525141 -0.981238 2.373767
65268 H 0.782203 0.775360 2.362061
65269 C 2.253094 1.468197 -0.004750
65270 O 1.740921 2.278429 -0.628300
65271 H -3.078198 -0.164668 -1.080370
65272 H 0.050132 0.536677 -1.256533
65273 O -0.825989 -1.125678 -0.671547
65274 O -1.253374 -1.814674 0.493980
65275 H -2.146090 -1.450493 0.610069
65276 H -1.411379 0.626423 1.431122
65277 H -0.621883 1.986474 0.608133

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65278 Rotational constants (GHz): 1.2227700 0.7260800 0.5921900
65279 Vibrational harmonic frequencies (cm-1):
65280 i325.2120 39.1608 74.7842
65281 96.4693 112.3364 134.5480
65282 164.2725 189.5925 194.7380
65283 220.3463 236.1051 244.4787
65284 268.9952 304.4495 320.3438
65285 364.6180 371.6555 425.5789
65286 443.6561 475.8558 549.7917
65287 564.4323 596.6585 665.1342
65288 833.3345 906.3145 950.9254
65289 974.2548 1006.3373 1050.6266
65290 1056.4506 1108.6144 1121.3462
65291 1144.3297 1240.6975 1309.6919
65292 1321.4605 1331.4799 1387.3087
65293 1406.9911 1408.9786 1420.6550
65294 1436.3383 1449.7607 1473.3874
65295 1486.1398 1494.5258 2056.1129
65296 3059.9431 3082.0688 3097.8501
65297 3132.6018 3138.0839 3156.9768
65298 3736.8535 3763.5142 3802.8154
65299 Zero-point correction (Hartree): 0.153559
65300
65301 TS.triHPacyl.COelim.pttpppppmu
65302 -----
65303 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16275097
65304 Electronic state : 2-A
65305 Cartesian coordinates (Angs):
65306 O 1.860702 -1.019175 -1.491430
65307 O 1.784359 -1.138880 -0.079843
65308 C 0.944730 -0.200563 0.445396
65309 C -0.326533 0.072037 -0.321493
65310 C -1.203463 1.110914 0.361060
65311 O -2.321063 1.457597 -0.431925
65312 O -3.288099 0.416826 -0.324046
65313 H 2.726043 -0.596826 -1.588453
65314 C 0.955031 -0.324218 1.934682
65315 H 1.980919 -0.426352 2.286196
65316 H 0.381174 -1.197276 2.249447
65317 H 0.520632 0.565041 2.388224
65318 C 1.990036 1.582248 0.145357
65319 O 3.041295 1.381789 -0.258046
65320 H -3.133069 -0.077736 -1.141027
65321 H -0.077830 0.429047 -1.322013
65322 O -1.041819 -1.128217 -0.610670
65323 O -1.531368 -1.681814 0.602462
65324 H -2.403742 -1.261250 0.666602
65325 H -1.543510 0.779941 1.342824
65326 H -0.641482 2.037899 0.476159
65327 Rotational constants (GHz): 1.4300000 0.6208300 0.5539800
65328 Vibrational harmonic frequencies (cm-1):
65329 i296.4434 44.6478 54.5239
65330 102.1948 121.8277 134.4059
65331 156.3284 190.3107 197.1038
65332 212.7494 229.5438 237.3827
65333 263.7489 283.6369 301.4505
65334 316.7257 366.9448 395.3877
65335 430.0900 495.6198 535.2207
65336 569.3709 597.4404 675.6488
65337 836.2662 905.2578 950.0234
65338 972.1493 1001.9582 1052.6681
65339 1055.6773 1106.8301 1120.6563
65340 1136.5864 1227.8693 1307.0634
65341 1316.7347 1329.5603 1380.1396
65342 1409.0510 1411.6406 1419.9001
65343 1425.7503 1446.9597 1478.0590
65344 1486.6957 1493.9495 2055.1428
65345 3063.8680 3086.9551 3105.4399
65346 3135.8232 3143.3753 3153.7083
65347 3723.5310 3791.2925 3791.6359
65348 Zero-point correction (Hartree): 0.153172
65349

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65350 TS.triHPacyl.COelim.pttpptppmu
65351 -----
65352 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16206488
65353 Electronic state : 2-A
65354 Cartesian coordinates (Angs):
65355 O 1.800922 -1.515237 -1.399528
65356 O 1.799808 -1.332311 0.004361
65357 C 1.058836 -0.238485 0.345187
65358 C -0.259604 -0.071444 -0.377202
65359 C -1.063741 1.112349 0.141438
65360 O -2.231318 1.329189 -0.624807
65361 O -3.208926 0.369811 -0.233967
65362 H 2.486239 -0.882957 -1.667641
65363 C 1.178137 0.006337 1.813906
65364 H 2.213604 -0.121735 2.124878
65365 H 0.549786 -0.694224 2.366612
65366 H 0.868299 1.022821 2.053888
65367 C 2.202378 1.275644 -0.494106
65368 O 2.088582 2.302635 -0.005840
65369 H -3.128204 -0.287538 -0.939343
65370 H -0.078280 0.066426 -1.444423
65371 O -1.022365 -1.276372 -0.368395
65372 O -1.415698 -1.566794 0.965029
65373 H -2.276545 -1.121858 1.012231
65374 H -1.333582 0.994707 1.191446
65375 H -0.485385 2.030574 0.032191
65376 Rotational constants (GHz): 1.2221200 0.6994900 0.5689200
65377 Vibrational harmonic frequencies (cm-1):
65378 1296.2682 49.2550 68.6921
65379 96.6527 124.4802 133.3108
65380 176.7063 192.1399 195.7931
65381 206.2557 223.8870 251.9110
65382 277.2613 304.0734 324.4156
65383 347.1462 363.7625 402.2301
65384 435.7678 483.7784 532.6989
65385 566.4444 599.4654 665.6063
65386 835.9717 905.3265 951.1822
65387 972.9001 1002.1548 1050.7721
65388 1056.6829 1107.3254 1121.5325
65389 1136.5385 1236.0720 1305.1361
65390 1317.3311 1335.4688 1381.4558
65391 1406.9421 1411.7356 1421.0997
65392 1433.1155 1443.1254 1476.6456
65393 1487.1655 1493.1839 2062.8763
65394 3062.4144 3086.2667 3101.9292
65395 3133.8017 3140.8440 3153.0628
65396 3746.8293 3747.4703 3790.0597
65397 Zero-point correction (Hartree): 0.153403
65398
65399 TS.triHPacyl.COelim.tmmmmmtmpu
65400 -----
65401 IRC pathway available
65402 expected
65403 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18781021
65404 E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07057440
65405 T1 diagnostic: 0.016826
65406 E(MP2/Aug-CC-pVTZ) (Hartree): -721.03109165
65407 E(MP3/Aug-CC-pVTZ) (Hartree): -721.04919953
65408 E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03632101
65409 E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05264744
65410 E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51187680
65411 E(UHF/Aug-CC-pVTZ) (Hartree): -718.50505950
65412 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16455115
65413 Electronic state : 2-A
65414 Cartesian coordinates (Angs):
65415 O -2.936177 -0.115783 0.808863
65416 O -1.553480 -0.143237 1.099836
65417 C -0.827665 -0.632892 0.045267
65418 C 0.592507 -0.843350 0.513547
65419 C 1.148747 0.305964 1.347762
65420 O 1.129756 1.557524 0.696957
65421 O 2.090190 1.526192 -0.353038

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65422      H      -3.039051      0.775099      0.441353
65423      C      -1.446105      -1.673990      -0.827018
65424      H      -2.356078      -1.311649      -1.297242
65425      H      -1.701862      -2.553651      -0.227886
65426      H      -0.730099      -1.962963      -1.591518
65427      C      -0.766995      1.049636      -1.266162
65428      O      -1.764218      1.605810      -1.202109
65429      H      1.525467      1.313115      -1.115351
65430      H      0.631796      -1.746814      1.140644
65431      O      1.325794      -1.083851      -0.679456
65432      O      2.675931      -1.325383      -0.338186
65433      H      3.044536      -0.428556      -0.393813
65434      H      0.518629      0.444128      2.225518
65435      H      2.161355      0.068902      1.674979
65436      Rotational constants (GHz):      1.3193800      0.7277400      0.6323900
65437      Vibrational harmonic frequencies (cm-1):
65438      i307.0615      47.5521      94.7868
65439      114.8783      133.0111      151.7519
65440      154.0193      167.9314      191.3573
65441      233.7337      240.3903      260.4583
65442      279.7984      307.4337      330.0774
65443      342.7844      391.2724      419.0890
65444      457.0907      477.9111      483.0200
65445      557.7587      620.4738      741.4178
65446      836.3618      881.2056      948.2096
65447      977.5665      1023.4180      1040.3149
65448      1067.6180      1088.8905      1122.4158
65449      1175.7372      1251.7211      1280.2247
65450      1297.0956      1359.3735      1380.8193
65451      1407.3730      1410.1745      1437.0299
65452      1441.0553      1455.2601      1478.8829
65453      1480.9551      1488.6930      2053.4374
65454      2990.1094      3043.4486      3092.3827
65455      3140.2389      3146.7930      3181.8525
65456      3702.0532      3719.9165      3767.3152
65457      Zero-point correction (Hartree): 0.153471
65458
65459      TS.triHPacyl.COelim.tmmmtttmpu
65460      -----
65461      IRC pathway available
65462      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -721.18793480
65463      E(CCSD/Aug-CC-pVTZ) (Hartree): -721.07069944
65464      T1 diagnostic: 0.016802
65465      E(MP2/Aug-CC-pVTZ) (Hartree): -721.03123845
65466      E(MP3/Aug-CC-pVTZ) (Hartree): -721.04944689
65467      E(PMP2/Aug-CC-pVTZ) (Hartree): -721.03660155
65468      E(PMP3/Aug-CC-pVTZ) (Hartree): -721.05295793
65469      E(PUHF/Aug-CC-pVTZ) (Hartree): -718.51223768
65470      E(UHF/Aug-CC-pVTZ) (Hartree): -718.50522630
65471      E(UMO62X/Aug-CC-pVTZ) (Hartree): -722.16454369
65472      Electronic state : 2-A
65473      Cartesian coordinates (Angs):
65474      O      -3.066680      -0.422407      -0.657359
65475      O      -1.799660      0.027336      -1.094400
65476      C      -1.058009      0.483795      -0.037648
65477      C      0.304109      0.874343      -0.564571
65478      C      0.946543      -0.171380      -1.469104
65479      O      1.179858      -1.410174      -0.832705
65480      O      2.294131      -1.259713      0.040683
65481      H      -2.831951      -1.273186      -0.251554
65482      C      -1.714537      1.392506      0.950381
65483      H      -2.625561      0.950356      1.343233
65484      H      -1.973917      2.337223      0.461540
65485      H      -1.025612      1.601520      1.764722
65486      C      -0.870317      -1.283109      1.103704
65487      O      -0.051136      -1.293333      1.900072
65488      H      1.858132      -1.223754      0.906607
65489      H      0.202243      1.799631      -1.152130
65490      O      1.074769      1.151052      0.594567
65491      O      2.338369      1.633973      0.182166
65492      H      2.848876      0.809087      0.137518
65493      H      0.265538      -0.404449      -2.286397

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65494      H      1.878313      0.212768      -1.884301
65495      Rotational constants (GHz):      1.2808700      0.7302000      0.6809000
65496      Vibrational harmonic frequencies (cm-1):
65497      i304.1293      59.4387      102.8584
65498      127.5937      131.8745      142.4957
65499      155.0896      173.1661      183.4588
65500      228.6422      232.9561      256.3800
65501      284.5336      316.0525      332.6133
65502      352.6227      398.5562      402.6151
65503      435.3909      459.1864      488.1645
65504      552.6637      617.4410      736.0593
65505      837.1017      882.1610      947.2488
65506      980.2356      1023.7606      1035.7637
65507      1062.7776      1088.8675      1121.0850
65508      1174.5381      1247.7213      1282.5235
65509      1294.3293      1361.2487      1376.4575
65510      1406.3120      1407.0858      1436.8994
65511      1444.1136      1454.5812      1477.3239
65512      1479.5278      1488.5252      2062.1685
65513      2988.6866      3041.9594      3094.8035
65514      3141.1016      3150.4615      3183.3960
65515      3723.8551      3728.9012      3753.0020
65516      Zero-point correction (Hartree): 0.153431
65517
65518      TS.triHPacyl.COelim.tmtmmmtmpu
65519      -----
65520      E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16054767
65521      Electronic state : 2-A
65522      Cartesian coordinates (Angs):
65523      O      -2.852218      -0.830983      -1.042736
65524      O      -1.451186      -0.879609      -0.848670
65525      C      -0.974034      0.329051      -0.411787
65526      C      0.529299      0.224916      -0.323954
65527      C      0.996486      -1.092773      0.286458
65528      O      2.386691      -1.085699      0.544955
65529      O      3.061207      -1.083583      -0.704441
65530      H      -3.171651      -1.176483      -0.195821
65531      C      -1.564460      1.579197      -0.970913
65532      H      -2.629000      1.643659      -0.763524
65533      H      -1.426472      1.601595      -2.056404
65534      H      -1.056938      2.431870      -0.528033
        C      -1.641804      0.375650      1.612134
        O      -2.397992      -0.463987      1.791797
        H      3.168501      -0.134276      -0.871016
        H      0.944602      0.342015      -1.332921
        O      0.949879      1.334323      0.457527
        O      2.311049      1.605557      0.149663
        H      2.757506      1.187890      0.900177
        H      0.542657      -1.228032      1.269650
        H      0.738427      -1.932632      -0.358486
        Rotational constants (GHz):      1.4232100      0.5757200      0.5451300
        Vibrational harmonic frequencies (cm-1):
        i304.3775      33.8982      48.8859
        94.2813      130.3864      138.9066
        155.6981      163.3267      170.3909
        194.6413      213.0057      242.9094
        258.3828      313.9737      338.4805
        355.3746      383.3002      410.4186
        424.9268      438.0716      493.0777
        524.8788      557.2982      669.7979
        889.0823      899.0738      956.4628
        992.2061      1025.5077      1052.0564
        1056.7523      1102.3090      1141.1687
        1155.6348      1261.3153      1275.6080
        1305.6774      1339.2388      1364.8155
        1407.5951      1417.6324      1426.6301
        1431.2847      1443.0554      1469.5672
        1478.2496      1487.5657      2047.6627
        3021.4843      3045.7762      3081.4603
        3140.0991      3142.4438      3182.3380
        3747.4035      3773.4007      3784.1327
        Zero-point correction (Hartree): 0.152863

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30
31 TS.triHPacyl.COelim.tmtmtpppu
32 -----
33 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16107728
34 Electronic state : 2-A
35 Cartesian coordinates (Angs):
36 O 2.700676 -1.587413 -0.276173
37 O 1.302245 -1.550122 -0.039514
38 C 0.930849 -0.312172 0.429896
39 C -0.576893 -0.337787 0.521611
40 C -1.252289 -0.768386 -0.787135
41 O -2.563208 -0.247354 -0.868722
42 O -3.321027 -0.800719 0.197467
43 H 2.730151 -1.478805 -1.236996
44 C 1.692484 0.267158 1.574370
45 H 2.758326 0.271754 1.365750
46 H 1.509997 -0.323733 2.477344
47 H 1.356101 1.286699 1.748950
48 C 1.499427 0.910469 -1.165837
49 O 2.120706 1.824411 -0.887450
50 H -3.216400 -0.124070 0.882424
51 H -0.856556 -1.033188 1.322485
52 O -1.107189 0.884083 0.998125
53 O -0.921383 1.884813 0.006456
54 H -1.728568 1.782712 -0.521385
55 H -0.737360 -0.343775 -1.647863
56 H -1.263730 -1.854882 -0.869646
57 Rotational constants (GHz): 1.3838400 0.6471500 0.5580200
58 Vibrational harmonic frequencies (cm-1):
59 1329.2815 48.4236 72.9157
60 86.2380 112.7586 132.3686
61 155.8168 175.8939 180.9969
62 193.4202 208.6773 264.5064
63 267.5163 294.6016 318.4892
64 348.5166 390.9154 405.2812
65 417.9673 469.3534 479.6567
66 495.0883 636.9504 724.8517
67 829.8259 914.1507 957.4500
68 982.7809 997.2790 1030.2690
69 1044.8662 1099.7258 1130.9245
70 1169.5687 1245.2332 1267.0474
71 1293.4187 1330.0802 1373.8949
72 1399.4427 1405.6065 1413.1607
73 1420.7442 1431.4153 1477.1758
74 1482.5607 1490.4373 2085.3243
75 3033.7639 3044.2995 3093.7554
76 3141.0797 3152.4546 3182.6671
77 3752.5599 3769.6038 3795.2042
78 Zero-point correction (Hartree): 0.152908
79
80 TS.triHPacyl.COelim.tmtmtttmpu
81 -----
82 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16097771
83 Electronic state : 2-A
84 Cartesian coordinates (Angs):
85 O 2.759537 -1.614671 0.057658
86 O 1.350842 -1.491496 0.178448
87 C 1.018352 -0.187090 0.437336
88 C -0.484048 -0.057720 0.383574
89 C -1.111038 -0.917423 -0.708332
90 O -2.477187 -0.604776 -0.899058
91 O -3.186563 -1.031891 0.254695
92 H 2.861864 -1.623101 -0.904563
93 C 1.747598 0.521868 1.529804
94 H 2.819241 0.519003 1.352212
95 H 1.550182 0.023799 2.483871
96 H 1.395755 1.549239 1.584818
97 C 1.670221 0.786982 -1.288388
98 O 2.141385 1.811678 -1.125529
99 H -3.165702 -0.235957 0.808142
100 H -0.902749 -0.315668 1.363905
101 O -0.724094 1.326696 0.154831

```

102	O	-2.044657	1.635762	0.578972		
103	H	-2.519253	1.621860	-0.264738		
104	H	-0.642350	-0.692121	-1.667090		
105	H	-0.997591	-1.977149	-0.480655		
106	Rotational constants (GHz):			1.3550600	0.6200300	0.5278300
107	Vibrational harmonic frequencies (cm-1):					
108	i325.9080		42.5481			53.1275
109	87.5855		112.5042			132.1490
110	148.4530		159.2580			169.8078
111	192.9258		197.2391			248.0641
112	262.6971		287.9111			317.2934
113	344.3107		383.0716			406.2703
114	409.6412		444.1709			491.8338
115	524.2147		558.5558			662.4060
116	888.5948		897.3281			954.9028
117	991.9419		1017.5014			1038.7985
118	1055.8507		1099.9313			1136.7084
119	1152.9023		1254.6483			1273.8599
120	1301.3914		1337.6864			1362.1626
121	1403.2854		1412.7539			1417.5651
122	1426.1371		1442.1834			1471.7821
123	1477.0601		1485.9302			2086.0822
124	3027.4261		3046.7529			3086.5859
125	3143.0978		3145.7162			3182.2738
126	3737.3075		3783.5533			3790.8134
127	Zero-point correction (Hartree):			0.152561		
128						
129	TS.triHPacyl.COelim.tmtppmppmu					
130	-----					
131	E(UM062X/Aug-CC-pVTZ) (Hartree):			-722.16130904		
132	Electronic state : 2-A					
133	Cartesian coordinates (Angs):					
134	O	-3.052520	-0.373181	-0.883783		
135	O	-1.655895	-0.476897	-1.087092		
136	C	-0.964416	0.414937	-0.301936		
137	C	0.497613	0.240068	-0.669796		
138	C	1.081981	-1.081230	-0.185549		
139	O	2.393281	-1.291998	-0.665379		
140	O	3.281796	-0.496130	0.114587		
141	H	-3.202804	-1.081872	-0.241170		
142	C	-1.494719	1.798302	-0.141561		
143	H	-2.536686	1.778383	0.164104		
144	H	-1.416794	2.341759	-1.088065		
145	H	-0.902830	2.316818	0.608056		
146	C	-1.278073	-0.396739	1.640988		
147	O	-1.943980	-1.326404	1.588622		
148	H	3.456176	0.243031	-0.484200		
149	H	0.570133	0.261561	-1.764107		
150	O	1.284152	1.353804	-0.295620		
151	O	1.353502	1.420080	1.121370		
152	H	2.130253	0.866620	1.303114		
153	H	1.072515	-1.150096	0.902744		
154	H	0.493032	-1.902430	-0.594989		
155	Rotational constants (GHz):			1.4331700	0.6063400	0.5676400
156	Vibrational harmonic frequencies (cm-1):					
157	i308.3546		34.6653			53.9452
158	93.8437		134.1362			159.6601
159	169.0794		177.4700			189.0197
160	208.9348		221.7344			249.9220
161	279.5244		310.3224			325.0137
162	341.8887		361.6853			379.5228
163	417.5528		489.8643			508.8030
164	537.3936		628.3726			677.5918
165	866.1110		902.4229			947.5171
166	978.1336		1001.1342			1043.1780
167	1050.0950		1117.4134			1129.4459
168	1159.8567		1230.4554			1280.3859
169	1308.8385		1313.9342			1381.4820
170	1404.3538		1408.4693			1414.0284
171	1430.3878		1445.1481			1477.3305
172	1481.0602		1487.1807			2043.8044
173	3038.6041		3047.6973			3087.0272

```

174          3141.8866          3145.8388          3186.8432
175          3731.9909          3780.1030          3796.6398
176 Zero-point correction (Hartree): 0.153113
177
178 TS.triHPacyl.COelim.tmtpmtppmu
179 -----
180 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16231965
181 Electronic state : 2-A
182 Cartesian coordinates (Angs):
183 O          2.886546          -1.351558          -0.182825
184 O          1.512757          -1.466181          0.152312
185 C          0.985053          -0.228257          0.437995
186 C          -0.502043          -0.434370          0.630738
187 C          -1.204693          -0.972780          -0.610663
188 O          -2.572042          -1.234626          -0.369609
189 O          -3.273725          0.006001          -0.399737
190 H          2.848958          -1.406955          -1.147854
191 C          1.705419          0.634471          1.419041
192 H          2.759550          0.700263          1.165945
193 H          1.604523          0.214648          2.424543
194 H          1.270010          1.630926          1.413389
195 C          1.300180          0.776314          -1.372092
196 O          1.812513          1.790582          -1.287722
197 H          -3.423066          0.164826          0.542357
198 H          -0.648018          -1.155012          1.445851
199 O          -1.124023          0.728102          1.144702
200 O          -1.040420          1.756253          0.167806
201 H          -1.856005          1.607207          -0.337714
202 H          -1.097853          -0.299063          -1.460126
203 H          -0.774452          -1.937703          -0.875917
204 Rotational constants (GHz):      1.3872700      0.6399600      0.5622800
205 Vibrational harmonic frequencies (cm-1):
206      i323.9136          47.7969          63.5103
207      86.5245          119.0055          137.0523
208      166.5569          182.0265          187.4621
209      200.7877          206.1151          219.5246
210      260.0128          283.4786          317.6002
211      328.7029          378.1706          400.9961
212      416.8293          467.3238          501.6113
213      542.8376          625.7951          671.6367
214      862.6209          904.8110          947.4102
215      977.0968          1000.0457          1031.3446
216      1047.7028          1115.7837          1126.5806
217      1157.1360          1234.0743          1268.0100
218      1300.3954          1313.7079          1374.4055
219      1401.4505          1406.1250          1412.7869
220      1413.2893          1441.5056          1476.4947
221      1477.8703          1481.6717          2085.7283
222      3027.9286          3045.5039          3098.6064
223      3142.4579          3152.5702          3184.6629
224      3741.4474          3793.6844          3798.2858
225 Zero-point correction (Hartree): 0.152762
226
227 TS.triHPacyl.COelim.tmtpmtpppu
228 -----
229 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16042610
230 Electronic state : 2-A
231 Cartesian coordinates (Angs):
232 O          2.880017          -1.351620          -0.283802
233 O          1.519515          -1.467093          0.102107
234 C          1.007638          -0.233827          0.433334
235 C          -0.472182          -0.433214          0.687747
236 C          -1.209494          -0.992313          -0.525288
237 O          -2.579583          -1.212255          -0.251916
238 O          -3.261213          0.033555          -0.379643
239 H          2.802191          -1.353812          -1.248062
240 C          1.772554          0.612846          1.394027
241 H          2.812859          0.690768          1.092038
242 H          1.722353          0.172790          2.394723
243 H          1.330201          1.605598          1.429686
244 C          1.248073          0.803413          -1.374268
245 O          1.757114          1.819683          -1.291532

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246	H	-3.849013	-0.151837	-1.122002	
247	H	-0.587791	-1.145235	1.514918	
248	O	-1.066949	0.730528	1.212805	
249	O	-1.055728	1.737921	0.210768	
250	H	-1.951272	1.636496	-0.147082	
251	H	-1.098437	-0.345904	-1.394700	
252	H	-0.806012	-1.976048	-0.763133	
253	Rotational constants (GHz):		1.3792000	0.6385700	0.5618200
254	Vibrational harmonic frequencies (cm-1):				
255	i321.0993		52.4799		69.6791
256	80.5167		121.9494		131.8505
257	164.4037		180.9725		190.7462
258	205.2894		209.8499		255.2295
259	275.3639		283.7350		293.5101
260	323.0687		328.9215		389.5321
261	406.3998		459.5406		492.7287
262	507.8412		625.1391		668.0538
263	857.7156		904.1311		948.6995
264	977.6506		1000.3066		1030.8223
265	1046.2668		1110.7469		1127.4506
266	1167.2700		1234.4557		1268.1037
267	1304.9234		1314.7227		1376.5930
268	1391.7368		1407.2614		1412.7419
269	1416.8312		1443.5883		1472.7261
270	1476.1438		1483.1065		2084.3075
271	3030.3839		3045.1783		3097.4054
272	3142.2602		3152.1829		3184.3147
273	3770.1272		3793.4367		3824.2819
274	Zero-point correction (Hartree): 0.152671				
275					
276	TS.triHPacyl.COelim.tmtpttmpu				
277	-----				
278	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.15927096				
279	Electronic state : 2-A				
280	Cartesian coordinates (Angs):				
281	O	-2.934788	-1.376475	-0.032079	
282	O	-1.554474	-1.373717	-0.361238	
283	C	-1.092214	-0.084584	-0.441763	
284	C	0.409246	-0.111922	-0.607192	
285	C	1.058167	-1.217354	0.218668	
286	O	2.457295	-1.300564	0.017808	
287	O	3.071578	-0.267916	0.788314	
288	H	-2.895500	-1.478450	0.929772	
289	C	-1.868807	0.892198	-1.259689	
290	H	-2.897669	0.961883	-0.918060	
291	H	-1.869470	0.572236	-2.306182	
292	H	-1.396818	1.868791	-1.187152	
293	C	-1.371453	0.603241	1.517165	
294	O	-1.679069	1.695939	1.613313	
295	H	3.737040	-0.767271	1.275370	
296	H	0.663488	-0.250606	-1.664962	
297	O	0.847976	1.182014	-0.223578	
298	O	1.993170	1.526656	-0.982503	
299	H	2.709415	1.188160	-0.421888	
300	H	0.839545	-1.084412	1.279373	
301	H	0.686821	-2.187298	-0.109709	
302	Rotational constants (GHz):		1.3307500	0.6149300	0.5458300
303	Vibrational harmonic frequencies (cm-1):				
304	i322.2244		42.0478		53.9362
305	65.3336		112.6932		128.3991
306	140.4766		157.7566		164.5148
307	176.4208		189.8377		232.7180
308	247.5902		291.8743		299.4322
309	315.8329		365.2326		380.0153
310	392.1946		449.8136		476.0709
311	521.2281		541.5055		655.3845
312	876.2782		905.1846		962.2038
313	980.0095		1018.6061		1044.8014
314	1056.4107		1103.4182		1121.5622
315	1156.6747		1244.0603		1269.2401
316	1308.6065		1324.9297		1364.2939
317	1388.6596		1403.3951		1413.8729

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318      1425.7439          1460.3722          1470.5166
319      1479.2549          1484.0946          2088.4810
320      3029.1001          3045.9817          3083.3625
321      3143.4162          3147.3090          3183.4064
322      3733.7211          3785.1112          3841.4161
323 Zero-point correction (Hartree): 0.152054
324
325 TS.triHPacyl.COelim.tmtppmpmpmu
326 -----
327 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16106227
328 Electronic state : 2-A
329 Cartesian coordinates (Angs):
330      O      2.851172      -1.302458      -0.305562
331      O      1.510718      -1.453947      0.149958
332      C      0.973208      -0.217164      0.424426
333      C     -0.511685      -0.434453      0.617328
334      C     -1.215032      -0.956460      -0.630696
335      O     -2.579602      -1.230742      -0.384563
336      O     -3.287943      0.006619      -0.397457
337      H      3.338389      -1.785941      0.373339
338      C      1.689817      0.651211      1.404754
339      H      2.731632      0.768526      1.118431
340      H      1.634195      0.210891      2.405662
341      H      1.221085      1.631801      1.432721
342      C      1.245668      0.801984      -1.374372
343      O      1.931865      1.709785      -1.316554
344      H     -3.425652      0.158998      0.547414
345      H     -0.656127      -1.168160      1.421274
346      O     -1.138974      0.716520      1.152702
347      O     -1.059563      1.764641      0.196890
348      H     -1.862808      1.609545      -0.326678
349      H     -1.116754      -0.267619      -1.467936
350      H     -0.777200      -1.912100      -0.916175
351 Rotational constants (GHz):      1.4057100      0.6327300      0.5608500
352 Vibrational harmonic frequencies (cm-1):
353      i340.6932          59.4463          78.0422
354      88.5540          114.4190          136.4718
355      163.8908          179.5373          192.7444
356      203.8260          211.9779          226.5977
357      255.9521          286.6763          321.2172
358      326.0072          375.8486          400.1063
359      415.9480          466.2477          501.4052
360      546.1301          624.9710          671.4957
361      861.6904          904.3706          946.4372
362      977.4609          998.8790          1023.1021
363      1045.3733          1113.5641          1126.4939
364      1155.4844          1231.3380          1261.7068
365      1294.4035          1311.8391          1375.6255
366      1398.9905          1401.4676          1411.4136
367      1416.5772          1441.0516          1476.3013
368      1479.5175          1484.6193          2086.6771
369      3024.6751          3038.7043          3104.5566
370      3140.8483          3157.4621          3179.3277
371      3739.4648          3798.6945          3822.2002
372 Zero-point correction (Hartree): 0.152815
373
374 TS.triHPacyl.COelim.tpmmmtmpu
375 -----
376 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16242643
377 Electronic state : 2-A
378 Cartesian coordinates (Angs):
379      O      1.920858      -1.368266      -1.158165
380      O      0.742941      -0.656647      -0.829899
381      C      0.756893      -0.267315      0.486134
382      C     -0.516431      0.463739      0.809159
383      C     -1.706247      -0.475564      1.015495
384      O     -1.897061      -1.413567      -0.017602
385      O     -2.239891      -0.699737      -1.199502
386      H      2.474493      -0.657449      -1.515199
387      C      1.302549      -1.214484      1.500719
388      H      2.348272      -1.441444      1.310628
389      H      0.743756      -2.154931      1.478436

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390      H      1.213731      -0.767597      2.489611
391      C      2.171334      1.326513      0.502160
392      O      2.782264      1.333718      -0.462966
393      H     -1.374038      -0.617216      -1.629242
394      H     -0.362436      1.008170      1.748182
395      O     -0.687976      1.392409      -0.253256
396      O     -1.928819      2.051524      -0.102115
397      H     -2.499832      1.498979      -0.659141
398      H     -1.516348      -1.085627      1.900005
399      H     -2.614708      0.104300      1.182752
400 Rotational constants (GHz):      1.2716600      0.7361300      0.6231000
401 Vibrational harmonic frequencies (cm-1):
402      i282.0345      47.5660      73.8634
403      82.2584      109.4208      134.1671
404      146.0409      169.9160      195.6488
405      208.7635      229.0842      240.4035
406      272.6628      316.5924      322.5356
407      371.1530      384.9044      409.4802
408      463.5265      470.3212      493.2780
409      533.2218      608.5990      775.9381
410      817.4600      868.0455      956.1618
411      973.7508      1024.5920      1036.6191
412      1061.1805      1073.7880      1125.5120
413      1171.4336      1233.5583      1287.0338
414      1303.0815      1347.0014      1381.7650
415      1404.5591      1415.9106      1429.9969
416      1436.2885      1444.8664      1468.4647
417      1479.0499      1497.0537      2065.0029
418      3038.8798      3046.2321      3083.5855
419      3129.6188      3130.8486      3166.4587
420      3735.9534      3754.3163      3770.1723
421 Zero-point correction (Hartree): 0.153133
422
423 TS.triHPacyl.COelim.tpmmmtmppu
424 -----
425 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16221972
426 Electronic state : 2-A
427 Cartesian coordinates (Angs):
428      O      0.884149      -1.936036      -1.452301
429      O      0.134920      -0.805896      -1.048422
430      C      0.447215      -0.457964      0.243031
431      C     -0.298298      0.801587      0.615762
432      C     -1.684917      0.498298      1.199147
433      O     -2.345534      -0.575290      0.574905
434      O     -2.777335      -0.153468      -0.708490
435      H      1.768400      -1.547362      -1.559553
436      C      0.558739      -1.532979      1.273528
437      H      1.318648      -2.264272      1.010594
438      H     -0.399069      -2.049757      1.374977
439      H      0.824460      -1.080793      2.229125
440      C      2.476510      0.065999      0.052648
441      O      2.909061      0.581680      0.972309
442      H     -2.027040      -0.406057      -1.267378
443      H      0.290003      1.333521      1.373282
444      O     -0.518545      1.651554      -0.492061
445      O      0.744029      2.072967      -0.983918
446      H      0.851424      1.500768      -1.756675
447      H     -1.572845      0.178248      2.235350
448      H     -2.295421      1.401965      1.159412
449 Rotational constants (GHz):      1.2073300      0.7537000      0.6643700
450 Vibrational harmonic frequencies (cm-1):
451      i290.1855      65.4310      85.6503
452      99.0926      123.7012      128.6839
453      155.1129      160.0471      200.2044
454      217.4231      236.2950      243.5560
455      266.8307      295.8462      327.7972
456      347.9551      368.9893      388.4957
457      402.0629      432.7583      475.0013
458      491.2905      605.9997      755.0606
459      812.6504      879.6568      956.6865
460      982.2081      1017.5824      1052.1455
461      1054.7464      1067.6717      1140.9141

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462      1172.1911      1242.8244      1283.5070
463      1304.4009      1331.2043      1378.1361
464      1404.2170      1407.6234      1414.8327
465      1442.6262      1448.9871      1461.0229
466      1475.1934      1497.4834      2088.4209
467      3035.1394      3055.1227      3079.5844
468      3128.7700      3136.4091      3161.0609
469      3722.1361      3765.4491      3788.4965
470 Zero-point correction (Hartree): 0.152779
471
472 TS.triHPacyl.COelim.tpmmmtmpu
473 -----
474 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16261646
475 Electronic state : 2-A
476 Cartesian coordinates (Angs):
477 O      1.654588      -1.842557      -1.202751
478 O      0.523972      -1.086094      -0.813762
479 C      0.817280      -0.328736      0.289640
480 C     -0.307461      0.628562      0.572303
481 C     -1.508885      -0.049807      1.234633
482 O     -1.958354      -1.210254      0.576262
483 O     -2.452393      -0.825704      -0.701351
484 H      2.190844      -1.161073      -1.640041
485 C      1.482377      -0.999435      1.445712
486 H      2.433349      -1.436541      1.152023
487 H      0.845877      -1.803589      1.827405
488 H      1.654913      -0.273949      2.239652
489 C      2.330648      0.944849      -0.430310
490 O      2.519993      1.845962      0.241138
491 H     -1.679919      -0.996999      -1.262909
492 H      0.060468      1.390856      1.270612
493 O     -0.599664      1.235063      -0.679591
494 O     -1.740442      2.058121      -0.546632
495 H     -2.441336      1.445663      -0.821446
496 H     -1.207648      -0.400567      2.222844
497 H     -2.321907      0.667313      1.353494
498 Rotational constants (GHz): 1.1798400 0.7732400 0.6201300
499 Vibrational harmonic frequencies (cm-1):
500      i290.1968      52.2179      70.4773
501      85.5228      96.0711      103.7340
502      132.3220      182.4136      192.2575
503      211.5064      222.8492      240.8922
504      283.7769      316.2356      332.3330
505      369.5648      381.5354      421.7919
506      468.9942      483.0964      484.7038
507      531.7290      607.2046      770.8457
508      816.9284      870.3879      958.7640
509      973.9420      1025.5228      1035.5245
510      1060.5448      1067.4313      1125.5483
511      1170.3831      1228.9883      1288.5411
512      1308.8752      1346.3240      1380.3676
513      1404.2181      1413.9680      1434.2222
514      1441.5282      1446.8685      1470.3964
515      1479.9109      1497.6761      2088.3610
516      3028.0283      3044.1361      3084.0623
517      3126.2459      3131.0607      3164.9289
518      3730.3113      3733.6823      3749.4009
519 Zero-point correction (Hartree): 0.153023
520
521 TS.triHPacyl.COelim.tppmpmpmpu
522 -----
523 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16059047
524 Electronic state : 2-A
525 Cartesian coordinates (Angs):
526 O      2.114777      -0.981783      -1.489367
527 O      1.131466      -0.050283      -1.074183
528 C      0.433677      -0.517036      0.015356
529 C     -0.595594      0.499512      0.435306
530 C     -1.799505      0.600814      -0.506866
531 O     -2.538221      -0.602356      -0.532842
532 O     -3.062128      -0.818960      0.773602
533 H      2.880011      -0.697546      -0.966965

```

534	C	0.101801	-1.969803	0.078595			
535	H	0.998533	-2.581140	0.152037			
536	H	-0.450501	-2.271378	-0.814186			
537	H	-0.528719	-2.148970	0.947345			
538	C	1.851222	-0.284394	1.595187			
539	O	2.883102	-0.045851	1.162984			
540	H	-4.007204	-0.694366	0.624518			
541	H	-0.953870	0.191194	1.418648			
542	O	-0.031115	1.778163	0.669998			
543	O	0.132809	2.462541	-0.565789			
544	H	0.975269	2.111274	-0.887067			
545	H	-2.423978	1.441390	-0.196478			
546	H	-1.484663	0.743208	-1.538546			
547	Rotational constants (GHz):				1.2375900	0.6766600	0.5854300
548	Vibrational harmonic frequencies (cm-1):						
549		i289.1300	31.1150			55.4172	
550		76.0832	144.6762			152.4570	
551		159.9571	163.3970			182.8986	
552		194.0002	208.3804			222.4632	
553		231.0971	250.9281			310.0335	
554		332.6412	365.3453			382.0922	
555		395.3705	400.1055			497.6481	
556		531.8268	586.4142			706.1058	
557		802.2920	930.9017			945.7558	
558		975.6990	1021.6541			1051.0612	
559		1065.0479	1099.5493			1117.0585	
560		1146.5447	1237.2433			1275.8532	
561		1292.0593	1322.1287			1381.1035	
562		1400.6915	1414.0665			1419.4291	
563		1432.7339	1434.1178			1468.0174	
564		1479.3550	1489.2582			2052.4169	
565		3061.1462	3071.3218			3110.6898	
566		3133.1332	3156.1852			3162.8113	
567		3768.2022	3785.0230			3827.2096	
568	Zero-point correction (Hartree):				0.152433		
569	TS.triHPacyl.COelim.tpppmtmpu						
570	-----						
571	E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16107826						
572	Electronic state : 2-A						
573	Cartesian coordinates (Angs):						
574	O	2.378042	-0.226882	-1.683459			
575	O	1.251275	0.439326	-1.141979			
576	C	0.566631	-0.393406	-0.289872			
577	C	-0.490747	0.378341	0.455597			
578	C	-1.731576	0.715704	-0.380326			
579	O	-2.433775	-0.448497	-0.760058			
580	O	-2.902616	-1.079803	0.427065			
581	H	2.955980	-0.279839	-0.903568			
582	C	0.277629	-1.786286	-0.742619			
583	H	1.194681	-2.346998	-0.911075			
584	H	-0.291722	-1.767332	-1.674935			
585	H	-0.324198	-2.290879	0.011522			
586	C	2.010401	-0.705914	1.207279			
587	O	1.586714	-1.106472	2.186526			
588	H	-3.855914	-0.952819	0.348879			
589	H	-0.808551	-0.246077	1.293506			
590	O	0.030516	1.539952	1.075577			
591	O	0.116909	2.590901	0.121201			
592	H	0.947802	2.388294	-0.332513			
593	H	-2.368615	1.392727	0.192972			
594	H	-1.460009	1.184086	-1.324130			
595	Rotational constants (GHz):				1.0534300	0.6987300	0.6468400
596	Vibrational harmonic frequencies (cm-1):						
597		i291.9948	36.6060			62.2389	
598		82.1090	113.6778			127.9161	
599		161.5389	165.4129			178.1451	
600		198.6511	207.0145			222.9921	
601		229.4731	295.9636			309.5166	
602		332.9124	371.0335			395.7371	
603		400.1600	428.8551			492.8915	
604		535.2402	582.5791			706.2309	

606	800.3483	934.2721	946.3743
607	976.4715	1021.2652	1047.5782
608	1059.1818	1098.4468	1117.8429
609	1145.8018	1234.8695	1275.1968
610	1297.7744	1323.2581	1380.8169
611	1399.5927	1411.4832	1418.1315
612	1434.5583	1445.1584	1467.3509
613	1479.7173	1486.8017	2087.1481
614	3056.5444	3072.7416	3096.0738
615	3128.4966	3155.8989	3159.5192
616	3713.9716	3778.2544	3827.0906

617 Zero-point correction (Hartree): 0.152443

618
619 TS.triHPacyl.COelim.ttpmmpmmu

620 -----
621 E(UM062X/Aug-CC-pVTZ) (Hartree): -722.16195622

622 Electronic state : 2-A

623 Cartesian coordinates (Angs):

624	O	-2.877454	0.087511	0.115228
625	O	-1.674968	0.447105	-0.538319
626	C	-0.567205	0.042591	0.162274
627	C	0.644400	0.595489	-0.563682
628	C	1.936531	0.502816	0.242595
629	O	2.223784	-0.801370	0.690492
630	O	2.525836	-1.591677	-0.450254
631	H	-3.076372	-0.766122	-0.297499
632	C	-0.647263	-0.002375	1.652799
633	H	-1.491110	-0.603199	1.980138
634	H	-0.768562	1.009226	2.050095
635	H	0.268803	-0.431976	2.049536
636	C	-0.497536	-1.993282	-0.323731
637	O	-1.559576	-2.411456	-0.410927
638	H	1.702900	-2.096968	-0.548719
639	H	0.766356	0.067673	-1.512859
640	O	0.453327	1.936270	-0.990776
641	O	0.110591	2.722821	0.144189
642	H	-0.837722	2.847231	0.001572
643	H	2.753689	0.885896	-0.369670
644	H	1.856130	1.103175	1.148810

645 Rotational constants (GHz): 1.0373300 0.8709600 0.5691500

646 Vibrational harmonic frequencies (cm-1):

647	i289.3920	45.5508	94.5536
648	116.8628	124.6763	145.6210
649	154.4556	167.8267	183.5615
650	198.5675	239.0906	254.5559
651	266.1150	289.5698	309.6963
652	344.0473	370.5549	374.0967
653	455.2911	476.5117	492.3859
654	499.0561	589.5728	722.9889
655	780.0642	939.9017	952.6344
656	977.3569	1024.8712	1044.7982
657	1069.5000	1093.7792	1123.0303
658	1153.5915	1246.0679	1276.2359
659	1312.0606	1344.0060	1378.3213
660	1405.9029	1408.2117	1415.2937
661	1430.2497	1442.4882	1478.3673
662	1487.8138	1498.7376	2046.3572
663	3054.1947	3082.9447	3086.0536
664	3143.5458	3145.3948	3179.9235
665	3709.6539	3775.9822	3794.0978

666 Zero-point correction (Hartree): 0.153131

667
668
669
670 #####
671 Raw quantum chemical M06-2X/aug-cc-pVTZ data for acyl radical O2-addition
672 #####
673

674 TS.triMeCO.triMe+CO

675 -----
676 E(UM062X/CC-pVDZ) (Hartree): -270.99334834

677 Electronic state : 2-A

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678 Cartesian coordinates (Angs):
679 C -0.554816 -0.011066 -0.056706
680 C 1.358067 0.141551 0.846263
681 C -0.418881 -1.320505 -0.778455
682 C -1.474787 0.015977 1.126742
683 C -0.530947 1.220777 -0.915598
684 O 2.210310 0.001820 0.090520
685 H -0.288171 -2.156843 -0.075553
686 H 0.436376 -1.306141 -1.470407
687 H -1.328423 -1.526193 -1.373877
688 H -1.350510 0.943898 1.703434
689 H -1.286519 -0.835459 1.796684
690 H -2.529556 -0.039855 0.799105
691 H 0.305189 1.193805 -1.630172
692 H -0.445258 2.133553 -0.307082
693 H -1.467419 1.298273 -1.499764
694 Rotational constants (GHz): 4.4239500 2.4499900 2.4436800
695 Vibrational harmonic frequencies (cm-1):
696 i382.9924 26.1486 166.8576
697 169.0603 185.0615 205.8343
698 219.5949 263.8121 355.5293
699 380.0507 402.7133 787.5729
700 923.9846 927.7798 955.7930
701 1016.6037 1020.7702 1109.4956
702 1288.2007 1298.7308 1380.2711
703 1384.4813 1394.3169 1436.0118
704 1446.7404 1448.4417 1466.5808
705 1470.1872 1473.6951 2083.3019
706 3018.3673 3020.7565 3026.6225
707 3100.8646 3101.4457 3109.8690
708 3143.0092 3144.3633 3149.7667
709 Zero-point correction (Hartree): 0.124166
710
711 HO0diMeCO.mm
712 -----
713 E(UM062X/CC-pVDZ) (Hartree): -382.02562393
714 Electronic state : 2-A
715 Cartesian coordinates (Angs):
716 C -0.044939 0.347927 0.023327
717 C -0.853920 -0.843670 -0.564620
718 C -0.690783 1.625533 -0.495058
719 C -0.032290 0.248927 1.542866
720 O 1.256064 0.353961 -0.529321
721 O -1.888457 -1.216873 -0.142582
722 H -1.718703 1.699752 -0.117519
723 H -0.703737 1.626054 -1.592791
724 H -0.109677 2.490689 -0.146694
725 H 0.472760 -0.672053 1.860926
726 H -1.062173 0.229414 1.922219
727 H 0.495929 1.117800 1.962565
728 O 1.855220 -0.903533 -0.238443
729 H 2.574567 -0.632391 0.354974
730 Rotational constants (GHz): 3.3912700 2.3104700 1.9542100
731 Vibrational harmonic frequencies (cm-1):
732 73.3489 151.1085 198.6679
733 210.2328 227.2574 256.2472
734 291.2570 340.5415 357.1883
735 443.7701 514.4637 597.7094
736 715.8100 876.5225 940.9633
737 955.9459 996.6803 1047.5492
738 1190.6206 1228.6410 1252.3911
739 1367.5271 1381.2452 1404.6484
740 1443.0567 1455.8815 1462.4636
741 1483.6477 1993.4628 3071.3635
742 3076.8822 3161.9676 3167.6445
743 3178.2999 3180.6153 3787.7189
744 Zero-point correction (Hartree): 0.108175
745
746 HO0diMeCO.mp
747 -----
748 E(UM062X/CC-pVDZ) (Hartree): -382.02908312
749 Electronic state : 2-A

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750 Cartesian coordinates (Angs):
751 C -0.037908 0.354245 0.017041
752 C -0.784700 -0.951866 -0.390958
753 C -0.747074 1.528056 -0.641642
754 C 0.000486 0.437278 1.536783
755 O 1.254572 0.334265 -0.556979
756 O -1.888192 -1.222768 -0.085243
757 H -1.774611 1.597091 -0.262546
758 H -0.768151 1.402387 -1.732156
759 H -0.203840 2.452728 -0.402773
760 H 0.570164 -0.404354 1.948413
761 H -1.021358 0.418820 1.938022
762 H 0.495142 1.375043 1.827474
763 O 1.941669 -0.807141 -0.073929
764 H 1.653439 -1.482846 -0.714562
765 Rotational constants (GHz): 3.4162500 2.2929400 1.9557000
766 Vibrational harmonic frequencies (cm-1):
767 85.2209 166.0018 198.1519
768 219.1884 247.9193 280.4953
769 306.8958 346.3173 372.4070
770 454.3937 502.0889 604.9654
771 697.0866 871.0023 943.1846
772 957.4214 997.3693 1046.9136
773 1184.0057 1233.9147 1253.7657
774 1369.0084 1383.1562 1423.7215
775 1440.7318 1455.0066 1461.2108
776 1482.3928 2002.6379 3076.2661
777 3077.9030 3166.8827 3168.6384
778 3180.8269 3187.3248 3728.9598
779 Zero-point correction (Hartree): 0.108380
780
781 HO0diMeC000.pmc
782 -----
783 E(UM062X/CC-pVDZ) (Hartree): -532.36033474
784 Electronic state : 2-A
785 Cartesian coordinates (Angs):
786 C -0.714381 0.039760 -0.283066
787 C 0.435191 0.828833 0.361329
788 C -1.990239 0.378342 0.479894
789 C -0.840429 0.361924 -1.769874
790 O -0.438139 -1.349846 -0.221965
791 O 0.340305 1.830510 0.986621
792 H -2.183099 1.457351 0.443999
793 H -1.897611 0.069048 1.528013
794 H -2.824586 -0.163192 0.015422
795 H 0.070954 0.081495 -2.307837
796 H -1.035247 1.435117 -1.898524
797 H -1.691551 -0.202660 -2.174136
798 O -0.175645 -1.665770 1.142592
799 H 0.756807 -1.937251 1.084751
800 O 1.748559 0.278003 0.260226
801 O 1.957854 -0.392029 -0.845148
802 Rotational constants (GHz): 1.9448500 1.6264600 1.4382000
803 Vibrational harmonic frequencies (cm-1):
804 81.6390 103.6669 154.5773
805 177.2830 214.8928 226.6203
806 258.8851 263.2623 285.5098
807 336.8836 364.4299 405.6917
808 504.3318 543.2729 628.0288
809 685.8652 753.8159 886.7206
810 944.3304 963.7107 1016.0975
811 1042.3630 1086.1285 1228.7729
812 1241.4530 1256.5700 1288.1352
813 1374.0427 1390.5965 1416.6504
814 1442.5593 1458.3085 1463.6247
815 1489.2241 1962.3544 3083.3988
816 3087.3109 3169.0921 3181.4570
817 3189.3192 3203.9182 3762.4085
818 Zero-point correction (Hartree): 0.117593
819
820 HO0diMeC000.pmm
821 -----

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822 E(UM062X/CC-pVDZ) (Hartree): -532.36032214
823 Electronic state : 2-A
824 Cartesian coordinates (Angs):
825 C -0.766734 -0.015575 0.234578
826 C 0.386104 -0.860405 -0.331466
827 C -1.983113 -0.200391 -0.660612
828 C -1.008485 -0.471788 1.672651
829 O -0.419025 1.347616 0.353612
830 O 0.286398 -1.769507 -1.082682
831 H -2.247403 -1.261008 -0.748683
832 H -1.772872 0.199514 -1.660026
833 H -2.821534 0.355255 -0.220626
834 H -0.100866 -0.339002 2.275739
835 H -1.314602 -1.525964 1.691677
836 H -1.811512 0.143962 2.099189
837 O 0.018365 1.796598 -0.919292
838 H 0.982353 1.793103 -0.761661
839 O 1.687144 -0.685111 0.258715
840 O 2.092094 0.550793 0.368834
841 Rotational constants (GHz): 1.9674500 1.6587500 1.3566300
842 Vibrational harmonic frequencies (cm-1):
843 52.3609 90.5153 176.0127
844 200.8632 218.3396 238.2404
845 264.2298 284.3723 328.7112
846 362.8763 400.1536 502.6185
847 533.4125 541.1992 584.2356
848 676.3503 765.6007 902.9003
849 946.4499 957.3687 1006.3605
850 1051.1323 1061.6676 1231.4527
851 1256.8431 1272.9632 1276.6740
852 1377.9195 1393.4823 1441.7420
853 1444.4404 1454.9934 1464.7695
854 1484.0858 1960.3222 3078.5909
855 3087.8104 3173.4182 3178.3669
856 3181.4172 3191.0220 3693.8735
857 Zero-point correction (Hartree): 0.117987
858
859 HO0diMeCOOO.pmt
860 -----
861 E(UM062X/CC-pVDZ) (Hartree): -532.36467361
862 Electronic state : 2-A
863 Cartesian coordinates (Angs):
864 C 0.858545 -0.233237 -0.147647
865 C -0.585990 -0.515049 0.256870
866 C 1.786405 -0.597925 1.000820
867 C 1.153026 -1.020316 -1.422919
868 O 1.000316 1.123708 -0.533739
869 O -0.989786 -1.362226 0.975597
870 H 1.612343 -1.634390 1.315344
871 H 1.604862 0.069053 1.852644
872 H 2.826117 -0.481380 0.667850
873 H 0.444562 -0.746033 -2.215745
874 H 1.082878 -2.097142 -1.221800
875 H 2.171123 -0.778668 -1.756246
876 O 0.585235 1.931600 0.560718
877 H -0.264019 2.263635 0.219675
878 O -1.464550 0.384100 -0.425393
879 O -2.724940 0.123329 -0.200242
880 Rotational constants (GHz): 2.2288400 1.4131400 1.1951400
881 Vibrational harmonic frequencies (cm-1):
882 54.7589 109.0973 176.6051
883 205.3574 214.7744 230.0833
884 251.9283 279.2156 329.9300
885 361.1642 381.7331 393.3141
886 482.2484 564.0314 606.7168
887 728.0274 832.4999 878.7783
888 945.9557 955.1736 1011.8668
889 1044.4575 1067.3636 1217.8919
890 1230.5383 1271.7968 1292.4613
891 1376.0364 1391.2013 1424.3952
892 1444.5711 1455.7562 1465.9505
893 1486.0878 1975.7978 3077.6391

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894          3086.1630          3171.9263          3178.0757
895          3180.8158          3188.3470          3755.2992
896 Zero-point correction (Hartree): 0.117954
897
898 HO0diMeC000.ppc
899 -----
900 E(UM062X/CC-pVDZ) (Hartree): -532.35834131
901 Electronic state : 2-A
902 Cartesian coordinates (Angs):
903   C      0.662829      0.103643      0.330089
904   C     -0.522455      0.769696     -0.389305
905   C      1.940685      0.619987     -0.322319
906   C      0.643589      0.392258      1.828991
907   O      0.564976     -1.308590      0.220030
908   O     -0.457555      1.751443     -1.054017
909   H      2.019127      1.707746     -0.207395
910   H      1.945460      0.392826     -1.395812
911   H      2.800261      0.138891      0.164155
912   H     -0.247258     -0.040824      2.294286
913   H      0.663117      1.477638      1.996574
914   H      1.542462     -0.049224      2.280923
915   O      0.363993     -1.611474     -1.156300
916   H      1.214126     -2.017790     -1.391763
917   O     -1.797645      0.167514     -0.299499
918   O     -1.959416     -0.614239      0.736573
919 Rotational constants (GHz):      1.9407700      1.6072000      1.4436000
920 Vibrational harmonic frequencies (cm-1):
921      78.9923      108.2025      136.8022
922     174.7140      215.9369      224.1138
923     248.6690      271.9842      281.2295
924     340.9680      369.8189      402.7325
925     513.1836      545.8103      635.1387
926     695.5901      746.4930      893.9291
927     943.1671      960.7150     1013.4272
928    1042.5991     1111.0694     1228.7352
929    1242.1515     1257.8076     1295.9824
930    1375.1865     1389.0125     1397.6536
931    1444.4415     1458.4217     1465.2366
932    1489.4264     1949.2578     3081.9473
933    3084.3566     3165.7000     3174.8153
934    3185.2587     3210.3228     3788.7072
935 Zero-point correction (Hartree): 0.117644
936
937 HO0diMeC000.ppt
938 -----
939 E(UM062X/CC-pVDZ) (Hartree): -532.36159550
940 Electronic state : 2-A
941 Cartesian coordinates (Angs):
942   C     -0.814716      0.297198     -0.163301
943   C      0.625208      0.401258      0.337087
944   C     -1.764772      0.676426      0.961049
945   C     -0.978653      1.172868     -1.402189
946   O     -1.046392     -1.022834     -0.637160
947   O      1.018168      0.983272      1.290594
948   H     -1.558702      1.696777      1.307309
949   H     -1.634824     -0.000841      1.814934
950   H     -2.798570      0.617589      0.593887
951   H     -0.269980      0.863283     -2.180587
952   H     -0.805935      2.225940     -1.143616
953   H     -2.002243      1.060859     -1.784559
954   O     -0.670891     -1.919246      0.401848
955   H     -1.536061     -2.248354      0.695945
956   O      1.485487     -0.268061     -0.564866
957   O      2.739117     -0.210849     -0.202815
958 Rotational constants (GHz):      2.2371800      1.3656600      1.2287900
959 Vibrational harmonic frequencies (cm-1):
960      58.9422      94.4250      142.8265
961     193.5608      200.2736      223.3989
962     247.9999      270.9774      289.0974
963     334.2686      361.6022      387.7623
964     500.9118      536.4124      607.4068
965     734.4015      851.8935      888.5402

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966          943.7020          951.0322          1008.6282
967          1043.5223          1082.8048          1218.9346
968          1227.0406          1273.5213          1301.6292
969          1379.2305          1391.4424          1398.9176
970          1445.7526          1456.2943          1466.0543
971          1486.0143          1966.0274          3078.8676
972          3081.6682          3170.7171          3173.0389
973          3181.2824          3182.6767          3784.2579
974 Zero-point correction (Hartree): 0.117594
975
976 HOodiMeC000.tpc
977 -----
978 E(UM062X/CC-pVDZ) (Hartree): -532.35489660
979 Electronic state : 2-A
980 Cartesian coordinates (Angs):
981 C      0.413866      0.363597      0.152785
982 C     -1.084666      0.507017     -0.143178
983 C      1.078342      1.701066     -0.146169
984 C      0.636416     -0.059096      1.607019
985 O      0.851071     -0.624649     -0.783153
986 O     -1.665429      1.532291     -0.279251
987 H      0.709199      2.476905      0.535860
988 H      0.865751      2.007031     -1.178096
989 H      2.161507      1.582213     -0.019823
990 H      0.238850     -1.063059      1.792001
991 H      0.144108      0.654996      2.282090
992 H      1.713839     -0.041691      1.815451
993 O      2.234270     -0.851819     -0.558616
994 H      2.212138     -1.759348     -0.212666
995 O     -1.873955     -0.661830     -0.282542
996 O     -1.334599     -1.760563      0.173868
997 Rotational constants (GHz):      2.1823200      1.5225300      1.1545200
998 Vibrational harmonic frequencies (cm-1):
999      70.6978      98.6716      135.0090
1000     173.1154      220.9500      239.1523
1001     255.2065      264.9494      300.5203
1002     330.4871      375.9696      423.4947
1003     441.2258      573.6197      634.6063
1004     720.4343      734.9728      859.7640
1005     941.7950      999.8503     1003.0132
1006    1043.3852     1102.7547     1215.2317
1007    1240.3340     1248.7251     1303.4029
1008    1370.8505     1391.6361     1410.5032
1009    1446.0943     1457.6455     1470.0980
1010    1488.0155     1954.9531     3083.4656
1011    3089.2227     3166.7534     3183.2090
1012    3188.1620     3196.2330     3783.2105
1013 Zero-point correction (Hartree): 0.117625
1014
1015 HOodiMeC000.tpt
1016 -----
1017 E(UM062X/CC-pVDZ) (Hartree): -532.35795095
1018 Electronic state : 2-A
1019 Cartesian coordinates (Angs):
1020 C      0.595439      0.292300      0.144546
1021 C     -0.906144      0.414374     -0.100190
1022 C      1.281697      1.582366     -0.269706
1023 C      0.824897     -0.061240      1.614308
1024 O      0.968996     -0.790292     -0.713045
1025 O     -1.522823      1.392498     -0.350694
1026 H      0.934007      2.416879      0.352363
1027 H      1.055120      1.807483     -1.319531
1028 H      2.365369      1.460984     -0.151386
1029 H      0.335764     -1.014048      1.857886
1030 H      0.419089      0.726031      2.264560
1031 H      1.903695     -0.144751      1.796497
1032 O      2.361790     -1.015631     -0.537071
1033 H      2.350816     -1.915476     -0.172277
1034 O     -1.515873     -0.852230      0.079497
1035 O     -2.809490     -0.822333     -0.098920
1036 Rotational constants (GHz):      2.6496300      1.1919400      1.0260000
1037 Vibrational harmonic frequencies (cm-1):

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1038      51.4438      107.0433      118.5802
1039      180.2612      217.9125      230.0835
1040      233.6925      256.6529      311.4278
1041      329.9169      374.5933      411.0401
1042      431.4878      498.9817      680.5180
1043      727.7528      827.1417      872.2354
1044      942.4887      988.5057      1000.2649
1045      1040.7724      1076.6297      1213.3527
1046      1216.5976      1251.2330      1314.3926
1047      1373.1134      1395.5031      1409.3548
1048      1445.7948      1457.5354      1472.2814
1049      1482.3726      1969.5731      3078.1315
1050      3088.9246      3168.1054      3178.7891
1051      3182.1674      3187.5425      3787.1176
1052 Zero-point correction (Hartree): 0.117511
1053
1054 HOdiMeCO.pm
1055 -----
1056 E(UM062X/CC-pVDZ) (Hartree): -382.02908308
1057 Electronic state : 2-A
1058 Cartesian coordinates (Angs):
1059 C      0.038022      0.354354      0.017049
1060 C      0.784782     -0.951451     -0.391274
1061 C     -0.000563      0.436964      1.536836
1062 C      0.746736      1.528552     -0.641368
1063 O     -1.254518      0.334144     -0.556919
1064 O      1.888046     -1.222985     -0.085350
1065 H      1.021201      0.417924      1.938228
1066 H     -0.570676     -0.404620      1.947992
1067 H     -0.494876      1.374816      1.827842
1068 H      0.768366      1.402941     -1.731880
1069 H      1.774056      1.598308     -0.261844
1070 H      0.202810      2.452889     -0.402734
1071 O     -1.941262     -0.807368     -0.074043
1072 H     -1.652859     -1.483099     -0.714562
1073 Rotational constants (GHz):      3.4156900      2.2934100      1.9558400
1074 Vibrational harmonic frequencies (cm-1):
1075      84.7843      165.9608      198.1394
1076      219.0488      247.9031      280.4073
1077      306.9100      346.3039      372.3878
1078      454.3901      502.1424      605.0521
1079      697.3316      871.0847      943.1930
1080      957.4754      997.3865      1047.2342
1081      1184.0915      1233.9412      1253.7083
1082      1369.0179      1383.1730      1423.7697
1083      1440.7348      1455.0097      1461.2100
1084      1482.3943      2002.8023      3076.2536
1085      3077.8876      3166.8377      3168.6144
1086      3180.8560      3187.2937      3728.9680
1087 Zero-point correction (Hartree): 0.108381
1088
1089 HOdiMeCO.pp
1090 -----
1091 E(UM062X/CC-pVDZ) (Hartree): -382.02562393
1092 Electronic state : 2-A
1093 Cartesian coordinates (Angs):
1094 C      0.044850      0.347840      0.023296
1095 C      0.853960     -0.843893     -0.564386
1096 C      0.032011      0.248894      1.542856
1097 C      0.690816      1.625400     -0.494980
1098 O     -1.256021      0.353882     -0.529568
1099 O      1.888789     -1.216483     -0.142547
1100 H      1.061868      0.230070      1.922295
1101 H     -0.472442     -0.672390      1.860982
1102 H     -0.496821      1.117466      1.962428
1103 H      0.703380      1.626149     -1.592719
1104 H      1.718883      1.699271     -0.117794
1105 H      0.110049      2.490628     -0.146212
1106 O     -1.855352     -0.903447     -0.238550
1107 H     -2.574072     -0.632257      0.355619
1108 Rotational constants (GHz):      3.3917500      2.3102100      1.9541900
1109 Vibrational harmonic frequencies (cm-1):

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1110      73.1980      151.0166      198.5824
1111      210.0358      227.1956      256.2262
1112      291.2128      340.5155      357.1490
1113      443.7739      514.4182      597.7319
1114      715.6942      876.4979      940.9544
1115      955.9747      996.6738     1047.6178
1116      1190.5684     1228.6910     1252.4422
1117      1367.5254     1381.2517     1404.6888
1118      1443.0547     1455.8844     1462.4644
1119      1483.6530     1993.4860     3071.3437
1120      3076.8857     3161.9570     3167.6266
1121      3178.3268     3180.6613     3787.5879
1122 Zero-point correction (Hartree): 0.108173
1123
1124 HOodiMeCO.tm
1125 -----
1126 E(UM062X/CC-pVDZ) (Hartree): -382.02355659
1127 Electronic state : 2-A
1128 Cartesian coordinates (Angs):
1129 C      0.052009      0.016548      0.053930
1130 C      1.337403     -0.055966     -0.794826
1131 C      0.011962     -1.195880      0.975373
1132 C      0.043935      1.347182      0.795496
1133 O     -0.979506     -0.031808     -0.931731
1134 O      2.430089     -0.071292     -0.355437
1135 H      0.883662     -1.185877      1.642736
1136 H      0.027431     -2.123326      0.385243
1137 H     -0.905753     -1.166284      1.577737
1138 H      0.123028      2.177274      0.080584
1139 H      0.887219      1.390863      1.497219
1140 H     -0.901812      1.444173      1.344604
1141 O     -2.223400      0.053935     -0.244792
1142 H     -2.603093     -0.814804     -0.452283
1143 Rotational constants (GHz):      4.6481800      1.8495300      1.8286400
1144 Vibrational harmonic frequencies (cm-1):
1145      80.4284      146.3187      196.4073
1146      202.6935      217.6388      247.7490
1147      306.9865      314.3650      371.1110
1148      448.2062      453.3803      597.1789
1149      752.6328      849.2091      940.1609
1150      981.5653      999.0172     1041.2133
1151      1207.9344     1210.5254     1239.5682
1152      1364.1213     1379.9755     1404.8973
1153      1443.3905     1456.8616     1465.2479
1154      1481.1643     1999.2855     3072.5941
1155      3078.0960     3161.6643     3170.7995
1156      3174.8150     3179.3588     3794.5832
1157 Zero-point correction (Hartree): 0.108056
1158
1159 HOodiMeCO.tp
1160 -----
1161 E(UM062X/CC-pVDZ) (Hartree): -382.02355657
1162 Electronic state : 2-A
1163 Cartesian coordinates (Angs):
1164 C      0.052035     -0.016839      0.054079
1165 C      1.337480      0.056404     -0.794727
1166 C      0.043306     -1.348465      0.793830
1167 C      0.012282      1.194476      0.976918
1168 O     -0.979360      0.033289     -0.931704
1169 O      2.430170      0.071996     -0.355369
1170 H      0.886646     -1.393580      1.495411
1171 H      0.121998     -2.177550      0.077716
1172 H     -0.902403     -1.445828      1.342905
1173 H      0.028530      2.122587      0.387896
1174 H      0.883574      1.183269      1.644807
1175 H     -0.905742      1.164654      1.578800
1176 O     -2.223298     -0.053093     -0.244876
1177 H     -2.603319      0.815450     -0.452550
1178 Rotational constants (GHz):      4.6477800      1.8495200      1.8286200
1179 Vibrational harmonic frequencies (cm-1):
1180      80.3908      146.2436      195.9957
1181      202.6722      217.3677      247.5869

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1182      306.9697      314.3693      371.0788
1183      448.1822      453.3746      597.1200
1184      752.5131      849.0820      940.1390
1185      981.5257      998.9607      1041.1988
1186      1207.8638      1210.6019      1239.4484
1187      1364.1608      1379.9798      1404.9440
1188      1443.4067      1456.8301      1465.2656
1189      1481.1257      1999.2834      3072.6180
1190      3078.1438      3161.7292      3170.8826
1191      3174.7517      3179.3187      3794.7569
1192 Zero-point correction (Hartree): 0.108053
1193
1194 O2
1195 --
1196 E(UM062X/CC-pVDZ) (Hartree): -150.27726911
1197 Point group : D*H
1198 Electronic state : 3-SGG
1199 Cartesian coordinates (Angs):
1200 O      0.000000      0.000000      0.595741
1201 O      0.000000      0.000000     -0.595741
1202 Rotational constants (GHz):  0.0000000  44.5133910  44.5133910
1203 Vibrational harmonic frequencies (cm-1):
1204      1777.0158 ( SGG)
1205 Zero-point correction (Hartree): 0.004048
1206
1207 triMeCO
1208 -----
1209 E(UM062X/CC-pVDZ) (Hartree): -271.01147966
1210 Electronic state : 2-A
1211 Cartesian coordinates (Angs):
1212 C      0.326151      0.000063      0.007244
1213 C     -1.039044     -0.002025     -0.717672
1214 C      0.096416      0.005122      1.518430
1215 C      1.071152     -1.258132     -0.445901
1216 C      1.072043      1.254615     -0.454087
1217 O     -2.108850     -0.000496     -0.222690
1218 H     -0.471357     -0.883004      1.829736
1219 H     -0.472184      0.894818      1.823587
1220 H      1.062698      0.007362      2.045885
1221 H      1.184486     -1.273526     -1.539286
1222 H      0.536884     -2.169148     -0.138885
1223 H      2.072449     -1.275248      0.010706
1224 H      0.539154      2.168164     -0.152309
1225 H      1.184640      1.263231     -1.547625
1226 H      2.073725      1.273456      0.001628
1227 Rotational constants (GHz):  4.5708700  2.7884600  2.7826200
1228 Vibrational harmonic frequencies (cm-1):
1229      31.0438      199.9801      247.0215
1230      261.9684      273.2618      339.0783
1231      345.5749      386.6280      443.8865
1232      566.9888      724.8938      842.3537
1233      947.9747      954.1493      958.4901
1234      1024.4339      1041.0020      1220.3698
1235      1243.5750      1265.8181      1374.8046
1236      1376.8123      1403.1487      1443.7560
1237      1453.4273      1457.7682      1469.2719
1238      1473.8322      1489.6781      1988.4947
1239      3058.5919      3058.8313      3062.3047
1240      3142.1730      3142.3235      3145.9083
1241      3151.3435      3152.9741      3157.0087
1242 Zero-point correction (Hartree): 0.128309
1243
1244 triMeCOOO.c
1245 -----
1246 E(UM062X/CC-pVDZ) (Hartree): -421.34630563
1247 Electronic state : 2-A
1248 Cartesian coordinates (Angs):
1249 C     -0.707885     -0.215982     -0.000016
1250 C      0.426034      0.801553     -0.000005
1251 C     -2.002698      0.604432      0.000016
1252 C     -0.660169     -1.082233     -1.270398
1253 C     -0.660100     -1.082162      1.270424

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1254	O	0.323041	1.985250	-0.000045	
1255	H	-2.063346	1.248407	-0.887602	
1256	H	-2.063301	1.248412	0.887630	
1257	H	-2.860857	-0.082415	0.000037	
1258	H	0.220111	-1.733438	-1.294704	
1259	H	-0.666878	-0.453863	-2.173536	
1260	H	-1.562660	-1.711067	-1.292785	
1261	H	-0.666757	-0.453753	2.173543	
1262	H	0.220160	-1.733388	1.294780	
1263	H	-1.562581	-1.711014	1.292963	
1264	O	1.787044	0.353855	0.000024	
1265	O	1.969293	-0.935547	-0.000034	
1266	Rotational constants (GHz):		2.6367700	1.9445800	1.4935700
1267	Vibrational harmonic frequencies (cm-1):				
1268		51.6780		109.9949	167.6011
1269		223.9510		243.3153	258.8080
1270		301.3712		307.8569	357.1505
1271		386.4972		395.9825	547.7016
1272		623.8644		679.1797	730.3825
1273		862.2373		956.3921	959.2845
1274		961.0688		1036.2907	1042.6706
1275		1081.7766		1246.0227	1258.2085
1276		1266.5701		1295.4679	1372.7824
1277		1381.7646		1410.1552	1446.2530
1278		1456.7380		1462.3572	1475.1632
1279		1475.4561		1500.0533	1941.4469
1280		3068.4635		3068.6237	3073.3162
1281		3142.5226		3142.9570	3160.5305
1282		3163.9234		3189.9983	3191.3235
1283	Zero-point correction (Hartree):		0.137773		
1284					
1285	triMeCOOO.t				
1286	-----				
1287	E(UM062X/CC-pVDZ) (Hartree):		-421.34983699		
1288	Electronic state :		2-A		
1289	Cartesian coordinates (Angs):				
1290	C	-0.903549	-0.088538	0.000005	
1291	C	0.511724	0.450853	-0.000005	
1292	C	-1.858870	1.103232	-0.000285	
1293	C	-1.102452	-0.946944	-1.259454	
1294	C	-1.102574	-0.946444	1.259777	
1295	O	0.888168	1.573938	-0.000019	
1296	H	-1.703633	1.731166	-0.888292	
1297	H	-1.703694	1.731544	0.887463	
1298	H	-2.896800	0.740709	-0.000246	
1299	H	-0.414679	-1.802919	-1.272942	
1300	H	-0.943517	-0.353221	-2.171633	
1301	H	-2.134578	-1.327010	-1.273610	
1302	H	-0.943811	-0.352346	2.171741	
1303	H	-0.414751	-1.802374	1.273717	
1304	H	-2.134674	-1.326584	1.273945	
1305	O	1.433510	-0.643859	-0.000055	
1306	O	2.681380	-0.264070	0.000028	
1307	Rotational constants (GHz):		3.1862700	1.5601500	1.3617800
1308	Vibrational harmonic frequencies (cm-1):				
1309		50.0791		102.7854	188.8804
1310		207.8852		234.8283	261.4463
1311		282.0656		327.5867	342.9883
1312		370.7601		384.1233	482.9446
1313		606.9432		734.1313	817.1913
1314		864.0455		955.9949	957.5436
1315		958.4359		1023.3495	1039.6708
1316		1069.0390		1230.0999	1244.0416
1317		1268.6793		1308.8600	1374.7906
1318		1384.3593		1410.2879	1445.3680
1319		1455.1646		1459.3491	1470.7225
1320		1475.8970		1497.7059	1961.6029
1321		3063.7906		3064.6110	3071.0045
1322		3145.4109		3146.0463	3157.1723
1323		3161.6701		3163.7222	3165.7510
1324	Zero-point correction (Hartree):		0.137576		
1325					

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1326 TS.HOOdiMeCO.HOOdiMe+CO.mm
1327 -----
1328 E(UM062X/CC-pVDZ) (Hartree): -382.01055256
1329 Electronic state : 2-A
1330 Cartesian coordinates (Angs):
1331 C      0.260934      0.505507      0.066515
1332 C     -1.400769     -0.502366     -0.783111
1333 C      0.133455      1.874487     -0.523513
1334 C      0.051617      0.314418      1.538266
1335 O      1.338486     -0.122614     -0.506792
1336 O     -2.223802     -0.739611     -0.018801
1337 H     -0.812347      2.331266     -0.201031
1338 H      0.149832      1.815400     -1.619752
1339 H      0.961348      2.526129     -0.193950
1340 H      0.108192     -0.747135      1.805726
1341 H     -0.938478      0.694433      1.823584
1342 H      0.817624      0.869253      2.109708
1343 O      1.289489     -1.511436     -0.176243
1344 H      2.209023     -1.652328      0.101458
1345 Rotational constants (GHz):   2.9429200   2.2511700   1.7951100
1346 Vibrational harmonic frequencies (cm-1):
1347 i324.6661      24.5570      49.2774
1348 114.7485      162.6127      184.0516
1349 187.3466      214.8431      268.2128
1350 345.6915      373.4305      404.7989
1351 541.9335      820.4249      938.6325
1352 948.2551      984.4209     1031.6271
1353 1092.0567     1286.0028     1288.8928
1354 1381.9163     1386.0935     1423.7910
1355 1437.6507     1451.3669     1456.2233
1356 1474.6961     2082.3723     3036.3661
1357 3041.0412     3127.1402     3137.9245
1358 3169.2576     3185.8708     3800.0990
1359 Zero-point correction (Hartree): 0.104462
1360
1361 TS.HOOdiMeCO.HOOdiMe+CO.mp
1362 -----
1363 E(UM062X/CC-pVDZ) (Hartree): -382.01563265
1364 Electronic state : 2-A
1365 Cartesian coordinates (Angs):
1366 C      0.191601      0.509292      0.021626
1367 C     -1.149577     -1.150130     -0.169481
1368 C     -0.497338      1.616939     -0.707545
1369 C      0.346369      0.596524      1.508685
1370 O      1.251939      0.052177     -0.718204
1371 O     -2.237256     -0.841789      0.027386
1372 H     -1.522737      1.725295     -0.325692
1373 H     -0.535066      1.402257     -1.783762
1374 H      0.030225      2.575011     -0.560400
1375 H      0.767287     -0.327944      1.919637
1376 H     -0.632125      0.791758      1.969007
1377 H      1.024651      1.429142      1.768449
1378 O      1.790240     -1.119270     -0.130133
1379 H      1.082058     -1.760223     -0.339347
1380 Rotational constants (GHz):   3.1656900   2.1069900   1.7649300
1381 Vibrational harmonic frequencies (cm-1):
1382 i275.3773      63.9224      132.4953
1383 149.5088      169.1340      201.6843
1384 223.1716      284.0215      339.3822
1385 366.5861      397.0889      425.8832
1386 556.2291      821.8349      940.0723
1387 954.5311      983.1158     1046.5636
1388 1094.3499     1291.6607     1312.5577
1389 1383.6452     1392.8005     1434.8346
1390 1446.5347     1452.9307     1458.0826
1391 1474.7502     2087.1566     3036.7020
1392 3043.0976     3124.7127     3132.0557
1393 3166.2819     3188.6579     3685.8797
1394 Zero-point correction (Hartree): 0.105392
1395
1396 TS.HOOdiMeCO.HOOdiMe+CO.pm
1397 -----

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1398 E(UM062X/CC-pVDZ) (Hartree): -382.01563265
1399 Electronic state : 2-A
1400 Cartesian coordinates (Angs):
1401 C -0.191600 0.509292 0.021626
1402 C 1.149579 -1.150130 -0.169473
1403 C -0.346377 0.596529 1.508683
1404 C 0.497339 1.616937 -0.707546
1405 O -1.251935 0.052174 -0.718208
1406 O 2.237258 -0.841787 0.027389
1407 H 0.632112 0.791776 1.969009
1408 H -0.767286 -0.327943 1.919638
1409 H -1.024671 1.429139 1.768440
1410 H 0.535081 1.402248 -1.783761
1411 H 1.522734 1.725303 -0.325683
1412 H -0.030231 2.575007 -0.560414
1413 O -1.790238 -1.119271 -0.130134
1414 H -1.082054 -1.760225 -0.339342
1415 Rotational constants (GHz): 3.1656900 2.1069900 1.7649300
1416 Vibrational harmonic frequencies (cm-1):
1417 i275.3780 63.9209 132.4936
1418 149.5082 169.1331 201.6827
1419 223.1713 284.0217 339.3822
1420 366.5862 397.0894 425.8835
1421 556.2292 821.8350 940.0723
1422 954.5309 983.1157 1046.5640
1423 1094.3502 1291.6608 1312.5575
1424 1383.6453 1392.8006 1434.8342
1425 1446.5349 1452.9308 1458.0825
1426 1474.7500 2087.1570 3036.7027
1427 3043.0985 3124.7137 3132.0565
1428 3166.2826 3188.6577 3685.8791
1429 Zero-point correction (Hartree): 0.105392
1430
1431 TS.HOOdiMeCO.HOOdiMe+CO.pp
1432 -----
1433 E(UM062X/CC-pVDZ) (Hartree): -382.01055256
1434 Electronic state : 2-A
1435 Cartesian coordinates (Angs):
1436 C -0.260934 0.505507 0.066515
1437 C 1.400768 -0.502367 -0.783112
1438 C -0.051615 0.314419 1.538266
1439 C -0.133455 1.874486 -0.523515
1440 O -1.338486 -0.122614 -0.506790
1441 O 2.223801 -0.739611 -0.018802
1442 H 0.938482 0.694431 1.823582
1443 H -0.108195 -0.747133 1.805728
1444 H -0.817619 0.869259 2.109708
1445 H -0.149833 1.815399 -1.619753
1446 H 0.812347 2.331265 -0.201034
1447 H -0.961348 2.526129 -0.193951
1448 O -1.289489 -1.511436 -0.176239
1449 H -2.209029 -1.652333 0.101438
1450 Rotational constants (GHz): 2.9429200 2.2511700 1.7951100
1451 Vibrational harmonic frequencies (cm-1):
1452 i324.6659 24.5574 49.2870
1453 114.7482 162.6122 184.0510
1454 187.3464 214.8432 268.2128
1455 345.6916 373.4304 404.7988
1456 541.9332 820.4248 938.6327
1457 948.2551 984.4210 1031.6275
1458 1092.0567 1286.0031 1288.8924
1459 1381.9162 1386.0934 1423.7913
1460 1437.6508 1451.3671 1456.2234
1461 1474.6964 2082.3721 3036.3661
1462 3041.0412 3127.1402 3137.9244
1463 3169.2575 3185.8711 3800.1009
1464 Zero-point correction (Hartree): 0.104462
1465
1466 TS.HOOdiMeCO.HOOdiMe+CO.tm
1467 -----
1468 E(UM062X/CC-pVDZ) (Hartree): -382.00590241
1469 Electronic state : 2-A

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1470 Cartesian coordinates (Angs):
1471 C -0.131879 -0.313537 0.069016
1472 C 1.721367 0.032209 -0.773744
1473 C -0.653945 -1.493614 -0.688987
1474 C 0.163086 -0.446898 1.530989
1475 O -0.666427 0.908512 -0.291079
1476 O 2.448781 0.621536 -0.112385
1477 H 0.004367 -2.361767 -0.547928
1478 H -0.700491 -1.258945 -1.761528
1479 H -1.663111 -1.760484 -0.335967
1480 H 0.732842 0.423012 1.883853
1481 H 0.727392 -1.365632 1.741907
1482 H -0.790648 -0.483831 2.085654
1483 O -2.087642 0.871051 0.025941
1484 H -2.459821 0.929899 -0.869449
1485 Rotational constants (GHz): 3.8050800 1.7872600 1.6841400
1486 Vibrational harmonic frequencies (cm-1):
1487 i390.8071 32.7146 61.1404
1488 167.1022 172.4159 188.2660
1489 207.2512 217.1810 264.9486
1490 314.5449 373.2905 454.5647
1491 553.2396 793.7152 838.8862
1492 927.2618 960.7939 1007.0835
1493 1084.1621 1253.2195 1277.1713
1494 1353.7838 1379.3825 1389.3371
1495 1435.3793 1449.9354 1454.7311
1496 1464.5708 2093.5201 3045.2035
1497 3056.4528 3131.1280 3137.5504
1498 3163.6636 3171.3936 3791.2382
1499 Zero-point correction (Hartree): 0.104035
1500
1501 TS.HOOdiMeCO.HOOdiMe+CO.tp
1502 -----
1503 E(UM062X/CC-pVDZ) (Hartree): -382.00590240
1504 Electronic state : 2-A
1505 Cartesian coordinates (Angs):
1506 C -0.131877 0.313519 0.069028
1507 C 1.721341 -0.032261 -0.773785
1508 C 0.163138 0.446825 1.530996
1509 C -0.653913 1.493636 -0.688932
1510 O -0.666479 -0.908499 -0.291091
1511 O 2.448808 -0.621503 -0.112407
1512 H 0.727485 1.365532 1.741921
1513 H 0.732875 -0.423116 1.883816
1514 H -0.790575 0.483775 2.085694
1515 H -0.700403 1.259030 -1.761490
1516 H 0.004381 2.361789 -0.547788
1517 H -1.663100 1.760473 -0.335948
1518 O -2.087694 -0.870998 0.025926
1519 H -2.459873 -0.929791 -0.869468
1520 Rotational constants (GHz): 3.8051600 1.7872300 1.6841200
1521 Vibrational harmonic frequencies (cm-1):
1522 i390.8044 32.7223 61.1308
1523 167.1028 172.4225 188.2682
1524 207.2604 217.1920 264.9495
1525 314.5504 373.2875 454.5606
1526 553.2373 793.7157 838.8835
1527 927.2593 960.7970 1007.0830
1528 1084.1620 1253.2201 1277.1721
1529 1353.7842 1379.3828 1389.3357
1530 1435.3788 1449.9366 1454.7306
1531 1464.5711 2093.5197 3045.2038
1532 3056.4525 3131.1292 3137.5498
1533 3163.6643 3171.3946 3791.2303
1534 Zero-point correction (Hartree): 0.104035
1535
1536 TS.HOOdiMeCO+O2.HOOdiMeCOO.pmc
1537 -----
1538 E(UM062X/CC-pVDZ) (Hartree): -532.31240872
1539 Electronic state : 2-A
1540 Cartesian coordinates (Angs):
1541 C -0.926589 -0.140720 -0.236126

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1542      C      -0.130980      0.985780      0.466465
1543      C      -2.136315      -0.503175      0.614815
1544      C      -1.281488      0.365517      -1.627958
1545      O      -0.070711      -1.238758      -0.447334
1546      O      -0.529396      1.944454      1.005433
1547      H      -2.742981      0.391082      0.808675
1548      H      -1.806964      -0.931864      1.568998
1549      H      -2.738224      -1.248925      0.076754
1550      H      -0.372952      0.662170      -2.168587
1551      H      -1.963189      1.222472      -1.553078
1552      H      -1.774699      -0.445764      -2.180684
1553      O      0.434461      -1.633745      0.820543
1554      H      1.371408      -1.378086      0.717226
1555      O      2.082616      0.806661      -0.373036
1556      O      2.693010      -0.193049      -0.077165
1557      Rotational constants (GHz):      2.0256600      1.2888600      1.0822700
1558      Vibrational harmonic frequencies (cm-1):
1559      i150.1904      50.8885      86.1785
1560      107.1204      145.7569      177.7375
1561      201.0923      229.0883      242.9804
1562      275.0964      303.2415      346.2054
1563      397.6873      446.6471      470.1159
1564      538.1466      604.5499      737.7110
1565      880.7258      943.9014      961.6964
1566      999.5176      1053.6105      1182.1844
1567      1230.6159      1249.3750      1369.5739
1568      1383.2017      1440.3820      1450.1922
1569      1455.1907      1459.6583      1483.1367
1570      1565.4492      2023.6969      3075.7261
1571      3078.0535      3168.3737      3170.1538
1572      3178.4461      3186.3656      3680.9887
1573      Zero-point correction (Hartree): 0.113978
1574
1575      TS.triMeCO+O2.triMeCOOO.c
1576      -----
1577      E(UM062X/CC-pVDZ) (Hartree): -421.29321070
1578      Electronic state : 2-A
1579      Cartesian coordinates (Angs):
1580      C      -0.863735      -0.313461      0.000000
1581      C      -0.056167      0.984586      -0.000003
1582      C      -2.354751      0.029997      0.000002
1583      C      -0.463382      -1.089390      -1.260421
1584      C      -0.463378      -1.089386      1.260423
1585      O      -0.397307      2.106051      -0.000003
1586      H      -2.621554      0.617143      -0.889931
1587      H      -2.621551      0.617145      0.889935
1588      H      -2.947411      -0.897361      0.000004
1589      H      0.614263      -1.299251      -1.267141
1590      H      -0.721359      -0.527831      -2.170042
1591      H      -1.008024      -2.045304      -1.280473
1592      H      -0.721352      -0.527825      2.170042
1593      H      0.614267      -1.299247      1.267140
1594      H      -1.008020      -2.045300      1.280479
1595      O      2.260307      0.545504      0.000004
1596      O      2.590653      -0.617336      -0.000004
1597      Rotational constants (GHz):      2.6279500      1.4290100      1.1632600
1598      Vibrational harmonic frequencies (cm-1):
1599      i156.1208      52.1460      74.6805
1600      109.1479      111.9505      199.5623
1601      219.1732      262.9247      263.8228
1602      277.5356      344.4905      345.6736
1603      400.3827      456.9154      580.9289
1604      756.2834      857.5942      948.7804
1605      956.2018      960.1794      1029.4534
1606      1041.3487      1229.4016      1241.8514
1607      1260.5944      1375.1404      1376.2698
1608      1402.5133      1445.2286      1454.6910
1609      1459.3746      1470.7213      1473.0254
1610      1492.0636      1565.3290      2012.7911
1611      3060.6820      3062.9905      3064.5818
1612      3143.4071      3143.7526      3147.3910
1613      3157.3505      3168.6357      3170.3116

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1614 Zero-point correction (Hartree): 0.133563
1615
1616 TS.triMeCO+O2.triMeCOO.t
1617 -----
1618 E(UM062X/CC-pVDZ) (Hartree): -421.29345851
1619 Electronic state : 2-A
1620 Cartesian coordinates (Angs):
1621 C -1.161570 -0.113007 -0.000000
1622 C 0.274762 0.412073 0.000000
1623 C -2.131888 1.069030 -0.000009
1624 C -1.315140 -0.975520 -1.256649
1625 C -1.315144 -0.975504 1.256659
1626 O 0.695768 1.507060 -0.000001
1627 H -1.982021 1.696752 -0.889626
1628 H -1.982023 1.696764 0.889600
1629 H -3.169373 0.701518 -0.000008
1630 H -0.564600 -1.778681 -1.271077
1631 H -1.198583 -0.373169 -2.169252
1632 H -2.317562 -1.428952 -1.266967
1633 H -1.198591 -0.373142 2.169255
1634 H -0.564605 -1.778665 1.271100
1635 H -2.317567 -1.428936 1.266979
1636 O 2.348129 -0.809398 -0.000001
1637 O 3.104704 0.122848 0.000001
1638 Rotational constants (GHz): 3.1934500 1.1251100 1.0179000
1639 Vibrational harmonic frequencies (cm-1):
1640 i77.1823 22.2830 46.4130
1641 85.8172 121.7894 195.4002
1642 229.7450 254.9424 269.5641
1643 285.1327 344.2420 347.6449
1644 398.8014 466.6598 579.8762
1645 758.9455 857.3582 948.1184
1646 955.2015 958.9098 1025.5058
1647 1041.4515 1229.5315 1242.0321
1648 1262.6146 1374.1944 1376.2503
1649 1403.1390 1443.2791 1452.7782
1650 1457.3431 1468.4091 1473.5193
1651 1490.1398 1652.2659 2006.1975
1652 3059.5428 3059.8102 3062.9507
1653 3144.9035 3146.0140 3148.5193
1654 3151.1400 3152.5908 3157.4197
1655 Zero-point correction (Hartree): 0.133520
1656
1657
1658 #####
1659 E-HOCH=CHCH2CH2OO ring closure
1660 #####
1661
1662 HOCHCHCH2CH2OO.Ecpmc
1663 ~~~~~
1664 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13875016
1665 Electronic state : 2-A
1666 Cartesian coordinates (Angs):
1667 C -1.464605 -0.422977 0.119382
1668 C -1.214437 0.847892 -0.164136
1669 C 0.132747 1.506700 -0.092726
1670 C 1.242428 0.655855 0.476854
1671 O 1.542377 -0.394003 -0.472187
1672 O 2.422013 -1.221736 -0.000305
1673 O -2.679471 -1.027466 0.067432
1674 H -0.700741 -1.127820 0.419328
1675 H -2.038291 1.479660 -0.483204
1676 H 0.436862 1.853511 -1.084376
1677 H 0.067173 2.402931 0.529284
1678 H 2.158746 1.227493 0.615094
1679 H 0.967614 0.177698 1.416724
1680 H -3.347513 -0.392658 -0.208613
1681 Rotational constants (GHz): 4.5202800 1.4779300 1.1717900
1682 Vibrational harmonic frequencies (cm-1):
1683 48.1026 124.2428 131.8012
1684 214.6629 263.0421 302.0468
1685 395.1256 448.3625 524.2222

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1686          619.2420          798.5684          872.2430
1687          939.1204          992.9402          1001.4340
1688          1064.1514         1112.3987          1161.7700
1689          1229.2525         1254.3525          1293.3706
1690          1297.0187         1350.5167          1387.6863
1691          1403.8246         1421.8062          1476.3599
1692          1506.1178         1767.7863          3052.5511
1693          3078.7936         3092.3963          3144.1966
1694          3156.9067         3222.3314          3857.5254
1695 Zero-point correction (Hartree): 0.111644
1696
1697 HOCHCHCH2CH200.Ecpmt
1698 ~~~~~
1699 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13755268
1700 Electronic state : 2-A
1701 Cartesian coordinates (Angs):
1702 C      -1.459720      -0.380138      0.100018
1703 C      -1.195673      0.890109      -0.161260
1704 C       0.160351      1.527147      -0.087119
1705 C       1.259783      0.656818      0.472133
1706 O       1.538632      -0.395509      -0.482336
1707 O       2.331305      -1.292747      0.015563
1708 O      -2.730887      -0.869703      0.027081
1709 H      -0.695940      -1.096969      0.379060
1710 H      -2.021999      1.524596      -0.459245
1711 H       0.465324      1.880214      -1.076448
1712 H       0.109175      2.419006      0.542606
1713 H       2.186733      1.212246      0.607498
1714 H       0.982718      0.178054      1.410801
1715 H      -2.726850      -1.817098      0.170634
1716 Rotational constants (GHz):  4.4196600      1.5059900      1.1816000
1717 Vibrational harmonic frequencies (cm-1):
1718      42.0257          126.7007          135.7249
1719      206.3338          235.5286          286.2958
1720      312.5589          394.5795          519.4377
1721      621.7216          802.1858          879.4116
1722      933.8539          972.8706          994.0134
1723      1062.5462         1111.2065         1185.9560
1724      1215.4124         1235.8830         1286.2828
1725      1299.1804         1353.5418         1387.9902
1726      1389.6808         1417.4445         1475.1009
1727      1504.8745         1790.0874         3052.1121
1728      3078.1940         3091.5871         3143.5744
1729      3188.7776         3190.6990         3917.2498
1730 Zero-point correction (Hartree): 0.111267
1731
1732 HOCHCHCH2CH200.Ecppc
1733 ~~~~~
1734 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13947030
1735 Electronic state : 2-A
1736 Cartesian coordinates (Angs):
1737 C      -1.529484      -0.302489      0.170987
1738 C      -1.034845      0.811980      -0.349991
1739 C       0.374698      1.300939      -0.188853
1740 C       1.232616      0.510313      0.773581
1741 O       1.481866      -0.830752      0.290517
1742 O       2.258116      -0.821903      -0.748450
1743 O      -2.804690      -0.750430      0.033491
1744 H      -0.945277      -0.991818      0.765712
1745 H      -1.686990      1.431986      -0.958476
1746 H       0.886349      1.319515      -1.154593
1747 H       0.364612      2.334302      0.167739
1748 H       2.203798      0.980548      0.914588
1749 H       0.745164      0.362278      1.736279
1750 H      -3.307907      -0.136598      -0.510058
1751 Rotational constants (GHz):  4.9983100      1.4387300      1.2663800
1752 Vibrational harmonic frequencies (cm-1):
1753      67.8308          117.8662          148.3515
1754      204.1084          269.3890          314.1250
1755      431.1025          446.1421          535.4174
1756      625.5700          811.4498          862.5680
1757      928.0912          984.7397          995.4913

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1758      1037.2588      1118.6221      1160.2299
1759      1227.7424      1248.8181      1283.3823
1760      1316.4783      1350.1384      1390.1106
1761      1399.1873      1413.6909      1474.9318
1762      1494.2587      1766.1610      3055.8556
1763      3083.2992      3099.4234      3154.0351
1764      3155.0453      3223.1537      3859.8894
1765 Zero-point correction (Hartree): 0.111753
1766
1767 HOCHCHCH2CH200.Ecppt
1768 ~~~~~
1769 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.1380200
1770 Electronic state : 2-A
1771 Cartesian coordinates (Angs):
1772   C      -1.529449      -0.270471      0.138609
1773   C      -1.022385      0.847727      -0.355323
1774   C       0.393919      1.310374      -0.189437
1775   C       1.239116      0.507328      0.773733
1776   O       1.461834      -0.842237      0.299354
1777   O       2.237854      -0.857438      -0.739800
1778   O      -2.840301      -0.599535      -0.051762
1779   H      -0.944052      -0.982245      0.709316
1780   H      -1.680273      1.480772      -0.939231
1781   H       0.906484      1.324864      -1.154913
1782   H       0.399687      2.343160      0.169092
1783   H       2.219956      0.958170      0.911539
1784   H       0.749641      0.373436      1.737641
1785   H      -3.013743      -1.474224      0.298727
1786 Rotational constants (GHz):  4.9691000      1.4437000      1.2654800
1787 Vibrational harmonic frequencies (cm-1):
1788      67.3447      120.3136      150.1679
1789      197.9145      232.0141      293.8005
1790      317.3200      440.0979      534.0222
1791      625.9645      814.0036      865.5497
1792      925.5620      971.6286      985.4511
1793     1035.0411     1118.1520     1185.3130
1794     1218.1745     1229.5988     1278.3390
1795     1313.1957     1355.4120     1387.3704
1796     1392.6868     1407.0145     1473.1566
1797     1491.9981     1788.7664     3055.7378
1798     3082.3562     3098.1625     3153.7357
1799     3187.0484     3189.4940     3917.0116
1800 Zero-point correction (Hartree): 0.111400
1801
1802 HOCHCHCH2CH200.Ectpc
1803 ~~~~~
1804 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13938546
1805 Electronic state : 2-A
1806 Cartesian coordinates (Angs):
1807   C       1.936312      -0.344147      -0.048058
1808   C       1.221437      0.766858      0.066513
1809   C      -0.268783      0.828034      0.220496
1810   C      -0.935101      -0.530449      0.227231
1811   O      -2.358621      -0.381508      0.409864
1812   O      -2.926371      0.085049      -0.659898
1813   O       3.285433      -0.418540      -0.190501
1814   H       1.502893      -1.335730      -0.039989
1815   H       1.740157      1.720866      0.048268
1816   H      -0.526798      1.344957      1.148427
1817   H      -0.706390      1.411545      -0.592537
1818   H      -0.780617      -1.069171      -0.707047
1819   H      -0.617071      -1.141356      1.070902
1820   H       3.661109      0.467113      -0.200841
1821 Rotational constants (GHz):  9.8150100      0.9944200      0.9536900
1822 Vibrational harmonic frequencies (cm-1):
1823      69.9008      110.5973      147.6182
1824     162.2996     271.1103     322.2673
1825     376.4266     438.7931     543.6010
1826     669.5200     774.6993     854.3725
1827     955.3967     987.5271     994.7808
1828     1101.3430     1108.4992     1158.9623
1829     1238.2333     1253.1820     1285.9201

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1830      1320.6570              1340.1831              1350.9176
1831      1403.4472              1422.6524              1492.0627
1832      1503.2176              1766.7069              3055.1602
1833      3089.3721              3090.7007              3150.9597
1834      3159.3541              3214.6008              3858.0659
1835      Zero-point correction (Hartree): 0.111728
1836
1837      HOCHCHCH2CH200.Ectpt
1838      ~~~~~
1839      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13741398
1840      Electronic state : 2-A
1841      Cartesian coordinates (Angs):
1842      C      1.939941      -0.306288      -0.043998
1843      C      1.212318      0.795109      0.054537
1844      C      -0.277420      0.841180      0.204218
1845      C      -0.931955      -0.522116      0.240755
1846      O      -2.357334      -0.384119      0.418383
1847      O      -2.929968      0.042776      -0.665264
1848      O      3.297206      -0.251505      -0.178406
1849      H      1.511880      -1.302568      -0.024448
1850      H      1.733897      1.744451      0.023800
1851      H      -0.541629      1.377099      1.119589
1852      H      -0.719151      1.403362      -0.621714
1853      H      -0.772293      -1.080333      -0.681255
1854      H      -0.609342      -1.110884      1.098530
1855      H      3.660101      -1.135645      -0.245271
1856      Rotational constants (GHz): 9.8556000      0.9914600      0.9518100
1857      Vibrational harmonic frequencies (cm-1):
1858      68.2076      106.6733      144.7125
1859      160.4354      191.3743      296.9736
1860      323.3690      370.0179      543.0483
1861      668.8520      773.9917      862.0336
1862      949.6565      970.6268      991.1841
1863      1100.9311      1106.9279      1182.2731
1864      1219.8489      1238.4636      1285.5997
1865      1318.8167      1339.1135      1355.0051
1866      1384.0531      1421.4667      1490.5967
1867      1501.8193      1787.9223      3055.0370
1868      3087.8865      3089.4569      3148.9799
1869      3179.5770      3191.1718      3919.9732
1870      Zero-point correction (Hartree): 0.111234
1871
1872      HOCHCHCH2CH200.Ecttc
1873      ~~~~~
1874      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13876938
1875      Point group : CS
1876      Electronic state : 2-A"
1877      Cartesian coordinates (Angs):
1878      C      -0.771975      -1.802408      0.000000
1879      C      0.515982      -1.485695      0.000000
1880      C      1.065624      -0.090714      0.000000
1881      C      -0.000000      0.979201      0.000000
1882      O      0.681606      2.250581      0.000000
1883      O      -0.157836      3.238907      0.000000
1884      O      -1.288633      -3.057915      0.000000
1885      H      -1.565508      -1.066926      0.000000
1886      H      1.246994      -2.288398      0.000000
1887      H      1.705699      0.056392      0.873368
1888      H      1.705699      0.056392      -0.873368
1889      H      -0.628043      0.945712      -0.890070
1890      H      -0.628043      0.945712      0.890070
1891      H      -0.575674      -3.703771      0.000000
1892      Rotational constants (GHz): 9.0291200      0.9776300      0.8918700
1893      Vibrational harmonic frequencies (cm-1):
1894      73.9734 ( A")      103.8979 ( A")      122.8267 ( A')
1895      131.4241 ( A")      268.2891 ( A")      288.7826 ( A')
1896      369.1405 ( A')      428.2408 ( A")      526.8094 ( A')
1897      646.7481 ( A')      765.5339 ( A")      849.9082 ( A")
1898      979.3574 ( A')      985.2831 ( A")      1031.1827 ( A')
1899      1082.6697 ( A")      1125.1460 ( A')      1161.8411 ( A')
1900      1227.6135 ( A")      1258.5921 ( A')      1296.4638 ( A')
1901      1307.5496 ( A")      1331.8992 ( A')      1351.7050 ( A')

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1902      1404.0158 ( A')      1431.0892 ( A')      1498.7546 ( A')
1903      1512.6102 ( A')      1765.5679 ( A')      3055.2827 ( A')
1904      3083.1958 ( A')      3084.1565 ( A'')      3140.6048 ( A'')
1905      3162.7702 ( A')      3218.6361 ( A')      3860.5767 ( A')
1906 Zero-point correction (Hartree): 0.111476
1907
1908 HOCHCHCH2CH2OO.Ecttt
1909 ~~~~~
1910 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13700871
1911 Point group : CS
1912 Electronic state : 2-A''
1913 Cartesian coordinates (Angs):
1914      C      -0.730667      -1.816974      0.000000
1915      C      0.550123      -1.482173      0.000000
1916      C      1.078835      -0.080256      0.000000
1917      C      -0.000000      0.976032      0.000000
1918      O      0.661347      2.258959      0.000000
1919      O      -0.193057      3.234275      0.000000
1920      O      -1.122947      -3.123534      0.000000
1921      H      -1.532954      -1.087177      0.000000
1922      H      1.278914      -2.283852      0.000000
1923      H      1.717525      0.073764      0.873326
1924      H      1.717525      0.073764      -0.873326
1925      H      -0.627193      0.934602      -0.890543
1926      H      -0.627193      0.934602      0.890543
1927      H      -2.079119      -3.183081      0.000000
1928 Rotational constants (GHz):      9.0451300      0.9756500      0.8903900
1929 Vibrational harmonic frequencies (cm-1):
1930      78.1147 ( A'')      105.6336 ( A'')      123.3877 ( A')
1931      141.6512 ( A'')      214.4010 ( A'')      288.1418 ( A')
1932      304.9511 ( A'')      364.9563 ( A')      524.9464 ( A')
1933      646.4276 ( A')      765.6786 ( A'')      858.0770 ( A'')
1934      969.0092 ( A'')      971.9698 ( A')      1029.4277 ( A')
1935      1082.5480 ( A'')      1124.5327 ( A')      1184.5187 ( A')
1936      1224.9998 ( A')      1228.0631 ( A'')      1296.3103 ( A')
1937      1306.9655 ( A'')      1329.6117 ( A')      1356.7021 ( A')
1938      1384.6632 ( A')      1429.1669 ( A')      1497.5473 ( A')
1939      1511.9850 ( A')      1787.3630 ( A')      3054.9617 ( A')
1940      3080.6423 ( A')      3083.6770 ( A'')      3137.9846 ( A'')
1941      3181.5268 ( A')      3193.1579 ( A')      3919.4957 ( A')
1942 Zero-point correction (Hartree): 0.111136
1943
1944 HOCHCHCH2CH2OO.Egppc
1945 ~~~~~
1946 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59741321
1947 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53562656
1948 T1 diagnostic: 0.021635
1949 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49135115
1950 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52284012
1951 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49450832
1952 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52470252
1953 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13366994
1954 E(UHF/Aug-CC-pVTZ) (Hartree): -380.12852112
1955 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14077322
1956 Electronic state : 2-A
1957 Cartesian coordinates (Angs):
1958      C      1.710511      -0.236631      0.326987
1959      C      0.944346      0.767676      -0.075868
1960      C      -0.364970      1.093381      0.572448
1961      C      -1.559565      0.810304      -0.322689
1962      O      -1.648835      -0.595790      -0.641420
1963      O      -1.913557      -1.302412      0.413399
1964      O      2.897580      -0.615656      -0.206873
1965      H      1.435802      -0.870144      1.161279
1966      H      1.254587      1.369726      -0.925861
1967      H      -0.486348      0.518270      1.490682
1968      H      -0.411223      2.150053      0.846885
1969      H      -2.497548      1.093650      0.152897
1970      H      -1.469744      1.294969      -1.293789
1971      H      3.111038      -0.054046      -0.958204
1972 Rotational constants (GHz):      4.8942000      1.4051200      1.2198500
1973 Vibrational harmonic frequencies (cm-1):

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1974      48.4327      73.9465      138.6868
1975      203.0000      282.0698      338.0806
1976      432.5349      464.7401      534.2373
1977      576.6960      817.7682      871.9379
1978      917.7207      978.5767      989.2948
1979      1056.1982      1130.6006      1160.8082
1980      1215.2377      1261.8162      1278.7131
1981      1308.6740      1341.0988      1362.0063
1982      1399.2443      1409.4212      1476.6644
1983      1490.7193      1764.6782      3063.6467
1984      3091.5359      3117.6738      3151.0787
1985      3153.2238      3205.8634      3858.7646
1986 Zero-point correction (Hartree): 0.111551
1987
1988 HOCHCHCH2CH2OO.Egppt
1989 ~~~~~
1990 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13943708
1991 Electronic state : 2-A
1992 Cartesian coordinates (Angs):
1993 C      1.687236      -0.201097      0.290896
1994 C      0.928303      0.817527      -0.079823
1995 C     -0.388725      1.111221      0.566132
1996 C     -1.573046      0.788725      -0.329917
1997 O     -1.625150      -0.623845      -0.632210
1998 O     -1.858347      -1.327385      0.431741
1999 O      2.875457      -0.478173      -0.312634
2000 H      1.391623      -0.864289      1.097960
2001 H      1.258737      1.441503      -0.902645
2002 H     -0.499833      0.540022      1.488258
2003 H     -0.463606      2.168069      0.832364
2004 H     -2.520100      1.052277      0.139199
2005 H     -1.491630      1.262981      -1.306601
2006 H      3.266520      -1.263601      0.072556
2007 Rotational constants (GHz):      4.8400900      1.4303100      1.2324500
2008 Vibrational harmonic frequencies (cm-1):
2009      47.9251      75.1564      145.3360
2010      199.4227      255.2148      299.2435
2011      337.1138      454.6666      532.7269
2012      576.7199      824.7387      880.4943
2013      914.9683      965.1112      979.4742
2014      1051.9435      1134.6384      1179.6874
2015      1207.3830      1246.9137      1270.9962
2016      1304.0541      1339.5274      1365.6406
2017      1395.8855      1399.3995      1477.7779
2018      1490.5910      1787.2229      3065.8359
2019      3092.1485      3116.9292      3153.6702
2020      3169.3150      3183.6903      3915.4862
2021 Zero-point correction (Hartree): 0.111259
2022
2023 HOCHCHCH2CH2OO.Egptt
2024 ~~~~~
2025 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13810416
2026 Electronic state : 2-A
2027 Cartesian coordinates (Angs):
2028 C      1.871289      -0.153176      0.329989
2029 C      1.054218      0.635267      -0.348775
2030 C     -0.127526      1.310639      0.274269
2031 C     -1.450685      0.761239      -0.222213
2032 O     -1.582532      -0.580829      0.295585
2033 O     -2.656826      -1.158544      -0.143306
2034 O      2.936654      -0.767166      -0.254017
2035 H      1.728227      -0.344927      1.388712
2036 H      1.232642      0.780890      -1.408353
2037 H     -0.094393      1.210822      1.360925
2038 H     -0.117389      2.380612      0.054960
2039 H     -2.303019      1.331426      0.145625
2040 H     -1.494215      0.695959      -1.308917
2041 H      3.386003      -1.326284      0.381331
2042 Rotational constants (GHz):      5.3088800      1.2317300      1.0613900
2043 Vibrational harmonic frequencies (cm-1):
2044      44.1585      72.5962      110.5274
2045      188.9176      240.8283      278.9011

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2046	332.8114	396.6938	537.4121			
2047	566.3702	818.6533	871.5105			
2048	917.0749	963.8968	1031.6287			
2049	1067.3404	1123.0761	1179.5649			
2050	1205.2590	1250.2644	1276.6812			
2051	1299.0977	1337.7871	1364.5492			
2052	1392.9945	1406.0468	1473.0211			
2053	1500.3771	1790.1720	3062.0313			
2054	3083.9850	3105.3708	3142.0309			
2055	3170.7630	3183.3007	3917.6972			
2056	Zero-point correction (Hartree): 0.110954					
2057						
2058	HOCHCH2CH2OO.Elmmc					
2059	~~~~~					
2060	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59783370					
2061	E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53613947					
2062	T1 diagnostic: 0.021613					
2063	E(MP2/Aug-CC-pVTZ) (Hartree): -381.49167334					
2064	E(MP3/Aug-CC-pVTZ) (Hartree): -381.52332066					
2065	E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49483364					
2066	E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52518461					
2067	E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13467350					
2068	E(UHF/Aug-CC-pVTZ) (Hartree): -380.12952628					
2069	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14119558					
2070	Electronic state : 2-A					
2071	Cartesian coordinates (Angs):					
2072	C	2.124153	0.276916	-0.042485		
2073	C	0.874173	-0.099991	-0.272337		
2074	C	-0.241856	0.871925	-0.502115		
2075	C	-1.331538	0.777029	0.551962		
2076	O	-1.920688	-0.543726	0.557753		
2077	O	-2.625917	-0.751207	-0.511793		
2078	O	3.188259	-0.535457	0.177972		
2079	H	2.419325	1.318728	-0.015007		
2080	H	0.628268	-1.157591	-0.294153		
2081	H	0.142333	1.893574	-0.495348		
2082	H	-0.708634	0.706852	-1.475186		
2083	H	-0.933191	0.894050	1.558058		
2084	H	-2.137311	1.487177	0.372899		
2085	H	2.906379	-1.454950	0.147128		
2086	Rotational constants (GHz):			7.1870100	1.0976100	1.0399700
2087	Vibrational harmonic frequencies (cm-1):					
2088		56.8155	83.9327			145.6926
2089		184.7958	282.8152			330.2073
2090		441.3317	475.5827			532.5543
2091		584.2154	819.8312			856.1046
2092		908.1255	989.8147			997.8385
2093		1093.6706	1120.4717			1158.1126
2094		1207.1273	1245.8661			1294.7724
2095		1306.4289	1340.7014			1365.5644
2096		1394.4322	1413.1006			1474.5714
2097		1489.2539	1763.9730			3068.0372
2098		3093.6743	3112.8341			3158.6898
2099		3163.9251	3203.8754			3858.7945
2100	Zero-point correction (Hartree): 0.111670					
2101						
2102	HOCHCH2CH2OO.Elmmt					
2103	~~~~~					
2104	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13870637					
2105	Electronic state : 2-A					
2106	Cartesian coordinates (Angs):					
2107	C	2.125235	0.248322	-0.058651		
2108	C	0.872717	-0.128232	-0.259321		
2109	C	-0.238762	0.845137	-0.498006		
2110	C	-1.328976	0.766348	0.557172		
2111	O	-1.950491	-0.538911	0.551717		
2112	O	-2.674554	-0.711942	-0.511242		
2113	O	3.126265	-0.649485	0.162286		
2114	H	2.416229	1.294412	-0.065456		
2115	H	0.636743	-1.185922	-0.247669		
2116	H	0.146936	1.866620	-0.504487		
2117	H	-0.709261	0.670049	-1.467856		


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2118      H      -0.927013      0.865361      1.563809
2119      H      -2.117523      1.497240      0.384897
2120      H      3.962841      -0.194512      0.267517
2121 Rotational constants (GHz):      7.4165000      1.0823000      1.0299300
2122 Vibrational harmonic frequencies (cm-1):
2123      58.1094      83.5004      145.1692
2124      179.0405      261.2688      283.6740
2125      343.9772      473.3522      529.3861
2126      579.8470      819.7825      865.7344
2127      908.1426      967.9874      997.4035
2128      1095.1717      1120.2871      1176.8371
2129      1197.1457      1237.6120      1272.9478
2130      1306.9577      1339.9534      1366.4940
2131      1393.0371      1401.3962      1474.2716
2132      1488.3671      1786.6412      3064.6038
2133      3092.0681      3109.0438      3157.2482
2134      3166.1291      3193.1663      3917.7310
2135 Zero-point correction (Hartree): 0.111296
2136
2137 HOCHCHCH2CH2OO.Elmpc
2138 ~~~~~
2139 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14045498
2140 Electronic state : 2-A
2141 Cartesian coordinates (Angs):
2142      C      1.990995      0.290723      0.147957
2143      C      0.783071      0.146789      -0.378955
2144      C     -0.267488      1.210011      -0.300446
2145      C     -1.511384      0.771514      0.459024
2146      O     -2.173244     -0.296686     -0.251029
2147      O     -1.760532     -1.467795      0.130963
2148      O      2.994221     -0.622237      0.132025
2149      H      2.297937      1.195879      0.657647
2150      H      0.524123     -0.780504     -0.880382
2151      H      0.132568      2.092020      0.204050
2152      H     -0.576875      1.525457     -1.299715
2153      H     -1.276596      0.401779      1.454863
2154      H     -2.249624      1.570606      0.506442
2155      H      2.693745     -1.425720     -0.304047
2156 Rotational constants (GHz):      5.3864800      1.3147700      1.1153500
2157 Vibrational harmonic frequencies (cm-1):
2158      63.8294      89.1137      132.6084
2159      185.0105      288.9820      340.3975
2160      444.6962      474.8875      529.9831
2161      562.1000      845.9667      860.7239
2162      884.3868      990.1286      1016.3122
2163      1084.0668      1116.5833      1160.1911
2164      1213.2703      1237.8761      1291.0053
2165      1322.3524      1344.0177      1370.2374
2166      1386.2854      1415.5074      1472.7173
2167      1485.0646      1763.5710      3057.6900
2168      3092.6181      3104.3023      3161.1612
2169      3167.6961      3201.1436      3857.5971
2170 Zero-point correction (Hartree): 0.111662
2171
2172 HOCHCHCH2CH2OO.Elmpc
2173 ~~~~~
2174 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13752742
2175 Electronic state : 2-A
2176 Cartesian coordinates (Angs):
2177      C      1.989507      0.262297      0.130044
2178      C      0.777124      0.125563     -0.382394
2179      C     -0.261349      1.198630     -0.291182
2180      C     -1.508613      0.770590      0.468626
2181      O     -2.193658     -0.275300     -0.251268
2182      O     -1.812128     -1.459012      0.124798
2183      O      2.930095     -0.719142      0.038424
2184      H      2.295569      1.168905      0.643384
2185      H      0.522343     -0.800812     -0.883005
2186      H      0.147817      2.075144      0.216406
2187      H     -0.571089      1.522324     -1.287893
2188      H     -1.275494      0.383278      1.458211
2189      H     -2.231510      1.582752      0.531264

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2190      H      3.737879      -0.446456      0.475440
2191 Rotational constants (GHz):      5.4572000      1.2998800      1.1070100
2192 Vibrational harmonic frequencies (cm-1):
2193      64.2559      86.3268      130.5274
2194      178.1882      258.9797      287.9710
2195      353.5359      474.4244      526.6953
2196      558.9309      844.4467      871.0567
2197      882.9824      970.8423      1018.2529
2198      1084.6321      1117.4167      1179.0426
2199      1201.6086      1237.9409      1264.4799
2200      1319.0775      1345.9730      1370.6756
2201      1385.7920      1403.8346      1472.6167
2202      1484.7002      1785.9588      3055.0045
2203      3090.6026      3101.1149      3159.7897
2204      3162.9384      3196.9708      3918.7962
2205 Zero-point correction (Hartree): 0.111280
2206
2207 HOCHCHCH2CH2OO.Elmtc
2208 ~~~~~
2209 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14044555
2210 Electronic state : 2-A
2211 Cartesian coordinates (Angs):
2212      C      2.175963      0.186009      0.179724
2213      C      0.978214      0.057207      -0.373761
2214      C     -0.069240      1.126498      -0.303036
2215      C     -1.324123      0.674537      0.417155
2216      O     -1.901820     -0.397832     -0.361864
2217      O     -2.954285     -0.892729      0.211247
2218      O      3.175990     -0.730064      0.170248
2219      H      2.475424      1.081714      0.710223
2220      H      0.723648     -0.859065     -0.897583
2221      H      0.322422      1.997960      0.224062
2222      H     -0.351103      1.458940     -1.304999
2223      H     -1.111008      0.276191      1.408134
2224      H     -2.073764      1.462124      0.484559
2225      H      2.890411     -1.518371     -0.301936
2226 Rotational constants (GHz):      7.0870600      1.0463600      0.9597700
2227 Vibrational harmonic frequencies (cm-1):
2228      49.5994      90.3886      116.2541
2229      189.2059      270.1401      329.0272
2230      396.3809      452.8971      546.4457
2231      570.7131      812.1939      856.0773
2232      929.8350      991.5934      1033.3265
2233      1078.2671      1125.6248      1160.3652
2234      1217.0645      1246.0738      1296.9406
2235      1298.3373      1341.4574      1365.5075
2236      1398.7018      1414.1608      1472.0318
2237      1501.0744      1763.3001      3060.7044
2238      3085.6154      3109.2440      3146.6216
2239      3165.8735      3201.7740      3857.2177
2240 Zero-point correction (Hartree): 0.111494
2241
2242 HOCHCHCH2CH2OO.Elmtt
2243 ~~~~~
2244 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13798496
2245 Electronic state : 2-A
2246 Cartesian coordinates (Angs):
2247      C      2.173117      0.167424      0.157258
2248      C      0.970963      0.041464     -0.381228
2249      C     -0.072376      1.111851     -0.290724
2250      C     -1.324757      0.656602      0.432221
2251      O     -1.926112     -0.388564     -0.364734
2252      O     -2.984436     -0.874250      0.205234
2253      O      3.112428     -0.815310      0.071604
2254      H      2.470110      1.065938      0.689801
2255      H      0.724771     -0.874854     -0.904278
2256      H      0.322664      1.978532      0.242455
2257      H     -0.361053      1.454522     -1.287458
2258      H     -1.105852      0.232019      1.411023
2259      H     -2.063330      1.451864      0.527200
2260      H      3.915968     -0.547075      0.519265
2261 Rotational constants (GHz):      7.2581100      1.0369700      0.9544000

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2262 Vibrational harmonic frequencies (cm-1):
2263     51.3622          91.4555          114.8537
2264     180.4182         259.3054         273.7506
2265     340.7793         398.9651         541.7653
2266     570.7578         811.9286         867.1642
2267     927.9807         970.4569        1033.7417
2268     1079.4163        1128.4707        1178.0868
2269     1206.8534        1237.1343        1279.3676
2270     1297.4922        1339.9602        1367.0724
2271     1398.1003        1403.2247        1471.8138
2272     1500.6779        1786.2808        3058.6410
2273     3085.1347        3105.6017        3145.9876
2274     3164.0356        3195.5698        3917.2662
2275 Zero-point correction (Hartree): 0.111131
2276
2277 HOCHCHCH2CH200.Elpmc
2278 ~~~~~
2279 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14031527
2280 Electronic state : 2-A
2281 Cartesian coordinates (Angs):
2282   C      -1.716898      0.146092      -0.385021
2283   C      -0.768732      0.610804      0.416624
2284   C       0.428961      1.348511     -0.088900
2285   C       1.742575      0.638342      0.211557
2286   O       1.802244     -0.622303     -0.477781
2287   O       1.259329     -1.577483      0.218050
2288   O      -2.823031     -0.544588     -0.015065
2289   H      -1.686140      0.288376     -1.458048
2290   H      -0.834430      0.427859      1.485386
2291   H       0.348477      1.499505     -1.166609
2292   H       0.496962      2.339651      0.368448
2293   H       2.593005      1.204843     -0.164387
2294   H       1.864156      0.433781      1.274056
2295   H      -2.805809     -0.701510      0.933953
2296 Rotational constants (GHz):  4.6279400    1.5523400    1.2629400
2297 Vibrational harmonic frequencies (cm-1):
2298     62.2880          96.0757          108.9101
2299     193.1536         290.6709         350.8344
2300     422.9886         466.9158         540.3184
2301     553.9728         824.1871         861.6162
2302     942.6393         983.8111         993.8037
2303     1040.3522        1132.5951        1164.1930
2304     1225.5704        1237.3195        1280.0041
2305     1318.0575        1343.4109        1360.5222
2306     1394.6357        1413.1371        1473.5582
2307     1485.7583        1764.5370        3051.7259
2308     3091.9388        3105.8278        3154.9038
2309     3159.3070        3207.7406        3860.3590
2310 Zero-point correction (Hartree): 0.111534
2311
2312 HOCHCHCH2CH200.Elpmt
2313 ~~~~~
2314 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13829904
2315 Electronic state : 2-A
2316 Cartesian coordinates (Angs):
2317   C       1.679246      0.110683      0.354616
2318   C       0.765612      0.682938     -0.412719
2319   C      -0.448739      1.353033      0.142140
2320   C      -1.743553      0.626339     -0.199469
2321   O      -1.783544     -0.650949      0.461241
2322   O      -1.236397     -1.586352     -0.258257
2323   O       2.781777     -0.496873     -0.162806
2324   H       1.592392      0.106015      1.436620
2325   H       0.886845      0.636445     -1.488836
2326   H      -0.374506      1.436458      1.227989
2327   H      -0.541797      2.369393     -0.249760
2328   H      -2.611147      1.164789      0.178867
2329   H      -1.844907      0.444686     -1.267936
2330   H       3.283043     -0.922361      0.534221
2331 Rotational constants (GHz):  4.5792500    1.5738300    1.2710500
2332 Vibrational harmonic frequencies (cm-1):
2333     56.7528          97.4223          108.0751

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2334      185.1658          241.9628          299.6491
2335      352.1428          462.0451          539.3009
2336      549.7923          828.6190          865.8652
2337      946.9980          961.6997          986.9639
2338      1038.2792         1136.0127         1180.7630
2339      1211.3605         1235.3846         1257.8402
2340      1313.9456         1340.3052         1361.4416
2341      1392.6747         1399.1790         1473.5968
2342      1484.3704         1787.1973         3054.9106
2343      3091.7525         3103.3339         3155.9447
2344      3170.1119         3189.6327         3917.6516
2345 Zero-point correction (Hartree): 0.111125
2346
2347 HOCHCHCH2CH200.Elptc
2348 ~~~~~
2349 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13968393
2350 Electronic state : 2-A
2351 Cartesian coordinates (Angs):
2352   C      -1.897069      -0.144664      -0.371056
2353   C      -1.056654       0.583217       0.350585
2354   C       0.114627       1.304085      -0.242630
2355   C       1.447573       0.762783       0.234917
2356   O       1.597683      -0.567063      -0.306902
2357   O       2.675606      -1.139922       0.129742
2358   O      -2.970820      -0.834603       0.085399
2359   H      -1.789832      -0.253802      -1.443022
2360   H      -1.197984       0.654553       1.425816
2361   H       0.080097       1.244268      -1.331847
2362   H       0.085634       2.364985       0.016705
2363   H       2.288937       1.353669      -0.125466
2364   H       1.498795       0.678604       1.320216
2365   H      -3.036259      -0.742095       1.040786
2366 Rotational constants (GHz):  5.3681500    1.2172800    1.0551600
2367 Vibrational harmonic frequencies (cm-1):
2368      47.1882          74.8600          110.7871
2369      204.1682         265.0175         334.2196
2370      391.4892         446.2482         540.5382
2371      567.6268         814.9271         863.6201
2372      917.8374         988.6263        1035.2476
2373     1069.2262        1122.3981        1159.4625
2374     1215.5601        1267.2054        1288.0298
2375     1298.6105        1341.6350        1362.4937
2376     1398.3535        1414.8400        1472.9430
2377     1500.9427        1766.3020        3062.0597
2378     3082.9820        3106.9162        3140.2931
2379     3153.5250        3208.4551        3860.2757
2380 Zero-point correction (Hartree): 0.111391
2381
2382 HOCHCHCH2CH200.Eltmc
2383 ~~~~~
2384 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59757712
2385 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53594843
2386 T1 diagnostic: 0.021541
2387 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49136426
2388 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52330142
2389 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49452390
2390 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52516264
2391 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13519483
2392 E(UHF/Aug-CC-pVTZ) (Hartree): -380.13005206
2393 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14085582
2394 Electronic state : 2-A
2395 Cartesian coordinates (Angs):
2396   C      -2.116996       0.458740       0.023049
2397   C      -1.201545      -0.458753       0.304944
2398   C       0.215959      -0.116171       0.646310
2399   C       1.167619      -0.590526      -0.439314
2400   O       2.539002      -0.357420      -0.056058
2401   O       2.828865       0.907518      -0.091009
2402   O      -3.413943       0.237036      -0.302756
2403   H      -1.893836       1.518356       0.037417
2404   H      -1.476744      -1.509855       0.279228
2405   H       0.330920       0.961839       0.759748

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2406      H      0.510763      -0.579923      1.590163
2407      H      1.107798      -1.667516      -0.590321
2408      H      0.992433      -0.071408      -1.380229
2409      H      -3.592948      -0.708296      -0.307352
2410      Rotational constants (GHz): 10.0368700      0.9316200      0.9000000
2411      Vibrational harmonic frequencies (cm-1):
2412      62.6193      86.0716      114.6904
2413      178.5780      307.7151      321.7048
2414      372.5639      446.0057      522.6093
2415      624.6712      795.8463      850.8975
2416      958.7976      991.0461      1019.8069
2417      1068.2658      1129.2750      1160.1231
2418      1220.7535      1266.9190      1283.4531
2419      1312.2745      1329.5215      1347.5466
2420      1395.5665      1412.2663      1485.2413
2421      1499.6656      1761.8549      3064.9628
2422      3093.7449      3118.4546      3151.9409
2423      3157.1601      3205.8173      3858.7043
2424      Zero-point correction (Hartree): 0.111578
2425
2426      HOCHCHCH2CH200.Eltmt
2427      ~~~~~
2428      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13929131
2429      Electronic state : 2-A
2430      Cartesian coordinates (Angs):
2431      C      -2.116572      0.416829      0.046261
2432      C      -1.191134      -0.498223      0.288145
2433      C      0.220217      -0.150112      0.644152
2434      C      1.178600      -0.580618      -0.453727
2435      O      2.546494      -0.334731      -0.064552
2436      O      2.817275      0.934757      -0.071963
2437      O      -3.393009      0.084359      -0.290855
2438      H      -1.898587      1.478277      0.110791
2439      H      -1.466099      -1.544455      0.212146
2440      H      0.326348      0.924914      0.792302
2441      H      0.517839      -0.642064      1.572851
2442      H      1.135422      -1.653914      -0.632830
2443      H      0.995182      -0.039785      -1.380697
2444      H      -3.922847      0.874692      -0.404589
2445      Rotational constants (GHz): 10.0574900      0.9318000      0.9003200
2446      Vibrational harmonic frequencies (cm-1):
2447      62.7043      88.0215      115.2441
2448      181.9248      265.8166      316.5343
2449      323.3749      385.1449      520.7013
2450      621.7596      796.6855      865.7763
2451      956.6579      970.6860      1017.8475
2452      1067.6172      1133.8664      1179.0186
2453      1212.3615      1246.3360      1283.4095
2454      1299.5434      1330.5167      1356.9055
2455      1382.7914      1407.6503      1484.8791
2456      1499.8352      1785.0922      3063.0106
2457      3094.1621      3115.4457      3156.4935
2458      3171.1139      3181.9716      3915.6844
2459      Zero-point correction (Hartree): 0.111303
2460
2461      HOCHCHCH2CH200.Eltpc
2462      ~~~~~
2463      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59774833
2464      E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53608544
2465      T1 diagnostic: 0.021615
2466      E(MP2/Aug-CC-pVTZ) (Hartree): -381.49148884
2467      E(MP3/Aug-CC-pVTZ) (Hartree): -381.52339626
2468      E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49466624
2469      E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52527544
2470      E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13522254
2471      E(UHF/Aug-CC-pVTZ) (Hartree): -380.13007016
2472      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14108463
2473      Electronic state : 2-A
2474      Cartesian coordinates (Angs):
2475      C      2.234338      0.135592      -0.357583
2476      C      1.152266      -0.409745      0.181764
2477      C      -0.208548      -0.304048      -0.433368

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2478	C	-1.139220	0.517425	0.443306	
2479	O	-2.467277	0.557499	-0.118814	
2480	O	-3.071055	-0.583770	0.015422	
2481	O	3.496844	0.090426	0.134221	
2482	H	2.198969	0.685380	-1.290008	
2483	H	1.240777	-0.954326	1.118051	
2484	H	-0.143183	0.158791	-1.418965	
2485	H	-0.656921	-1.291129	-0.560283	
2486	H	-1.221690	0.101001	1.446713	
2487	H	-0.828505	1.559128	0.495662	
2488	H	3.509436	-0.407433	0.957481	
2489	Rotational constants (GHz):			13.1446600	0.8826300 0.8713100
2490	Vibrational harmonic frequencies (cm-1):				
2491		67.8392	71.8809		132.1719
2492		170.9503	293.7329		332.8483
2493		372.3254	440.9682		536.2726
2494		616.7591	789.1311		849.8083
2495		973.1622	989.9596		1014.5884
2496		1068.2345	1126.4066		1158.0426
2497		1225.3138	1255.7702		1293.0913
2498		1309.0186	1331.2088		1346.1744
2499		1393.1945	1412.4869		1483.8683
2500		1498.2063	1764.3313		3068.2706
2501		3092.7231	3113.9544		3151.3558
2502		3158.2694	3205.3995		3859.9303
2503	Zero-point correction (Hartree): 0.111557				
2504	HOCHCH2CH200.Eltpt				
2505	~~~~~				
2507	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13930049				
2508	Electronic state : 2-A				
2509	Cartesian coordinates (Angs):				
2510	C	-2.230972	0.064200	0.344730	
2511	C	-1.142923	-0.387317	-0.259035	
2512	C	0.211479	-0.361046	0.375652	
2513	C	1.147173	0.565479	-0.382958	
2514	O	2.467725	0.545511	0.198395	
2515	O	3.082314	-0.567691	-0.062484	
2516	O	-3.453504	0.041539	-0.254464	
2517	H	-2.198295	0.469898	1.351149	
2518	H	-1.236164	-0.785712	-1.263260	
2519	H	0.141500	-0.028243	1.412508	
2520	H	0.660147	-1.356295	0.376634	
2521	H	1.244648	0.273692	-1.427997	
2522	H	0.830008	1.604246	-0.313275	
2523	H	-4.122658	0.379656	0.342337	
2524	Rotational constants (GHz):			13.3164800	0.8817100 0.8703500
2525	Vibrational harmonic frequencies (cm-1):				
2526		68.0919	72.1152		131.6989
2527		167.9317	240.6208		305.5826
2528		330.2599	384.9810		534.3830
2529		612.6315	793.2149		862.2344
2530		970.0369	973.8711		1011.7579
2531		1068.5068	1129.8299		1178.0602
2532		1214.5548	1242.4344		1280.3932
2533		1305.1409	1331.0117		1354.6634
2534		1382.6060	1408.1982		1484.8761
2535		1499.3454	1785.4662		3065.4744
2536		3093.5087	3110.7624		3157.8435
2537		3168.6656	3184.8947		3916.5030
2538	Zero-point correction (Hartree): 0.111225				
2539	HOCHCH2CH200.Elttc				
2541	~~~~~				
2542	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14004222				
2543	Electronic state : 2-A				
2544	Cartesian coordinates (Angs):				
2545	C	-2.275809	0.148690	-0.367891	
2546	C	-1.260724	0.112279	0.484643	
2547	C	0.071423	0.733498	0.193929	
2548	C	1.150763	-0.325924	0.094412	
2549	O	2.412869	0.349900	-0.093776	

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2550      O      3.395681      -0.491871      -0.180792
2551      O      -3.506287      -0.390315      -0.187617
2552      H      -2.204780      0.644611      -1.328060
2553      H      -1.382734      -0.396042      1.437314
2554      H      0.028218      1.293552      -0.740915
2555      H      0.348530      1.438096      0.981051
2556      H      1.231526      -0.919900      1.004892
2557      H      0.998327      -0.988116      -0.756826
2558      H      -3.551102      -0.825174      0.669474
2559      Rotational constants (GHz): 13.6874400      0.8329600      0.8191700
2560      Vibrational harmonic frequencies (cm-1):
2561      60.8092      90.3699      93.3198
2562      165.2775      280.7597      313.8347
2563      355.1919      453.9746      528.9095
2564      593.7630      785.7557      851.2485
2565      989.6390      993.0427      1029.7627
2566      1104.1590      1122.0018      1159.0048
2567      1206.0828      1269.0806      1294.2590
2568      1309.3283      1318.2802      1346.6675
2569      1397.3583      1419.6101      1490.8330
2570      1507.2386      1765.0976      3063.5670
2571      3084.8968      3108.9567      3144.2032
2572      3154.2420      3207.2976      3859.5147
2573      Zero-point correction (Hartree): 0.111442
2574
2575      HOCHCHCH2CH2OO.Elttt
2576      ~~~~~
2577      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13833875
2578      Electronic state : 2-A
2579      Cartesian coordinates (Angs):
2580      C      -2.273429      0.105513      -0.345910
2581      C      -1.250519      0.154109      0.492492
2582      C      0.075477      0.744656      0.126087
2583      C      1.158404      -0.315660      0.135892
2584      O      2.416046      0.340116      -0.137218
2585      O      3.400500      -0.503981      -0.153931
2586      O      -3.469088      -0.443689      0.003341
2587      H      -2.206311      0.507793      -1.351936
2588      H      -1.375714      -0.260890      1.486384
2589      H      0.027645      1.201252      -0.863577
2590      H      0.354735      1.529938      0.832104
2591      H      1.248309      -0.804624      1.105828
2592      H      1.003251      -1.068940      -0.635313
2593      H      -4.091178      -0.375805      -0.722381
2594      Rotational constants (GHz): 13.8484500      0.8326000      0.8185100
2595      Vibrational harmonic frequencies (cm-1):
2596      57.7469      90.3574      103.0039
2597      158.1623      229.2563      299.1034
2598      314.3737      359.8705      526.9658
2599      590.0482      784.7093      863.0777
2600      967.4995      986.9136      1029.3380
2601      1103.2365      1124.1121      1179.2551
2602      1199.0412      1244.0592      1293.4717
2603      1302.6613      1312.7888      1355.5095
2604      1382.0788      1415.5474      1491.3168
2605      1507.2022      1788.3995      3061.7607
2606      3086.0660      3106.1688      3145.2990
2607      3169.8118      3184.8758      3916.9350
2608      Zero-point correction (Hartree): 0.111015
2609
2610
2611      TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Ec.b
2612      ~~~~~
2613      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.10724016
2614      Electronic state : 2-A
2615      Cartesian coordinates (Angs):
2616      C      1.217486      0.279742      0.364305
2617      C      0.341773      1.097742      -0.320596
2618      C      -1.027092      1.246613      0.229747
2619      C      -1.844235      -0.064593      -0.045476
2620      O      -0.992753      -1.095210      -0.485394
2621      O      0.005605      -1.255843      0.439528

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2622      O      2.391428      -0.139894      -0.136307
2623      H      1.213890      0.247341      1.445253
2624      H      0.518331      1.286381      -1.373712
2625      H      -0.974047      1.394725      1.307886
2626      H      -1.549034      2.096788      -0.204608
2627      H      -2.361650      -0.370132      0.865237
2628      H      -2.563582      0.066706      -0.852405
2629      H      2.354263      -0.151259      -1.098142
2630      Rotational constants (GHz):      4.7724200      2.2768000      1.7445200
2631      Vibrational harmonic frequencies (cm-1):
2632      i685.0331      79.5739      248.9258
2633      266.7727      368.0530      402.7393
2634      421.1075      441.7393      542.8748
2635      651.4000      781.5885      819.2272
2636      891.5753      903.7398      977.2995
2637      1039.4828      1100.8839      1133.4693
2638      1159.3361      1225.4296      1268.0599
2639      1279.5097      1296.2485      1321.3174
2640      1371.2509      1405.3781      1487.8162
2641      1504.3742      1563.6009      3068.4393
2642      3087.8182      3127.3766      3146.3952
2643      3173.8162      3211.4429      3854.2426
2644      Zero-point correction (Hartree): 0.110770
2645
2646      TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Ec
2647      ~~~~~
2648      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.57644612
2649      E(CCSD/Aug-CC-pVTZ) (Hartree): -381.50999223
2650      T1 diagnostic: 0.028421
2651      E(MP2/Aug-CC-pVTZ) (Hartree): -381.46077651
2652      E(MP3/Aug-CC-pVTZ) (Hartree): -381.49072084
2653      E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47834524
2654      E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50387730
2655      E(PUHF/Aug-CC-pVTZ) (Hartree): -380.10921509
2656      E(UHF/Aug-CC-pVTZ) (Hartree): -380.08883155
2657      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11687402
2658      Electronic state : 2-A
2659      Cartesian coordinates (Angs):
2660      C      1.155879      0.174702      0.396882
2661      C      0.378016      1.143937      -0.200909
2662      C      -1.050426      1.263609      0.187134
2663      C      -1.791931      -0.024462      -0.246750
2664      O      -1.122666      -1.127408      0.316294
2665      O      0.084327      -1.281446      -0.319510
2666      O      2.404324      -0.122337      0.004603
2667      H      0.959046      -0.158255      1.406366
2668      H      0.705464      1.550892      -1.151471
2669      H      -1.160467      1.353572      1.268525
2670      H      -1.521335      2.128324      -0.278811
2671      H      -2.806017      -0.050121      0.151243
2672      H      -1.807149      -0.117482      -1.333491
2673      H      2.553350      0.195881      -0.891592
2674      Rotational constants (GHz):      4.8099700      2.3018300      1.7081900
2675      Vibrational harmonic frequencies (cm-1):
2676      i612.2148      155.8931      259.5245
2677      308.9601      339.9696      400.6085
2678      432.1901      440.3496      541.4172
2679      590.7723      747.5627      862.9943
2680      933.5439      972.9901      987.3404
2681      1024.8407      1090.4612      1128.1823
2682      1165.3542      1214.9112      1262.3010
2683      1277.6477      1318.6330      1327.6199
2684      1367.9829      1403.7461      1484.0993
2685      1488.6522      1571.1142      3073.6098
2686      3076.3357      3128.1857      3139.6010
2687      3172.6958      3222.8911      3853.6386
2688      Zero-point correction (Hartree): 0.111099
2689
2690      TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Et.b
2691      ~~~~~
2692      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.10677807
2693      Electronic state : 2-A

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2694 Cartesian coordinates (Angs):
2695 C 1.214263 0.289700 0.332681
2696 C 0.326195 1.114648 -0.316324
2697 C -1.033088 1.235463 0.261697
2698 C -1.845033 -0.070021 -0.053565
2699 O -0.991057 -1.100931 -0.491333
2700 O 0.004584 -1.260867 0.433509
2701 O 2.353683 -0.063418 -0.294347
2702 H 1.212212 0.218401 1.414086
2703 H 0.498114 1.324250 -1.363766
2704 H -0.967915 1.341177 1.344097
2705 H -1.571161 2.095330 -0.132183
2706 H -2.385987 -0.385297 0.840440
2707 H -2.544451 0.076333 -0.875285
2708 H 2.847487 -0.687210 0.243044
2709 Rotational constants (GHz): 4.7508600 2.2809700 1.7416400
2710 Vibrational harmonic frequencies (cm-1):
2711 1672.3229 91.4225 248.4742
2712 275.6830 318.7083 368.7678
2713 416.8751 431.7870 540.0841
2714 655.4871 795.1183 823.1929
2715 885.9184 903.5206 972.9894
2716 1036.2457 1094.7108 1133.0696
2717 1177.5571 1217.2911 1251.4219
2718 1276.5256 1297.2793 1318.4758
2719 1357.5098 1390.8892 1487.3773
2720 1503.7334 1588.4282 3065.0986
2721 3087.2872 3126.5789 3145.9153
2722 3174.3288 3205.5509 3893.7939
2723 Zero-point correction (Hartree): 0.110621
2724
2725 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Et
2726 ~~~~~
2727 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -381.57685956
2728 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -381.51053770
2729 T1 diagnostic: 0.028927
2730 E(MP2/Aug-CC-pVTZ) (Hartree): -381.46051972
2731 E(MP3/Aug-CC-pVTZ) (Hartree): -381.49081210
2732 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47833678
2733 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50423593
2734 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.11048561
2735 E(UHF/Aug-CC-pVTZ) (Hartree): -380.08990202
2736 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11743003
2737 Electronic state : 2-A
2738 Cartesian coordinates (Angs):
2739 C 1.147043 0.214569 0.362170
2740 C 0.350660 1.166516 -0.223427
2741 C -1.071962 1.255057 0.192903
2742 C -1.791056 -0.052670 -0.223763
2743 O -1.091404 -1.144407 0.327652
2744 O 0.098491 -1.285160 -0.343113
2745 O 2.388067 0.005591 -0.115672
2746 H 0.939296 -0.138660 1.365124
2747 H 0.673943 1.583833 -1.167781
2748 H -1.167356 1.347532 1.275518
2749 H -1.573728 2.104419 -0.268728
2750 H -2.797301 -0.098079 0.192044
2751 H -1.822870 -0.148961 -1.309517
2752 H 2.778671 -0.759101 0.315106
2753 Rotational constants (GHz): 4.7651800 2.3156100 1.7036200
2754 Vibrational harmonic frequencies (cm-1):
2755 1590.6847 159.4186 269.6552
2756 294.5891 342.8123 374.2063
2757 399.9901 435.6672 538.4892
2758 595.4815 773.5039 860.5234
2759 934.0770 971.0382 982.5272
2760 1020.8763 1084.1233 1128.2875
2761 1182.8838 1208.9500 1256.2854
2762 1265.7570 1319.9350 1332.9792
2763 1358.1819 1384.0530 1483.8822
2764 1488.5767 1600.3175 3075.6803
2765 3076.1514 3129.3890 3140.5615

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2766          3185.3172          3208.4006          3884.7204
2767 Zero-point correction (Hartree): 0.111054
2768
2769
2770 #####
2771 Z-HOCH=CHCH2CH2OO ring closure
2772 #####
2773
2774 HOCHCHCH2CH2OO.Zcptt
2775 ~~~~~
2776 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13711336
2777 Electronic state : 2-A
2778 Cartesian coordinates (Angs):
2779 C      -1.776794      -0.554659      -0.256263
2780 C      -1.493800      0.732244      -0.393931
2781 C      -0.341202      1.507229      0.179422
2782 C      0.865022      0.702094      0.611509
2783 O      1.362636      0.001504      -0.550034
2784 O      2.306136      -0.829333      -0.236274
2785 O      -1.045956      -1.415474      0.509502
2786 H      -2.641959      -0.983117      -0.748092
2787 H      -2.189973      1.293835      -1.001782
2788 H      -0.017457      2.242074      -0.560669
2789 H      -0.672659      2.085016      1.047217
2790 H      1.667247      1.352616      0.959066
2791 H      0.637097      -0.043564      1.366069
2792 H      -1.284185      -2.321888      0.308221
2793 Rotational constants (GHz): 3.9278800      2.0404800      1.5310900
2794 Vibrational harmonic frequencies (cm-1):
2795 45.9236      64.9179      135.0800
2796 247.0910      265.4998      269.3807
2797 385.3755      449.8302      535.0364
2798 742.0012      759.3706      851.3365
2799 877.4570      975.0962      1014.7206
2800 1055.0647      1080.1995      1130.9052
2801 1232.4978      1259.8112      1284.3392
2802 1303.6282      1317.0023      1385.4671
2803 1420.2666      1446.4422      1472.3424
2804 1505.9929      1788.8382      3052.2248
2805 3086.2696      3096.1607      3178.5278
2806 3182.7917      3214.4693      3910.7664
2807 Zero-point correction (Hartree): 0.111681
2808
2809 HOCHCHCH2CH2OO.Zcptt
2810 ~~~~~
2811 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13858979
2812 Electronic state : 2-A
2813 Cartesian coordinates (Angs):
2814 C      2.258555      0.186620      -0.159502
2815 C      1.324382      1.115087      -0.020896
2816 C      -0.138910      0.947789      0.264829
2817 C      -0.670348      -0.470054      0.176316
2818 O      -2.097451      -0.455162      0.413555
2819 O      -2.742614      0.049252      -0.592871
2820 O      2.019007      -1.155385      -0.046563
2821 H      3.284895      0.462810      -0.367898
2822 H      1.671553      2.134578      -0.122294
2823 H      -0.365199      1.344959      1.258467
2824 H      -0.708414      1.553057      -0.443552
2825 H      -0.503577      -0.913031      -0.802703
2826 H      -0.273150      -1.120533      0.949555
2827 H      2.820279      -1.648133      -0.229019
2828 Rotational constants (GHz): 6.2539000      1.3314300      1.1658700
2829 Vibrational harmonic frequencies (cm-1):
2830 21.5428      88.9392      136.3872
2831 180.6831      222.3307      282.7500
2832 372.7885      454.7840      567.1876
2833 745.0536      765.6149      806.7722
2834 929.2624      975.1060      977.1411
2835 1054.0019      1098.4514      1128.5862
2836 1236.7695      1247.2451      1290.1310
2837 1310.8892      1328.5947      1348.8740

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2838      1422.8371          1441.6560          1484.8573
2839      1496.2722          1791.5757          3050.7558
2840      3091.2172          3117.6643          3185.2642
2841      3187.6863          3213.3065          3917.4230
2842 Zero-point correction (Hartree): 0.111563
2843
2844 HOCHCHCH2CH2OO.Zcttc
2845 ~~~~~
2846 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13442233
2847 Point group : CS
2848 Electronic state : 2-A''
2849 Cartesian coordinates (Angs):
2850      C      -0.377205      -2.307271      0.000000
2851      C      0.796415      -1.684238      0.000000
2852      C      1.154718      -0.224566      0.000000
2853      C      -0.000000      0.750786      0.000000
2854      O      0.571304      2.076013      0.000000
2855      O      -0.349166      2.989418      0.000000
2856      O      -1.641430      -1.809192      0.000000
2857      H      -0.408505      -3.388123      0.000000
2858      H      1.648626      -2.350758      0.000000
2859      H      1.777089      -0.010247      0.872495
2860      H      1.777089      -0.010247     -0.872495
2861      H      -0.617134      0.675760     -0.897332
2862      H      -0.617134      0.675760      0.897332
2863      H      -1.649264      -0.850327      0.000000
2864 Rotational constants (GHz):      5.8449000      1.2754700      1.0608800
2865 Vibrational harmonic frequencies (cm-1):
2866      43.1149 ( A'')      81.4073 ( A'')      129.0539 ( A')
2867      149.1265 ( A'')      268.3374 ( A')      311.4776 ( A'')
2868      379.5594 ( A')      482.1220 ( A'')      508.2954 ( A')
2869      751.1183 ( A'')      767.0594 ( A')      814.7686 ( A'')
2870      913.8562 ( A')      1003.6698 ( A'')      1031.8930 ( A')
2871      1073.4671 ( A')      1088.9370 ( A'')      1145.5511 ( A')
2872      1230.7542 ( A')      1253.1947 ( A'')      1290.3416 ( A')
2873      1317.5934 ( A'')      1342.4242 ( A')      1362.1290 ( A')
2874      1427.3542 ( A')      1444.3698 ( A')      1497.6006 ( A')
2875      1532.5811 ( A')      1767.2677 ( A')      3052.1786 ( A')
2876      3061.3874 ( A')      3082.0577 ( A'')      3121.4614 ( A'')
2877      3196.9164 ( A')      3224.9995 ( A')      3910.9139 ( A')
2878 Zero-point correction (Hartree): 0.111763
2879
2880 HOCHCHCH2CH2OO.Zcttt
2881 ~~~~~
2882 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13769930
2883 Point group : CS
2884 Electronic state : 2-A''
2885 Cartesian coordinates (Angs):
2886      C      -0.410643      -2.264632      0.000000
2887      C      0.790060      -1.705198      0.000000
2888      C      1.158136      -0.250913      0.000000
2889      C      0.000000      0.723795      0.000000
2890      O      0.595745      2.042813      0.000000
2891      O      -0.306243      2.973965      0.000000
2892      O      -1.579759      -1.557348      0.000000
2893      H      -0.514846      -3.342783      0.000000
2894      H      1.619897      -2.399009      0.000000
2895      H      1.783976      -0.042358      0.871782
2896      H      1.783976      -0.042358     -0.871782
2897      H      -0.624334      0.644558     -0.886550
2898      H      -0.624334      0.644558      0.886550
2899      H      -2.327588      -2.156356      0.000000
2900 Rotational constants (GHz):      5.8453500      1.3275400      1.0964700
2901 Vibrational harmonic frequencies (cm-1):
2902      17.2363 ( A'')      78.2270 ( A'')      128.1975 ( A'')
2903      138.3477 ( A')      253.4598 ( A')      270.7581 ( A'')
2904      380.3751 ( A')      456.1568 ( A'')      510.4761 ( A')
2905      745.6136 ( A'')      770.0082 ( A')      803.5707 ( A'')
2906      930.3358 ( A')      978.1798 ( A'')      1016.3361 ( A')
2907      1069.1464 ( A')      1076.6634 ( A'')      1144.0290 ( A')
2908      1221.3629 ( A'')      1252.0845 ( A')      1299.7341 ( A')
2909      1314.2764 ( A')      1315.9130 ( A'')      1340.0882 ( A')

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2910      1428.7474 ( A')          1443.9492 ( A')          1493.9967 ( A')
2911      1503.7163 ( A')          1792.5665 ( A')          3051.8416 ( A')
2912      3079.8236 ( A'')         3111.9295 ( A')          3171.9629 ( A'')
2913      3187.6752 ( A')          3213.1564 ( A')          3916.7245 ( A')
2914 Zero-point correction (Hartree): 0.111418
2915
2916 HOCHCHCH2CH2OO.Zgpmc
2917 ~~~~~
2918 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14139996
2919 Electronic state : 2-A
2920 Cartesian coordinates (Angs):
2921 C      -1.737468      -0.146900      0.370704
2922 C      -0.997116      0.936025      0.587248
2923 C      0.077260      1.427802     -0.337557
2924 C      1.434514      0.783067     -0.094846
2925 O      1.333949     -0.627424     -0.393721
2926 O      1.297258     -1.365867      0.677108
2927 O     -1.644538     -0.999462     -0.676321
2928 H     -2.531448     -0.435613      1.045857
2929 H     -1.192722      1.491430      1.493099
2930 H     -0.201334      1.255270     -1.380993
2931 H      0.200699      2.505915     -0.228546
2932 H      2.192512      1.171852     -0.773936
2933 H      1.761229      0.867044      0.938717
2934 H     -0.785432     -0.913843     -1.104020
2935 Rotational constants (GHz):      3.6140200      2.2889700      1.7079300
2936 Vibrational harmonic frequencies (cm-1):
2937      58.2574          93.1132          123.1605
2938      232.3401         265.0035         361.0549
2939      456.4881         524.6469         582.7744
2940      657.9690         761.3718         837.5371
2941      919.5851         981.6888         992.3137
2942     1035.9988        1083.2694        1141.7043
2943     1223.1119        1228.6007        1276.7832
2944     1312.6929        1350.0219        1370.6682
2945     1383.0603        1438.3066        1483.6831
2946     1488.0368        1742.8540        3054.4239
2947     3091.7480        3110.0397        3163.6564
2948     3210.9156        3231.1092        3838.7502
2949 Zero-point correction (Hartree): 0.111873
2950
2951 HOCHCHCH2CH2OO.Zgppt
2952 ~~~~~
2953 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13954204
2954 Electronic state : 2-A
2955 Cartesian coordinates (Angs):
2956 C      1.914859      0.090571     -0.431387
2957 C      0.985666      1.025018     -0.298066
2958 C     -0.116046      0.973688      0.714388
2959 C     -1.485281      0.843125      0.071006
2960 O     -1.596557     -0.397079     -0.661614
2961 O     -1.635879     -1.415766      0.141001
2962 O      1.969504     -0.998001      0.385586
2963 H      2.684108      0.156570     -1.191408
2964 H      1.022074      1.860050     -0.985306
2965 H      0.028552      0.133836      1.392152
2966 H     -0.126916      1.885411      1.316826
2967 H     -2.284305      0.853205      0.810695
2968 H     -1.659541      1.610620     -0.682013
2969 H      2.644287     -1.607334      0.083620
2970 Rotational constants (GHz):      4.1422700      1.8180600      1.4550000
2971 Vibrational harmonic frequencies (cm-1):
2972      28.3230          59.2797          144.7891
2973     214.5535         252.6226         295.0937
2974     378.7974         519.7864         568.4510
2975     668.2856         766.4669         861.6718
2976     890.9170         973.7082         995.9278
2977    1047.5808        1076.0585        1148.4667
2978    1215.0584        1257.7825        1277.3019
2979    1296.0053        1313.5432        1357.1520
2980    1398.7465        1444.7125        1481.0926
2981    1490.7725        1785.2217        3064.5679

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2982      3089.8000      3132.9715      3151.1366
2983      3184.5111      3210.8037      3919.8909
2984 Zero-point correction (Hartree): 0.111543
2985
2986 HOCHCHCH2CH2OO.Zgptc
2987 ~~~~~
2988 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14241976
2989 Electronic state : 2-A
2990 Cartesian coordinates (Angs):
2991 C      1.897914      -0.385648      -0.365766
2992 C      1.383603      0.840262      -0.401496
2993 C      0.264452      1.332044      0.474141
2994 C     -1.122747      0.977069      -0.024651
2995 O     -1.262451      -0.455486      0.137606
2996 O     -2.386318      -0.899974      -0.330991
2997 O      1.496806      -1.417339      0.410545
2998 H      2.743478      -0.659416      -0.982587
2999 H      1.826601      1.532954      -1.102642
3000 H      0.369226      0.941970      1.491084
3001 H      0.315083      2.417337      0.557387
3002 H     -1.913850      1.441070      0.563359
3003 H     -1.261010      1.196692      -1.081776
3004 H      0.596840      -1.270578      0.724538
3005 Rotational constants (GHz):  4.0906500      1.8775300      1.4146100
3006 Vibrational harmonic frequencies (cm-1):
3007      68.9838      87.6903      136.6126
3008      229.9296      265.9066      335.7055
3009      440.9411      503.4870      609.9387
3010      656.8277      765.8418      844.7707
3011      899.0257      994.9890      1024.7678
3012      1053.7330      1087.6190      1138.3086
3013      1222.6732      1254.0154      1290.0043
3014      1295.5010      1353.6839      1378.2692
3015      1396.6054      1439.7699      1481.4740
3016      1500.2293      1746.2514      3053.1188
3017      3087.8198      3118.3686      3150.7968
3018      3205.2596      3225.7012      3823.1965
3019 Zero-point correction (Hartree): 0.112013
3020
3021 HOCHCHCH2CH2OO.Zgmtt
3022 ~~~~~
3023 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14019926
3024 Electronic state : 2-A
3025 Cartesian coordinates (Angs):
3026 C      2.270326      -0.081809      0.116109
3027 C      1.368345      -1.008545      -0.173754
3028 C     -0.033049      -0.679805      -0.596835
3029 C     -0.912228      -0.443690      0.621475
3030 O     -2.280375      -0.204704      0.228308
3031 O     -2.418909      0.964599      -0.318224
3032 O      1.972686      1.245837      0.034722
3033 H      3.276542      -0.331255      0.429921
3034 H      1.665202      -2.041996      -0.067885
3035 H     -0.047455      0.226657      -1.201609
3036 H     -0.455768      -1.491488      -1.188285
3037 H     -0.964202      -1.321549      1.263055
3038 H     -0.572122      0.420624      1.189408
3039 H      2.750225      1.776249      0.214973
3040 Rotational constants (GHz):  5.5989900      1.3520200      1.1808600
3041 Vibrational harmonic frequencies (cm-1):
3042      43.3704      65.7348      120.2632
3043      202.9634      257.3635      286.3124
3044      355.0370      527.0481      572.4761
3045      679.5690      764.8308      817.1081
3046      959.4980      972.6762      985.8933
3047      1066.5337      1079.6370      1137.5424
3048      1223.2900      1259.5267      1290.9339
3049      1294.5599      1306.4462      1335.8659
3050      1399.4687      1434.0395      1485.8825
3051      1502.2942      1772.3973      3082.3660
3052      3098.7856      3130.6060      3162.4014
3053      3191.4227      3226.1186      3915.6145

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3054 Zero-point correction (Hartree): 0.111644
3055
3056 HOCHCHCH2CH2OO.Zgtpc
3057 ~~~~~
3058 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14075752
3059 Electronic state : 2-A
3060 Cartesian coordinates (Angs):
3061 C -2.374942 0.337594 0.155917
3062 C -1.213663 0.969303 0.026282
3063 C 0.051787 0.353347 -0.491740
3064 C 0.940906 -0.095044 0.658214
3065 O 2.162758 -0.680760 0.162951
3066 O 2.948064 0.222433 -0.339989
3067 O -2.645564 -0.950933 -0.168538
3068 H -3.253375 0.830196 0.548466
3069 H -1.180539 2.000982 0.346920
3070 H -0.142237 -0.503852 -1.142065
3071 H 0.609705 1.072998 -1.090594
3072 H 1.211162 0.739468 1.303249
3073 H 0.474510 -0.883184 1.247021
3074 H -1.865818 -1.373723 -0.540433
3075 Rotational constants (GHz): 7.9091100 1.1060900 1.0406700
3076 Vibrational harmonic frequencies (cm-1):
3077 27.6412 67.0647 124.0091
3078 202.9161 276.6980 353.9663
3079 400.0936 544.5398 578.0624
3080 659.8564 773.9056 803.7664
3081 971.0301 980.5378 995.6468
3082 1062.8364 1078.2751 1139.3897
3083 1219.6081 1248.4100 1274.1562
3084 1303.1465 1327.5545 1348.3426
3085 1397.1146 1436.2636 1488.9787
3086 1512.6791 1754.1465 3055.7317
3087 3094.2064 3114.3684 3156.7534
3088 3212.0556 3233.4812 3862.2667
3089 Zero-point correction (Hartree): 0.111811
3090
3091 HOCHCHCH2CH2OO.Zgtpt
3092 ~~~~~
3093 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14074793
3094 Electronic state : 2-A
3095 Cartesian coordinates (Angs):
3096 C -2.324227 0.311436 0.177412
3097 C -1.219788 1.035274 0.068940
3098 C 0.059043 0.494489 -0.498552
3099 C 0.866340 -0.199202 0.587154
3100 O 2.103565 -0.717299 0.053086
3101 O 2.945104 0.237649 -0.200539
3102 O -2.363701 -0.988806 -0.234841
3103 H -3.239998 0.710018 0.596257
3104 H -1.251137 2.050569 0.437250
3105 H -0.153083 -0.226551 -1.288160
3106 H 0.664985 1.295553 -0.919357
3107 H 1.120232 0.478128 1.401064
3108 H 0.342422 -1.072435 0.970777
3109 H -3.251384 -1.339617 -0.149199
3110 Rotational constants (GHz): 7.5430100 1.1750500 1.0826100
3111 Vibrational harmonic frequencies (cm-1):
3112 24.4640 68.1809 125.1362
3113 203.0655 252.2195 270.6904
3114 363.9977 526.6943 578.7486
3115 676.4526 766.1211 809.5074
3116 966.7978 974.4646 988.3892
3117 1065.2591 1078.1403 1135.2163
3118 1225.4347 1262.0164 1288.1527
3119 1294.5643 1310.5307 1334.8408
3120 1397.7532 1434.8279 1485.8232
3121 1501.1418 1774.3630 3082.8514
3122 3097.4074 3132.3512 3162.7554
3123 3193.8803 3228.2664 3916.4641
3124 Zero-point correction (Hartree): 0.111623
3125

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3126 HOCHCHCH2CH2OO.Zgttc
3127 ~~~~~
3128 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13967776
3129 Electronic state : 2-A
3130 Cartesian coordinates (Angs):
3131 C 2.398795 0.120656 -0.319230
3132 C 1.388901 0.958388 -0.113563
3133 C 0.123169 0.616565 0.617809
3134 C -0.960737 0.190896 -0.354749
3135 O -2.151912 -0.090414 0.411191
3136 O -3.129570 -0.472234 -0.351222
3137 O 2.490714 -1.166102 0.096813
3138 H 3.285422 0.415956 -0.862452
3139 H 1.484300 1.951272 -0.529376
3140 H 0.277657 -0.180984 1.349411
3141 H -0.228776 1.479200 1.183930
3142 H -1.203033 0.978332 -1.067333
3143 H -0.693941 -0.714815 -0.898969
3144 H 1.703757 -1.418004 0.588932
3145 Rotational constants (GHz): 7.1967100 1.0749200 1.0053600
3146 Vibrational harmonic frequencies (cm-1):
3147 27.6140 75.3062 103.2976
3148 164.6930 279.9752 327.4172
3149 409.5551 486.7181 584.7638
3150 659.6895 772.5865 798.5818
3151 963.9454 998.3189 1023.3267
3152 1066.5952 1102.6237 1135.4684
3153 1203.3977 1251.5210 1290.0301
3154 1301.4801 1310.1920 1349.7321
3155 1403.9103 1437.3067 1501.7698
3156 1515.9947 1754.9348 3056.6056
3157 3086.3611 3107.6039 3144.8072
3158 3213.9386 3234.4311 3863.8149
3159 Zero-point correction (Hartree): 0.111649
3160
3161 HOCHCHCH2CH2OO.Zgttt
3162 ~~~~~
3163 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13973051
3164 Electronic state : 2-A
3165 Cartesian coordinates (Angs):
3166 C 2.351439 0.076127 -0.312571
3167 C 1.403691 0.990183 -0.166351
3168 C 0.127070 0.732235 0.579489
3169 C -0.917596 0.150776 -0.353388
3170 O -2.130330 -0.040952 0.408884
3171 O -3.082366 -0.527365 -0.325056
3172 O 2.223606 -1.171407 0.223381
3173 H 3.264418 0.272205 -0.861180
3174 H 1.560642 1.950948 -0.635060
3175 H 0.303140 0.027431 1.391986
3176 H -0.254728 1.656223 1.013054
3177 H -1.154796 0.818428 -1.180964
3178 H -0.613335 -0.819983 -0.742173
3179 H 3.019754 -1.683391 0.073604
3180 Rotational constants (GHz): 6.8219700 1.1327600 1.0449100
3181 Vibrational harmonic frequencies (cm-1):
3182 17.7531 75.6068 100.6331
3183 163.6008 251.6023 256.2517
3184 357.1504 470.8270 578.0969
3185 671.1409 764.7380 804.8320
3186 967.3141 972.8733 1022.0913
3187 1068.3820 1103.5542 1130.0493
3188 1208.6234 1269.6215 1292.2993
3189 1293.7736 1312.5331 1316.4638
3190 1403.7061 1435.9979 1494.8269
3191 1505.7502 1776.5340 3080.9903
3192 3090.6090 3125.2729 3151.1963
3193 3192.8048 3228.0659 3916.2471
3194 Zero-point correction (Hartree): 0.111338
3195
3196 HOCHCHCH2CH2OO.Zlmmc
3197 ~~~~~

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3198 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13994056
3199 Electronic state : 2-A
3200 Cartesian coordinates (Angs):
3201 C 2.143768 -0.664679 0.139343
3202 C 0.823500 -0.626813 0.007766
3203 C 0.009027 0.560010 -0.410802
3204 C -1.165145 0.807557 0.521676
3205 O -2.073223 -0.316307 0.501905
3206 O -2.704934 -0.391193 -0.629406
3207 O 3.028093 0.339703 -0.091022
3208 H 2.655945 -1.560534 0.461000
3209 H 0.286885 -1.541015 0.221674
3210 H 0.598678 1.479894 -0.427379
3211 H -0.393321 0.426727 -1.417786
3212 H -0.850580 0.878497 1.561091
3213 H -1.737194 1.687549 0.232840
3214 H 2.573202 1.114817 -0.431159
3215 Rotational constants (GHz): 8.3236200 1.1198900 1.0759200
3216 Vibrational harmonic frequencies (cm-1):
3217 17.6350 67.8239 141.9868
3218 214.7837 252.1685 318.5315
3219 428.7667 524.9213 588.2432
3220 647.9435 778.0323 823.9482
3221 899.4037 997.0807 1004.6641
3222 1043.3525 1106.6705 1128.8582
3223 1219.1224 1238.5768 1279.6884
3224 1305.2664 1337.6068 1369.0230
3225 1397.5003 1441.7449 1472.6402
3226 1491.9527 1760.7025 3057.5479
3227 3090.4578 3101.2578 3159.9774
3228 3209.5933 3231.4405 3876.0568
3229 Zero-point correction (Hartree): 0.111687
3230
3231 HOCHCHCH2CH2OO.Zlmmt
3232 ~~~~~
3233 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14069596
3234 Electronic state : 2-A
3235 Cartesian coordinates (Angs):
3236 C -2.088309 -0.661230 -0.159614
3237 C -0.799558 -0.727793 0.137412
3238 C 0.004714 0.427704 0.647944
3239 C 1.058514 0.886017 -0.344729
3240 O 1.993842 -0.180062 -0.630865
3241 O 2.748805 -0.433773 0.393502
3242 O -2.807425 0.491902 -0.019341
3243 H -2.635411 -1.519816 -0.529306
3244 H -0.303212 -1.676494 -0.011978
3245 H -0.647327 1.274451 0.860453
3246 H 0.514923 0.159490 1.574692
3247 H 0.624742 1.125067 -1.313747
3248 H 1.637611 1.726756 0.033916
3249 H -3.725278 0.337827 -0.246486
3250 Rotational constants (GHz): 8.0364600 1.1756500 1.1218800
3251 Vibrational harmonic frequencies (cm-1):
3252 23.9377 62.4069 135.4223
3253 205.8432 253.4339 279.2227
3254 389.6089 524.3234 602.4719
3255 656.0122 778.7954 827.2330
3256 890.9544 976.7741 1004.8483
3257 1048.0315 1099.1372 1132.7352
3258 1211.3681 1247.2811 1294.7766
3259 1300.3257 1305.2226 1357.3751
3260 1392.5991 1444.6908 1480.8993
3261 1489.5894 1781.4930 3077.5404
3262 3094.8937 3130.4073 3159.1728
3263 3191.1439 3224.0324 3920.0462
3264 Zero-point correction (Hartree): 0.111617
3265
3266 HOCHCHCH2CH2OO.Zlmpc
3267 ~~~~~
3268 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13868808
3269 Electronic state : 2-A

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3270 Cartesian coordinates (Angs):
3271 C -1.989705 -0.744530 0.029943
3272 C -0.720256 -0.485431 0.318009
3273 C -0.087986 0.872455 0.366130
3274 C 1.236003 0.929434 -0.382633
3275 O 2.209234 0.096137 0.280618
3276 O 2.301386 -1.081886 -0.259005
3277 O -2.973361 0.146858 -0.259003
3278 H -2.368788 -1.756248 0.000843
3279 H -0.087874 -1.335139 0.534889
3280 H -0.728776 1.638039 -0.079650
3281 H 0.094512 1.182833 1.398414
3282 H 1.147655 0.572355 -1.406187
3283 H 1.661348 1.931503 -0.357447
3284 H -2.644486 1.046223 -0.180442
3285 Rotational constants (GHz): 6.7689600 1.2445200 1.1083900
3286 Vibrational harmonic frequencies (cm-1):
3287 18.0344 91.5867 105.7143
3288 226.4445 232.0717 322.9611
3289 433.7305 515.3716 568.8543
3290 651.4993 779.4896 844.9060
3291 878.1583 999.1262 1017.5783
3292 1051.9170 1093.4299 1129.7210
3293 1230.1992 1236.6756 1271.0215
3294 1318.5707 1345.2177 1372.6220
3295 1390.8427 1445.6145 1469.7737
3296 1485.7653 1760.8773 3047.9076
3297 3082.0069 3098.8408 3163.8554
3298 3211.9308 3234.1030 3877.2726
3299 Zero-point correction (Hartree): 0.111639
3300
3301 HOCHCHCH2CH200.Zlmp
3302 ~~~~~
3303 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13978773
3304 Electronic state : 2-A
3305 Cartesian coordinates (Angs):
3306 C -1.922704 -0.708652 0.104527
3307 C -0.703461 -0.461169 0.557734
3308 C -0.057498 0.888661 0.521306
3309 C 1.167248 0.936171 -0.379521
3310 O 2.204704 0.079601 0.144661
3311 O 2.144685 -1.121019 -0.347727
3312 O -2.709907 0.267767 -0.438055
3313 H -2.355496 -1.700688 0.142598
3314 H -0.144789 -1.293540 0.961654
3315 H -0.767207 1.631260 0.156524
3316 H 0.247172 1.192543 1.525260
3317 H 0.948198 0.597554 -1.389685
3318 H 1.610516 1.930687 -0.392956
3319 H -3.555761 -0.098666 -0.698706
3320 Rotational constants (GHz): 6.1146800 1.3366200 1.2016300
3321 Vibrational harmonic frequencies (cm-1):
3322 27.3716 88.2057 114.5263
3323 221.3444 238.6604 267.6976
3324 403.9375 513.5193 587.8196
3325 654.3555 781.7969 849.4386
3326 877.1053 977.9788 1013.9296
3327 1054.9938 1090.2377 1130.0488
3328 1216.4038 1236.8401 1291.6605
3329 1297.7336 1321.4059 1361.5667
3330 1385.6273 1446.8172 1479.1669
3331 1485.9362 1781.7754 3066.5438
3332 3096.1160 3123.3747 3162.6365
3333 3192.2612 3226.0934 3921.1846
3334 Zero-point correction (Hartree): 0.111599
3335
3336 HOCHCHCH2CH200.Zlmtc
3337 ~~~~~
3338 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13905289
3339 Electronic state : 2-A
3340 Cartesian coordinates (Angs):
3341 C -2.192234 -0.718371 -0.080291

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3342      C      -0.903735      -0.591983      0.212102
3343      C      -0.170168      0.700361      0.418640
3344      C      1.165032      0.721580     -0.299271
3345      O      1.997363      -0.285070      0.318060
3346      O      3.143934      -0.386438     -0.278970
3347      O     -3.107001      0.273427     -0.230218
3348      H     -2.647185     -1.686944     -0.232436
3349      H     -0.333417     -1.505117      0.311545
3350      H     -0.739251      1.555554      0.046180
3351      H      0.009899      0.884330      1.481313
3352      H      1.071934      0.464778     -1.353488
3353      H      1.680731      1.674843     -0.191820
3354      H     -2.710451      1.127670     -0.039355
3355      Rotational constants (GHz):      9.7604000      1.0288300      0.9728300
3356      Vibrational harmonic frequencies (cm-1):
3357          19.6535          66.5428          120.1996
3358          217.3154          241.8543          313.8582
3359          388.7097          501.0476          578.1024
3360          661.9453          779.6506          823.0225
3361          908.1268          998.9615         1044.1810
3362         1051.8555         1090.0733         1136.9804
3363         1229.3177         1236.2048         1287.8689
3364         1296.4890         1335.1353         1372.6237
3365         1400.6148         1444.0866         1469.3469
3366         1501.9053         1759.4537         3050.8456
3367         3083.3175         3094.3059         3148.6704
3368         3211.1193         3233.2802         3875.4610
3369      Zero-point correction (Hartree): 0.111567
3370
3371      HOCHCHCH2CH2OO.Zlmtt
3372      ~~~~~
3373      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14001114
3374      Electronic state : 2-A
3375      Cartesian coordinates (Angs):
3376      C      -2.129890      -0.693101      -0.078516
3377      C      -0.912971      -0.635025      0.440602
3378      C      -0.162846      0.640650      0.675647
3379      C      1.084324      0.746825     -0.178450
3380      O      1.976008     -0.318638      0.223395
3381      O      3.051639     -0.340873     -0.499865
3382      O     -2.819622      0.428371     -0.441076
3383      H     -2.637773     -1.636103     -0.239607
3384      H     -0.434511     -1.570323      0.694454
3385      H     -0.799649      1.494655      0.448190
3386      H      0.129922      0.721365      1.724899
3387      H      0.872470      0.609029     -1.237642
3388      H      1.616475      1.684755     -0.024412
3389      H     -3.682831      0.189645     -0.781210
3390      Rotational constants (GHz):      8.1761600      1.0884600      1.0485000
3391      Vibrational harmonic frequencies (cm-1):
3392          23.2548          68.7763          118.9651
3393          204.1627          245.2082          274.0911
3394          350.5013          480.3196          602.0876
3395          655.5972          780.3875          824.4920
3396          907.0490          976.6682         1041.0311
3397         1052.1215         1085.7309         1138.5377
3398         1217.7992         1245.1212         1293.7441
3399         1300.0195         1304.5116         1356.4493
3400         1395.4060         1446.1590         1480.4572
3401         1500.4784         1781.5388         3067.6293
3402         3086.9684         3129.9267         3147.0592
3403         3191.7444         3226.1869         3920.6148
3404      Zero-point correction (Hartree): 0.111450
3405
3406      HOCHCHCH2CH2OO.Zlpmt
3407      ~~~~~
3408      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13945018
3409      Electronic state : 2-A
3410      Cartesian coordinates (Angs):
3411      C      -1.792042      -0.245705      0.497000
3412      C      -0.763719      0.514753      0.840462
3413      C      0.080855      1.269692     -0.135131

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3414 C 1.532826 0.812047 -0.131362
3415 O 1.629254 -0.554384 -0.573924
3416 O 1.511557 -1.390915 0.414204
3417 O -2.197243 -0.376930 -0.798829
3418 H -2.365981 -0.794326 1.233637
3419 H -0.507953 0.557576 1.890440
3420 H -0.322875 1.165542 -1.141313
3421 H 0.084996 2.336127 0.106554
3422 H 2.127656 1.380476 -0.844490
3423 H 1.979199 0.862095 0.860435
3424 H -2.891109 -1.034385 -0.862684
3425 Rotational constants (GHz): 4.2484800 1.7298900 1.5147800
3426 Vibrational harmonic frequencies (cm-1):
3427 17.9802 96.2996 108.0144
3428 219.1300 246.6748 290.6683
3429 387.2275 523.5856 545.1065
3430 672.0064 766.3136 846.1595
3431 923.9577 971.3979 991.2150
3432 1047.3391 1068.3295 1149.5674
3433 1225.9786 1235.6111 1284.1883
3434 1297.3051 1318.1810 1360.7644
3435 1393.2404 1446.2410 1477.8737
3436 1486.1508 1782.0974 3058.1557
3437 3092.6592 3127.6936 3155.3540
3438 3189.6091 3217.7380 3919.5797
3439 Zero-point correction (Hartree): 0.111492
3440
3441 HOCHCH2CH200.Zlptt
3442 ~~~~~
3443 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13906481
3444 Electronic state : 2-A
3445 Cartesian coordinates (Angs):
3446 C -2.005846 -0.189901 0.557402
3447 C -1.055449 0.728700 0.636447
3448 C -0.149303 1.104773 -0.494933
3449 C 1.307147 0.824153 -0.185709
3450 O 1.465252 -0.607883 -0.080592
3451 O 2.673323 -0.927575 0.263857
3452 O -2.267356 -0.865206 -0.597161
3453 H -2.627361 -0.440774 1.408355
3454 H -0.920009 1.219966 1.591008
3455 H -0.434299 0.569448 -1.399886
3456 H -0.232266 2.172840 -0.710148
3457 H 1.972741 1.163634 -0.978403
3458 H 1.622660 1.253347 0.765125
3459 H -2.930518 -1.539498 -0.444117
3460 Rotational constants (GHz): 5.0261900 1.3870900 1.2335400
3461 Vibrational harmonic frequencies (cm-1):
3462 21.3258 66.7347 117.6948
3463 209.2188 235.3191 293.1693
3464 337.7011 470.2339 570.4101
3465 675.2776 764.1390 852.0397
3466 890.5305 971.6337 1039.7919
3467 1062.8667 1072.7564 1140.2453
3468 1216.0551 1265.2629 1288.7033
3469 1296.4313 1299.1031 1356.4039
3470 1399.5920 1448.0565 1478.8844
3471 1502.9722 1786.2420 3066.2634
3472 3082.7260 3125.5137 3141.4267
3473 3187.1186 3213.1129 3920.4763
3474 Zero-point correction (Hartree): 0.111324
3475
3476 HOCHCH2CH200.Zpmmc
3477 ~~~~~
3478 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.60037010
3479 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53772838
3480 T1 diagnostic: 0.022191
3481 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49448818
3482 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52479655
3483 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49774632
3484 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52669599
3485 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13149271

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3486 E(UHF/Aug-CC-pVTZ) (Hartree): -380.12616632
3487 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14414641
3488 Electronic state : 2-A
3489 Cartesian coordinates (Angs):
3490 C 1.838020 0.079555 0.342809
3491 C 1.016432 1.117681 0.218070
3492 C -0.200990 1.144807 -0.658951
3493 C -1.489617 0.807122 0.068881
3494 O -1.451380 -0.522535 0.649006
3495 O -1.199537 -1.432397 -0.236220
3496 O 1.729213 -1.129048 -0.251044
3497 H 2.725321 0.135368 0.959152
3498 H 1.258623 2.004009 0.787568
3499 H -0.332366 2.141817 -1.082837
3500 H -0.092628 0.466424 -1.506073
3501 H -1.657397 1.451712 0.929058
3502 H -2.353180 0.834791 -0.595467
3503 H 0.842185 -1.257284 -0.610196
3504 Rotational constants (GHz): 3.8427200 2.2415600 1.6192300
3505 Vibrational harmonic frequencies (cm-1):
3506 53.1930 131.5021 148.7968
3507 214.3796 291.8812 357.7868
3508 466.1477 541.8760 599.5496
3509 667.3210 761.4688 849.8795
3510 886.5390 981.9506 996.2389
3511 1037.1786 1088.8224 1148.0690
3512 1222.6972 1260.3105 1275.4686
3513 1306.3988 1351.2209 1373.7689
3514 1404.3696 1442.6719 1490.4872
3515 1495.2118 1747.8273 3075.1083
3516 3090.8924 3114.1355 3157.0129
3517 3205.6803 3226.0874 3797.6382
3518 Zero-point correction (Hartree): 0.112222
3519
3520 HOCHCHCH2CH2OO.Zptpc
3521 ~~~~~
3522 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14299943
3523 Electronic state : 2-A
3524 Cartesian coordinates (Angs):
3525 C 1.990719 -0.256495 0.149012
3526 C 1.485695 0.947781 -0.106531
3527 C 0.056334 1.134753 -0.529354
3528 C -0.937822 0.806510 0.595548
3529 O -2.050788 0.022964 0.099607
3530 O -1.651134 -1.141169 -0.305940
3531 O 1.331854 -1.432158 0.068728
3532 H 3.017806 -0.397564 0.456449
3533 H 2.133420 1.803863 0.003447
3534 H -0.110610 2.147300 -0.887896
3535 H -0.173160 0.466885 -1.364114
3536 H -0.471153 0.216023 1.382390
3537 H -1.404024 1.688816 1.026043
3538 H 0.398713 -1.317709 -0.167528
3539 Rotational constants (GHz): 4.3235600 1.9772300 1.4811700
3540 Vibrational harmonic frequencies (cm-1):
3541 86.7356 102.9580 196.4536
3542 219.3773 324.4331 366.9969
3543 522.0243 568.6202 624.7459
3544 707.6098 753.2826 813.2521
3545 954.6509 992.7960 1003.1022
3546 1032.6939 1079.1186 1135.4807
3547 1230.2006 1263.6910 1287.2719
3548 1308.1613 1339.8173 1375.1774
3549 1399.4617 1431.3431 1493.5697
3550 1509.4091 1733.6295 3059.1022
3551 3101.0760 3136.5884 3168.4579
3552 3216.8284 3242.0571 3721.9528
3553 Zero-point correction (Hartree): 0.112774
3554
3555
3556 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Zp
3557 ~~~~~

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3558 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.57530128
3559 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.50813416
3560 T1 diagnostic: 0.028163
3561 E(MP2/Aug-CC-pVTZ) (Hartree): -381.46065809
3562 E(MP3/Aug-CC-pVTZ) (Hartree): -381.48930848
3563 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47781124
3564 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50213210
3565 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.10312287
3566 E(UHF/Aug-CC-pVTZ) (Hartree): -380.08321231
3567 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11528532
3568 Electronic state : 2-A
3569 Cartesian coordinates (Angs):
3570 C -1.313651 0.291233 0.341855
3571 C -0.290224 1.192205 0.597926
3572 C 0.894511 1.228012 -0.296765
3573 C 1.630403 -0.125664 -0.144674
3574 O 0.687093 -1.170389 -0.292135
3575 O -0.130432 -1.179717 0.824619
3576 O -1.677701 -0.116515 -0.885788
3577 H -2.107594 0.163169 1.065677
3578 H -0.202646 1.551906 1.612946
3579 H 0.601424 1.347293 -1.342140
3580 H 1.571932 2.041338 -0.041842
3581 H 2.372267 -0.273285 -0.929519
3582 H 2.096557 -0.203814 0.837668
3583 H -0.889856 -0.408346 -1.366413
3584 Rotational constants (GHz): 3.8895600 2.8846500 2.2593700
3585 Vibrational harmonic frequencies (cm-1):
3586 1623.4638 177.6328 248.3701
3587 280.9721 391.9599 432.6138
3588 452.0873 500.3075 587.6845
3589 663.9523 737.8072 875.1450
3590 919.1406 932.5186 979.4588
3591 1017.9830 1061.3809 1077.5628
3592 1148.8220 1210.9937 1256.2309
3593 1268.3454 1318.6422 1340.3793
3594 1369.6287 1434.1885 1484.4078
3595 1497.9549 1538.4045 3065.6462
3596 3076.6998 3128.7866 3140.1905
3597 3209.6855 3225.6704 3759.1579
3598 Zero-point correction (Hartree): 0.111198
3599
3600 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.zt
3601 ~~~~~
3602 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11419635
3603 Electronic state : 2-A
3604 Cartesian coordinates (Angs):
3605 C -1.287511 0.259883 0.386557
3606 C -0.294591 1.181154 0.633815
3607 C 0.851787 1.247950 -0.305377
3608 C 1.636262 -0.084230 -0.149982
3609 O 0.753486 -1.169180 -0.328771
3610 O -0.090769 -1.241275 0.751995
3611 O -1.630822 -0.007392 -0.891770
3612 H -2.019276 0.015380 1.147963
3613 H -0.171789 1.509338 1.655646
3614 H 0.518979 1.326247 -1.338814
3615 H 1.519237 2.078630 -0.080707
3616 H 2.397095 -0.186422 -0.923444
3617 H 2.090673 -0.145555 0.840312
3618 H -2.025769 -0.883393 -0.942661
3619 Rotational constants (GHz): 3.8492700 2.8899600 2.2304200
3620 Vibrational harmonic frequencies (cm-1):
3621 1636.9546 172.7885 237.3710
3622 258.3095 345.3806 425.8914
3623 446.6402 470.7412 581.9767
3624 665.6133 750.0642 868.5386
3625 930.9654 944.1562 984.0003
3626 1021.3281 1065.7209 1080.7316
3627 1155.5223 1207.5550 1260.3485
3628 1273.2681 1283.4913 1320.2074
3629 1368.5899 1434.2763 1481.3443

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3630      1490.0791      1559.9629      3068.6534
3631      3091.3822      3132.4485      3147.5517
3632      3178.7540      3223.6184      3862.1701
3633 Zero-point correction (Hartree): 0.111151
3634
3635
3636 #####
3637 E-HOCH=C(CH3)CH2CH2OO ring closure and H-shift
3638 #####
3639
3640 HOCHCCH3CH2CH2OO.Ecppc
3641 ~~~~~
3642 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45033361
3643 Electronic state : 2-A
3644 Cartesian coordinates (Angs):
3645 C      -1.103065      -0.871471      0.191141
3646 C      -0.923169      0.437989      0.049117
3647 C      0.395924      1.105234      0.334463
3648 C      1.491277      0.242106      0.917800
3649 O      1.954620      -0.751298      -0.027162
3650 O      2.592063      -0.202878      -1.014324
3651 O      -2.250252      -1.571520      -0.021246
3652 H      -0.307885      -1.538884      0.491128
3653 C      -1.996493      1.381879      -0.412544
3654 H      0.784451      1.565845      -0.579038
3655 H      0.231319      1.930178      1.035728
3656 H      2.356948      0.841506      1.192988
3657 H      1.153244      -0.338338      1.774789
3658 H      -2.959546      -0.976412      -0.277049
3659 H      -2.282302      2.070261      0.386228
3660 H      -2.903590      0.887905      -0.759677
3661 H      -1.630930      1.989086      -1.243099
3662 Rotational constants (GHz): 3.2229900 1.1959300 1.0071900
3663 Vibrational harmonic frequencies (cm-1):
3664      51.8982      69.8197      73.8428
3665      147.1759      217.6721      261.0593
3666      300.7799      325.5790      340.9710
3667      477.0424      492.8291      545.1056
3668      613.4975      792.7749      844.9085
3669      922.6439      972.1016      990.6421
3670      1022.9268      1055.5205      1118.1250
3671      1179.2911      1217.1855      1231.9348
3672      1277.5549      1296.8105      1317.5123
3673      1396.5873      1402.2311      1423.3292
3674      1438.1956      1472.3417      1478.9286
3675      1496.0521      1505.6938      1781.0266
3676      3038.5655      3048.2013      3068.5338
3677      3098.9307      3100.1948      3124.0822
3678      3154.6785      3232.9326      3881.6709
3679 Zero-point correction (Hartree): 0.139650
3680
3681 HOCHCCH3CH2CH2OO.Ecppt
3682 ~~~~~
3683 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45049488
3684 Electronic state : 2-A
3685 Cartesian coordinates (Angs):
3686 C      -1.104756      -0.841832      0.194140
3687 C      -0.917761      0.462519      0.041328
3688 C      0.404086      1.129509      0.303331
3689 C      1.497118      0.278838      0.908852
3690 O      1.943860      -0.756505      0.000620
3691 O      2.585868      -0.256450      -1.009129
3692 O      -2.321172      -1.428384      -0.034035
3693 H      -0.313292      -1.514921      0.498488
3694 C      -2.014262      1.373580      -0.423936
3695 H      0.789235      1.563549      -0.624469
3696 H      0.244566      1.974288      0.981369
3697 H      2.371537      0.878173      1.155111
3698 H      1.158947      -0.265689      1.789342
3699 H      -2.238138      -2.380469      0.030156
3700 H      -2.237775      2.126436      0.335668
3701 H      -2.924844      0.823720      -0.643640

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3702      H      -1.705234      1.909941      -1.323966
3703 Rotational constants (GHz):      3.2608800      1.1933500      1.0065700
3704 Vibrational harmonic frequencies (cm-1):
3705      64.2134      69.7592      128.4212
3706      147.9245      202.7073      220.2890
3707      280.1259      304.5266      309.7661
3708      459.1385      476.7862      545.6244
3709      617.3729      804.5104      838.1869
3710      894.5427      972.8820      987.6513
3711      1020.9739      1061.4689      1119.3137
3712      1187.0261      1200.6626      1231.1333
3713      1279.8442      1304.1932      1315.6101
3714      1387.4788      1398.6469      1409.4114
3715      1438.5514      1469.9868      1491.9479
3716      1493.7130      1495.7324      1800.1772
3717      3041.0298      3049.1693      3070.3455
3718      3095.7183      3097.7090      3153.4042
3719      3168.7181      3202.3506      3921.7865
3720 Zero-point correction (Hartree): 0.139493
3721
3722 HOCHCCH3CH2CH2OO.Ecptc
3723 ~~~~~
3724 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44964409
3725 Electronic state : 2-A
3726 Cartesian coordinates (Angs):
3727      C      0.958460      0.920769      0.176224
3728      C      1.056457      -0.394701      0.011636
3729      C      -0.134754      -1.309029      0.129860
3730      C      -1.439234      -0.683554      0.559397
3731      O      -1.928124      0.141653      -0.523660
3732      O      -3.012965      0.767980      -0.188622
3733      O      1.964580      1.833701      0.114548
3734      H      0.017272      1.414141      0.372494
3735      C      2.341567      -1.103477      -0.306493
3736      H      -0.295534      -1.825626      -0.822258
3737      H      0.096126      -2.096372      0.854757
3738      H      -2.201540      -1.437712      0.748404
3739      H      -1.336795      -0.046262      1.437080
3740      H      2.803597      1.393954      -0.044874
3741      H      2.649076      -1.746589      0.521495
3742      H      3.173599      -0.436166      -0.529254
3743      H      2.211299      -1.746085      -1.179711
3744 Rotational constants (GHz):      3.3065000      1.1620200      0.9115700
3745 Vibrational harmonic frequencies (cm-1):
3746      39.4128      52.5256      72.1304
3747      128.7292      228.7058      257.5636
3748      290.8939      323.7623      338.1896
3749      394.0621      493.4623      563.6174
3750      607.2767      795.5039      831.6187
3751      933.5204      977.2514      1009.9132
3752      1030.1231      1074.5935      1109.3652
3753      1180.0895      1216.7749      1236.2106
3754      1283.9118      1295.7526      1302.1399
3755      1391.7808      1407.0620      1424.9217
3756      1441.9287      1471.4976      1479.7302
3757      1505.3723      1508.0329      1781.5179
3758      3035.6387      3047.6372      3061.6866
3759      3090.1179      3098.7149      3125.4747
3760      3142.3662      3234.4097      3881.7042
3761 Zero-point correction (Hartree): 0.139416
3762
3763 HOCHCCH3CH2CH2OO.Ecptt
3764 ~~~~~
3765 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45008565
3766 Electronic state : 2-A
3767 Cartesian coordinates (Angs):
3768      C      0.949245      0.896312      0.173511
3769      C      1.049244      -0.416643      0.012924
3770      C      -0.135912      -1.337351      0.118120
3771      C      -1.445615      -0.719812      0.542801
3772      O      -1.925296      0.123323      -0.531726
3773      O      -2.955198      0.820810      -0.165589

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3774 O 2.041054 1.717938 0.093176
3775 H 0.007111 1.392579 0.368978
3776 C 2.355536 -1.083852 -0.297378
3777 H -0.284575 -1.849886 -0.838045
3778 H 0.095114 -2.126970 0.840052
3779 H -2.210711 -1.475964 0.713060
3780 H -1.351997 -0.094804 1.430111
3781 H 1.762803 2.632521 0.154340
3782 H 2.621025 -1.794855 0.488654
3783 H 3.160225 -0.360887 -0.395257
3784 H 2.281535 -1.650231 -1.228646
3785 Rotational constants (GHz): 3.3040500 1.1760800 0.9184100
3786 Vibrational harmonic frequencies (cm-1):
3787 39.1216 64.6219 128.1937
3788 134.5810 219.8758 237.7368
3789 275.3857 299.8364 306.6485
3790 395.6929 461.5607 564.4930
3791 611.0092 806.0451 825.4997
3792 902.5628 978.5088 1008.2744
3793 1030.0588 1075.5645 1111.3507
3794 1188.2078 1201.5821 1235.4196
3795 1286.3389 1298.9974 1305.7658
3796 1387.2775 1395.9645 1413.2556
3797 1443.2880 1469.1613 1493.2110
3798 1494.0080 1506.8397 1800.8022
3799 3038.4796 3048.6987 3064.8658
3800 3089.6645 3094.9998 3142.0858
3801 3168.8376 3203.8529 3920.8200
3802 Zero-point correction (Hartree): 0.139353
3803
3804 HOHCCH3CH2CH2OO.Ectpc
3805 ~~~~~
3806 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45041178
3807 Electronic state : 2-A
3808 Cartesian coordinates (Angs):
3809 C 1.572068 -0.848306 -0.035840
3810 C 1.048365 0.370431 0.058022
3811 C -0.430853 0.592940 0.216823
3812 C -1.275230 -0.662205 0.231476
3813 O -2.664912 -0.314663 0.411511
3814 O -3.163533 0.215424 -0.662995
3815 O 2.883973 -1.174345 -0.191749
3816 H 0.970192 -1.745366 0.005025
3817 C 1.858942 1.633757 0.008171
3818 H -0.617029 1.146169 1.142711
3819 H -0.792868 1.228042 -0.596810
3820 H -1.198296 -1.223420 -0.698772
3821 H -1.047709 -1.305710 1.079830
3822 H 3.418857 -0.378750 -0.252772
3823 H 2.936081 1.471320 -0.013281
3824 H 1.647700 2.253607 0.881680
3825 H 1.599093 2.223085 -0.873668
3826 Rotational constants (GHz): 4.4348700 0.9033900 0.7892900
3827 Vibrational harmonic frequencies (cm-1):
3828 53.6282 69.9208 88.4423
3829 135.7319 170.3219 257.5520
3830 290.1776 336.9574 353.7257
3831 404.0617 491.8700 547.3106
3832 647.4542 792.2281 844.8403
3833 918.2831 977.5671 1004.5079
3834 1035.6693 1091.3277 1117.8562
3835 1178.3510 1218.5345 1240.8101
3836 1279.3550 1293.0455 1329.7371
3837 1349.0943 1410.2839 1426.3496
3838 1442.5403 1479.1171 1490.3443
3839 1503.1670 1506.4381 1778.2516
3840 3040.4836 3052.2854 3075.5687
3841 3093.2477 3105.0726 3127.5160
3842 3154.5866 3227.0072 3881.4336
3843 Zero-point correction (Hartree): 0.139679
3844
3845 HOHCCH3CH2CH2OO.Ectpt

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3846 ~~~~~
3847 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45000645
3848 Electronic state : 2-A
3849 Cartesian coordinates (Angs):
3850 C 1.577852 -0.819250 -0.040591
3851 C 1.039649 0.390526 0.048849
3852 C -0.439288 0.606583 0.202344
3853 C -1.275694 -0.652926 0.243520
3854 O -2.668115 -0.314816 0.420538
3855 O -3.177044 0.179949 -0.665932
3856 O 2.928480 -1.001619 -0.177833
3857 H 0.988561 -1.727576 -0.009288
3858 C 1.873460 1.636055 0.003073
3859 H -0.626141 1.177823 1.116948
3860 H -0.803352 1.224427 -0.623312
3861 H -1.197913 -1.231149 -0.676395
3862 H -1.040261 -1.278141 1.103607
3863 H 3.126312 -1.936141 -0.247113
3864 H 2.928756 1.407436 -0.114273
3865 H 1.742175 2.216290 0.919033
3866 H 1.559429 2.272992 -0.826568
3867 Rotational constants (GHz): 4.5430900 0.8957900 0.7869900
3868 Vibrational harmonic frequencies (cm-1):
3869 66.1054 81.8442 118.2333
3870 133.7300 168.4497 211.6414
3871 270.5425 300.3762 340.0182
3872 401.4638 463.2389 548.0668
3873 655.0680 787.2887 856.5622
3874 882.6100 976.6554 1004.0975
3875 1038.8936 1090.5760 1119.9076
3876 1183.3872 1200.1907 1240.4372
3877 1284.8237 1297.3005 1328.9850
3878 1344.8630 1391.9456 1417.1383
3879 1441.1149 1486.2883 1493.8206
3880 1495.3588 1502.2354 1796.0394
3881 3042.9124 3052.9699 3078.1945
3882 3090.6331 3100.8132 3151.6730
3883 3170.4785 3193.7375 3923.0461
3884 Zero-point correction (Hartree): 0.139478
3885
3886 HOCHCCH3CH2CH2OO.Ecttc
3887 ~~~~~
3888 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44977810
3889 Electronic state : 2-A
3890 Cartesian coordinates (Angs):
3891 C 1.488099 -0.916064 -0.005446
3892 C 1.157250 0.372000 -0.004153
3893 C -0.277382 0.825472 -0.006417
3894 C -1.301472 -0.284018 0.000130
3895 O -2.599710 0.348790 0.000616
3896 O -3.555657 -0.527145 0.004487
3897 O 2.740169 -1.447403 0.002084
3898 H 0.750225 -1.706120 -0.013362
3899 C 2.156681 1.492604 0.004339
3900 H -0.453841 1.465276 0.863764
3901 H -0.454740 1.456607 -0.882589
3902 H -1.248142 -0.912948 -0.888009
3903 H -1.243594 -0.906166 0.892763
3904 H 3.398381 -0.748000 0.022418
3905 H 3.194147 1.164942 -0.051675
3906 H 2.053967 2.092384 0.911142
3907 H 1.986132 2.160124 -0.842661
3908 Rotational constants (GHz): 4.5196000 0.8584100 0.7311900
3909 Vibrational harmonic frequencies (cm-1):
3910 39.9873 66.4798 104.0525
3911 118.0175 126.4742 258.2234
3912 277.4712 336.0857 345.7019
3913 356.7540 491.5233 552.7374
3914 628.5252 781.4722 838.9029
3915 916.1860 1004.7024 1027.4762
3916 1032.3684 1102.6472 1113.7519
3917 1180.2951 1219.2221 1231.7335

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3918      1285.5998          1297.2377          1310.4639
3919      1346.4920          1411.7788          1429.2141
3920      1447.0180          1479.5478          1495.7512
3921      1506.2214          1512.9631          1778.6707
3922      3041.0038          3052.2032          3069.5630
3923      3084.7357          3103.9782          3128.5020
3924      3142.6828          3227.4756          3881.6338
3925      Zero-point correction (Hartree): 0.139386
3926
3927      HOCHCCH3CH2CH2OO.Ecttt
3928      ~~~~~
3929      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44960190
3930      Electronic state : 2-A
3931      Cartesian coordinates (Angs):
3932      C      1.497402      -0.887783      0.000047
3933      C      1.149149      0.392873      -0.000195
3934      C      -0.286555      0.836909      -0.000243
3935      C      -1.302947      -0.279254      0.000509
3936      O      -2.608087      0.338922      0.000809
3937      O      -3.554154      -0.547667      -0.000566
3938      O      2.808980      -1.279956      0.000127
3939      H      0.772529      -1.692773      0.000239
3940      C      2.167038      1.493856      -0.000459
3941      H      -0.464979      1.472336      0.872425
3942      H      -0.465223      1.471424      -0.873521
3943      H      -1.242267      -0.904675      -0.889847
3944      H      -1.241502      -0.903978      0.891323
3945      H      2.863827      -2.236095      0.000007
3946      H      3.180058      1.102198      -0.000860
3947      H      2.039886      2.130695      0.877666
3948      H      2.039237      2.130865      -0.878364
3949      Rotational constants (GHz):      4.6297500      0.8525500      0.7297200
3950      Vibrational harmonic frequencies (cm-1):
3951      61.1190          98.7035          106.0269
3952      120.7515          124.9046          216.6812
3953      263.0903          301.9858          333.7557
3954      352.6867          461.9462          551.4865
3955      637.3932          777.7230          851.1881
3956      881.7542          1005.5986          1027.6191
3957      1032.6477          1105.6258          1112.9235
3958      1188.1821          1201.6842          1231.4127
3959      1295.4491          1297.7054          1308.7258
3960      1343.6335          1393.4035          1420.2363
3961      1446.5771          1489.3928          1494.3233
3962      1498.0086          1512.2925          1796.4653
3963      3043.6363          3052.7079          3072.4169
3964      3082.2130          3100.2050          3139.7630
3965      3170.4924          3194.7409          3923.5816
3966      Zero-point correction (Hartree): 0.139248
3967
3968      HOCHCCH3CH2CH2OO.Egmpc
3969      ~~~~~
3970      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45079312
3971      Electronic state : 2-A
3972      Cartesian coordinates (Angs):
3973      C      -1.828722          0.593462          -0.318153
3974      C      -0.749123          0.228923          0.366273
3975      C      0.356813          1.221157          0.592489
3976      C      1.588782          1.000573          -0.274274
3977      O      2.226603          -0.254941          0.045546
3978      O      1.867639          -1.208950          -0.758884
3979      O      -2.888998          -0.203964          -0.611804
3980      H      -1.967069          1.592998          -0.708991
3981      C      -0.625813          -1.165153          0.928019
3982      H      0.001192          2.230566          0.374814
3983      H      0.665992          1.211051          1.640907
3984      H      1.340216          0.972306          -1.333044
3985      H      2.348091          1.756234          -0.075769
3986      H      -2.717138          -1.099473          -0.304838
3987      H      -0.474526          -1.911017          0.144251
3988      H      -1.516950          -1.442277          1.497998
3989      H      0.226614          -1.241311          1.599681

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3990 Rotational constants (GHz):    3.5834100    1.2111900    1.0713800
3991 Vibrational harmonic frequencies (cm-1):
3992     39.9458      73.1485      128.2640
3993     167.4782     175.8704     263.8396
3994     308.0215     339.6564     396.1107
3995     471.1996     520.2774     540.9332
3996     609.5298     795.0616     861.5924
3997     923.9655     937.1037    1016.3156
3998     1031.4899    1050.5768    1093.6730
3999     1179.3530    1227.8926    1241.8213
4000     1251.0525    1320.3644    1328.3232
4001     1378.4174    1391.6522    1405.0569
4002     1421.3944    1470.4582    1481.4939
4003     1496.5170    1502.0666    1765.0900
4004     3040.3305    3053.9698    3088.4239
4005     3093.0150    3102.2243    3146.0031
4006     3158.5547    3212.6987    3861.4501
4007 Zero-point correction (Hartree): 0.139792
4008
4009 HOCHCCH3CH2CH2OO.Elmmc
4010 ~~~~~
4011 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45242156
4012 Electronic state : 2-A
4013 Cartesian coordinates (Angs):
4014 C      2.013050    -0.583300     0.048600
4015 C      0.822405    -0.037761     0.280218
4016 C     -0.330897    -0.920787     0.665404
4017 C     -1.401168    -1.046745    -0.407538
4018 O     -2.022990     0.228051    -0.691483
4019 O     -2.717012     0.653555     0.318701
4020 O      3.144830     0.064818    -0.333535
4021 H      2.192013    -1.644901     0.158839
4022 C      0.576416     1.443144     0.170143
4023 H      0.025312    -1.930256     0.878572
4024 H     -0.813437    -0.547858     1.572093
4025 H     -0.979016    -1.352464    -1.363281
4026 H     -2.195381    -1.728309    -0.105657
4027 H      2.954627     0.995628    -0.481461
4028 H      0.217636     1.728786    -0.820826
4029 H      1.471402     2.028463     0.390908
4030 H     -0.190622     1.752218     0.880397
4031 Rotational constants (GHz):    4.6129000    1.0605600    0.9487100
4032 Vibrational harmonic frequencies (cm-1):
4033     38.6505      77.3705      130.5209
4034     169.8811     176.6163     264.7294
4035     311.8036     328.6012     402.1490
4036     459.2398     517.9373     551.3201
4037     617.6214     797.0893     847.4594
4038     928.4938     943.3898     996.1643
4039     1036.3604    1052.8646    1106.3434
4040     1176.3255    1219.7146    1234.3742
4041     1269.0028    1305.5852    1318.0439
4042     1378.3035    1395.9793    1409.7986
4043     1426.5379    1469.6655    1485.0410
4044     1489.3419    1505.1048    1769.2464
4045     3047.6348    3061.1003    3088.9961
4046     3104.5789    3110.0293    3124.2378
4047     3153.5715    3211.4230    3868.8059
4048 Zero-point correction (Hartree): 0.139827
4049
4050 HOCHCCH3CH2CH2OO.Elmtt
4051 ~~~~~
4052 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45107126
4053 Electronic state : 2-A
4054 Cartesian coordinates (Angs):
4055 C     -2.045545    -0.556310    -0.080610
4056 C     -0.840502    -0.020493    -0.231501
4057 C      0.320886    -0.905756    -0.581414
4058 C      1.398805    -0.977272     0.489546
4059 O      2.113025     0.274231     0.616461
4060 O      2.827360     0.521781    -0.437538
4061 O     -3.140708     0.192148     0.252576

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4062      H      -2.218904      -1.618909      -0.211558
4063      C      -0.596830      1.451270      -0.071279
4064      H      -0.024704      -1.925997      -0.758613
4065      H      0.802291      -0.563348      -1.501394
4066      H      0.977864      -1.144065      1.479792
4067      H      2.140528      -1.740460      0.258152
4068      H      -3.929223      -0.350927      0.223254
4069      H      -0.062021      1.665449      0.855983
4070      H      -1.533593      2.002421      -0.061156
4071      H      0.029452      1.821923      -0.884911
4072      Rotational constants (GHz):      4.9357000      1.0140300      0.9163200
4073      Vibrational harmonic frequencies (cm-1):
4074          36.7960          71.9341          147.3537
4075          166.4145          200.7384          220.6476
4076          267.5188          297.9678          374.2763
4077          433.4844          506.7578          553.2612
4078          611.9254          806.4659          851.1981
4079          888.6263          946.0686          989.6621
4080          1041.5967          1058.7229          1110.1534
4081          1180.1000          1210.4322          1229.0814
4082          1272.1106          1305.5993          1308.5329
4083          1380.5998          1394.8994          1397.4725
4084          1430.8916          1468.7159          1487.8996
4085          1493.0969          1493.7255          1791.2177
4086          3056.7129          3057.7261          3087.8331
4087          3106.6378          3107.8842          3152.1624
4088          3161.8569          3175.6031          3920.5807
4089      Zero-point correction (Hartree): 0.139544
4090
4091      HOCHCCH3CH2CH2OO.Elmtc
4092      ~~~~~
4093      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45103902
4094      Electronic state : 2-A
4095      Cartesian coordinates (Angs):
4096      C      2.057130      -0.569428      -0.201725
4097      C      0.932723      -0.082448      0.315439
4098      C      -0.172671      -1.032065      0.687609
4099      C      -1.412079      -0.918236      -0.180575
4100      O      -2.063491      0.337284      0.123070
4101      O      -3.099629      0.531724      -0.632015
4102      O      3.138556      0.138524      -0.620488
4103      H      2.215710      -1.631877      -0.333222
4104      C      0.710421      1.388304      0.540609
4105      H      0.181427      -2.060750      0.604398
4106      H      -0.471987      -0.880858      1.728956
4107      H      -1.171835      -0.910268      -1.243110
4108      H      -2.133812      -1.706963      0.029789
4109      H      2.960188      1.080858      -0.554230
4110      H      0.152950      1.849424      -0.276981
4111      H      1.646002      1.936518      0.665775
4112      H      0.124727      1.546901      1.445953
4113      Rotational constants (GHz):      4.5600900      0.9613500      0.8826200
4114      Vibrational harmonic frequencies (cm-1):
4115          33.2861          60.1466          98.9528
4116          149.4043          179.0129          256.2755
4117          302.3820          334.3240          390.1704
4118          410.9641          501.4042          575.1685
4119          600.9007          797.4821          840.6084
4120          925.9919          961.2699          1025.1453
4121          1044.0113          1059.1274          1093.6388
4122          1180.0190          1218.9880          1237.1159
4123          1276.0249          1295.5166          1318.5902
4124          1380.5161          1398.0782          1412.0442
4125          1428.2151          1467.6952          1485.1955
4126          1498.0731          1503.1657          1769.5168
4127          3049.7919          3050.6693          3082.3847
4128          3107.0257          3108.5436          3125.5393
4129          3142.4746          3209.4681          3871.6575
4130      Zero-point correction (Hartree): 0.139551
4131
4132      HOCHCCH3CH2CH2OO.Elmtt
4133      ~~~~~

```

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4134 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44993064
4135 Electronic state : 2-A
4136 Cartesian coordinates (Angs):
4137 C -2.102942 0.538206 -0.143436
4138 C -0.937721 0.060986 0.276054
4139 C 0.166425 1.019365 0.624421
4140 C 1.406567 0.886346 -0.241243
4141 O 2.135432 -0.287980 0.187571
4142 O 3.181418 -0.493893 -0.550088
4143 O -3.144905 -0.277302 -0.488645
4144 H -2.283931 1.603643 -0.234672
4145 C -0.681508 -1.410118 0.417318
4146 H -0.189171 2.046483 0.528509
4147 H 0.472598 0.885162 1.666565
4148 H 1.166525 0.752649 -1.295559
4149 H 2.081468 1.733116 -0.121316
4150 H -3.916446 0.249339 -0.700408
4151 H 0.027256 -1.761330 -0.335032
4152 H -1.602277 -1.977775 0.312444
4153 H -0.236502 -1.626603 1.390083
4154 Rotational constants (GHz): 4.9541800 0.9345000 0.8533500
4155 Vibrational harmonic frequencies (cm-1):
4156 38.2223 60.7487 118.7998
4157 167.5998 208.7623 239.9630
4158 253.9018 295.9806 369.6034
4159 380.9865 471.5233 579.6108
4160 597.9815 807.2849 841.7321
4161 891.1782 958.9019 1021.9535
4162 1049.8199 1064.5119 1098.2331
4163 1185.8944 1209.9780 1231.6886
4164 1279.2776 1296.1262 1305.4640
4165 1382.0083 1397.4037 1398.7941
4166 1432.0567 1465.6511 1490.4287
4167 1496.2937 1500.0287 1794.8727
4168 3047.2310 3058.8339 3081.9629
4169 3106.0061 3109.1757 3141.2796
4170 3163.4507 3177.9344 3921.3390
4171 Zero-point correction (Hartree): 0.139402
4172
4173 HOCHCCH3CH2CH2OO.Elpmc
4174 ~~~~~
4175 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -420.84408640
4176 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -420.77348661
4177 T1 diagnostic: 0.020724
4178 E(MP2/Aug-CC-pVTZ) (Hartree): -420.72102249
4179 E(MP3/Aug-CC-pVTZ) (Hartree): -420.76040125
4180 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72446597
4181 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76254263
4182 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18070042
4183 E(UHF/Aug-CC-pVTZ) (Hartree): -419.17544253
4184 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45265451
4185 Electronic state : 2-A
4186 Cartesian coordinates (Angs):
4187 C -1.517607 -0.283437 -0.753321
4188 C -0.688102 0.550324 -0.133217
4189 C 0.538745 1.038517 -0.843823
4190 C 1.838957 0.611526 -0.173038
4191 O 1.985009 -0.818500 -0.218460
4192 O 1.354129 -1.396059 0.761167
4193 O -2.645530 -0.839962 -0.241593
4194 H -1.353689 -0.601333 -1.774347
4195 C -0.894450 1.005527 1.283658
4196 H 0.547096 0.688579 -1.876849
4197 H 0.549588 2.133239 -0.871075
4198 H 2.704278 0.996970 -0.709256
4199 H 1.882456 0.910749 0.873250
4200 H -2.716026 -0.636878 0.695306
4201 H -0.360153 0.364472 1.988530
4202 H -1.947769 1.023448 1.568417
4203 H -0.519904 2.022190 1.415556
4204 Rotational constants (GHz): 3.0806800 1.3277200 1.2131600
4205 Vibrational harmonic frequencies (cm-1):

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4206      63.9862      104.7020      108.6729
4207      122.1413      201.4260      273.4201
4208      300.7804      361.7789      395.4514
4209      458.0915      513.3197      555.9277
4210      598.5636      800.0066      863.5417
4211      918.9867      962.5085      1003.3209
4212      1035.1931      1053.7956      1078.6200
4213      1184.2846      1224.9307      1237.2872
4214      1246.1949      1314.7995      1323.2196
4215      1372.5476      1393.5532      1406.8474
4216      1425.4227      1469.2816      1484.0931
4217      1495.6961      1505.2614      1772.5644
4218      3040.6819      3046.7273      3093.4939
4219      3107.1019      3108.7996      3113.8965
4220      3154.7250      3216.3431      3873.0163
4221 Zero-point correction (Hartree): 0.139845
4222
4223 HOCHCCH3CH2CH2OO.Elpm
4224 ~~~~~
4225 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45177275
4226 Electronic state : 2-A
4227 Cartesian coordinates (Angs):
4228 C      -1.510210      -0.336826      -0.690902
4229 C      -0.683259      0.546226      -0.145920
4230 C      0.539959      0.977063      -0.898706
4231 C      1.847651      0.597746      -0.214740
4232 O      2.000095      -0.831905      -0.179810
4233 O      1.380285      -1.354796      0.837605
4234 O      -2.640887      -0.764850      -0.055396
4235 H      -1.323918      -0.761340      -1.671016
4236 C      -0.911633      1.122466      1.218494
4237 H      0.541037      0.556366      -1.905497
4238 H      0.548957      2.066978      -1.003651
4239 H      2.705532      0.954743      -0.781869
4240 H      1.899584      0.958318      0.811076
4241 H      -3.092511      -1.415167      -0.594411
4242 H      -0.205936      0.698501      1.936264
4243 H      -1.917224      0.908862      1.570994
4244 H      -0.766517      2.205095      1.209553
4245 Rotational constants (GHz): 3.1009500 1.3187700 1.1980700
4246 Vibrational harmonic frequencies (cm-1):
4247 57.1189 93.4475 104.6185
4248 131.9094 219.1160 232.0021
4249 276.1121 311.2246 387.5974
4250 438.8327 494.0006 557.1893
4251 600.1569 807.2122 858.7543
4252 894.0112 961.8466 999.8902
4253 1036.6439 1062.5751 1080.2574
4254 1193.8357 1210.0610 1235.1229
4255 1248.8211 1303.8493 1319.1174
4256 1375.2739 1390.0143 1398.2793
4257 1430.4524 1469.6591 1486.2454
4258 1489.9780 1504.9210 1796.2725
4259 3041.9251 3050.8094 3095.6879
4260 3102.2293 3104.9275 3157.8622
4261 3162.0273 3180.0152 3922.6773
4262 Zero-point correction (Hartree): 0.139594
4263
4264 HOCHCCH3CH2CH2OO.Elppc
4265 ~~~~~
4266 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45195093
4267 Electronic state : 2-A
4268 Cartesian coordinates (Angs):
4269 C      1.459781      -0.776614      0.420568
4270 C      0.809440      0.376741      0.306445
4271 C      -0.482178      0.573410      1.045944
4272 C      -1.666117      0.819506      0.124995
4273 O      -1.850534      -0.277332      -0.795413
4274 O      -2.187652      -1.364440      -0.172854
4275 O      2.617064      -1.127776      -0.198308
4276 H      1.098108      -1.575173      1.054509
4277 C      1.280687      1.502085      -0.571500

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4278      H      -0.703645      -0.293698      1.667310
4279      H      -0.414759      1.443134      1.707674
4280      H      -2.593160      0.935477      0.684486
4281      H      -1.513927      1.681988      -0.522449
4282      H      2.881434      -0.442781      -0.818407
4283      H      0.815043      1.470810      -1.560068
4284      H      2.362349      1.500720      -0.714819
4285      H      1.027859      2.465136      -0.124337
4286      Rotational constants (GHz):      3.1403500      1.2648500      1.0636500
4287      Vibrational harmonic frequencies (cm-1):
4288          36.8765          52.5879          118.8400
4289          127.2007          205.7481          263.7766
4290          302.9698          348.2542          391.2698
4291          454.1732          509.8571          554.3828
4292          615.8995          799.6879          843.0226
4293          929.9481          956.6517          993.0827
4294          1035.7560          1052.2483          1089.8522
4295          1182.5724          1223.8758          1230.1082
4296          1265.2094          1299.6920          1317.9795
4297          1377.4525          1396.8678          1410.5049
4298          1426.5641          1472.3962          1486.1949
4299          1496.9209          1505.0832          1778.0527
4300          3041.6380          3043.2119          3093.3491
4301          3098.9139          3114.6308          3121.5831
4302          3151.6504          3215.2843          3874.0553
4303      Zero-point correction (Hartree): 0.139665
4304
4305      HOCHCCH3CH2CH2OO.Elpppt
4306      ~~~~~
4307      E(CCS(D)/Aug-CC-pVTZ) (Hartree): -420.84385432
4308      E(CCS(D)/Aug-CC-pVTZ) (Hartree): -420.77372382
4309      T1 diagnostic: 0.020573
4310      E(MP2/Aug-CC-pVTZ) (Hartree): -420.72095663
4311      E(MP3/Aug-CC-pVTZ) (Hartree): -420.76066693
4312      E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72411407
4313      E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76253098
4314      E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18205719
4315      E(UHF/Aug-CC-pVTZ) (Hartree): -419.17690718
4316      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45188619
4317      Electronic state : 2-A
4318      Cartesian coordinates (Angs):
4319      C      1.428909      -0.761649      0.387917
4320      C      0.808286      0.406145      0.287379
4321      C      -0.489208      0.617197      1.011743
4322      C      -1.672006      0.827860      0.080720
4323      O      -1.862434      -0.311367      -0.786966
4324      O      -2.193385      -1.369017      -0.113317
4325      O      2.607110      -1.019542      -0.254484
4326      H      1.022622      -1.570406      0.984909
4327      C      1.341535      1.528230      -0.552156
4328      H      -0.712932      -0.230656      1.658873
4329      H      -0.426996      1.506181      1.647335
4330      H      -2.598217      0.971458      0.635324
4331      H      -1.517559      1.658184      -0.605961
4332      H      2.895243      -1.912333      -0.060989
4333      H      0.735260      1.673752      -1.449666
4334      H      2.361263      1.329288      -0.871014
4335      H      1.325889      2.467235      0.005707
4336      Rotational constants (GHz):      3.1486200      1.2674200      1.0540300
4337      Vibrational harmonic frequencies (cm-1):
4338          26.7941          45.7261          108.2875
4339          130.5170          215.3615          233.3374
4340          275.5859          299.0623          385.1109
4341          433.3619          493.0776          557.0090
4342          615.4538          807.4477          840.0362
4343          902.1129          957.7869          984.3953
4344          1035.1859          1063.0966          1089.2179
4345          1192.4548          1208.3106          1233.7179
4346          1266.7916          1301.9615          1305.5584
4347          1381.0377          1389.3788          1401.8280
4348          1430.7164          1471.4674          1487.7331
4349          1490.5883          1502.7339          1800.3064

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4350      3046.1368          3048.2779          3093.5697
4351      3097.0945          3117.7039          3155.1559
4352      3161.9043          3180.8921          3921.9245
4353 Zero-point correction (Hartree): 0.139390
4354
4355 HOCHCCH3CH2CH2OO.Elptc
4356 ~~~~~
4357 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45093535
4358 Electronic state : 2-A
4359 Cartesian coordinates (Angs):
4360   C      -1.721411      -0.587870      -0.547802
4361   C      -0.916644       0.407847      -0.192202
4362   C       0.248419       0.773116      -1.068863
4363   C       1.585035       0.661313      -0.362510
4364   O       1.784646      -0.724568      -0.010541
4365   O       2.857524      -0.884493       0.700195
4366   O      -2.797669      -1.055815       0.136247
4367   H      -1.576378      -1.138501      -1.467638
4368   C      -1.090617       1.192064       1.078120
4369   H       0.263101       0.147565      -1.962174
4370   H       0.157778       1.811407      -1.403676
4371   H       2.415615       0.956359      -1.002489
4372   H       1.620835       1.237491       0.561719
4373   H      -2.868588      -0.611774       0.985637
4374   H      -0.462934       0.806120       1.885350
4375   H      -2.122091       1.195651       1.433353
4376   H      -0.812046       2.235865       0.922256
4377 Rotational constants (GHz):   3.4451300      1.0522800      0.9883000
4378 Vibrational harmonic frequencies (cm-1):
4379      41.6818          55.6782          95.2414
4380      122.1272         225.6290         255.4193
4381      298.1443         341.1793         386.6297
4382      405.9443         500.7129         568.1586
4383      599.1119         800.1281         838.2699
4384      929.8089         959.6360        1024.2254
4385     1049.3828        1067.1277        1077.5407
4386     1181.2537        1223.4907        1231.4619
4387     1276.1074        1297.0730        1318.4225
4388     1380.2345        1394.1162        1412.8135
4389     1428.6500        1470.7367        1488.4428
4390     1503.7162        1508.9518        1777.2567
4391     3043.4882        3044.8136        3085.8243
4392     3100.1926        3108.8349        3116.2341
4393     3140.7489        3215.3730        3874.7341
4394 Zero-point correction (Hartree): 0.139571
4395
4396 HOCHCCH3CH2CH2OO.Elptt
4397 ~~~~~
4398 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45062207
4399 Electronic state : 2-A
4400 Cartesian coordinates (Angs):
4401   C       1.687998      -0.618795       0.492881
4402   C       0.915542       0.416456       0.192925
4403   C      -0.259700       0.749108       1.067999
4404   C      -1.591353       0.659142       0.349459
4405   O      -1.802077      -0.723348      -0.011109
4406   O      -2.887151      -0.874508      -0.704725
4407   O       2.769767      -0.965716      -0.266504
4408   H       1.492458      -1.242616       1.357736
4409   C       1.163201       1.278087      -1.009050
4410   H      -0.285528       0.095656       1.941473
4411   H      -0.170140       1.775429       1.437329
4412   H      -2.423692       0.956840       0.985921
4413   H      -1.613993       1.241844      -0.570464
4414   H       3.198522      -1.736052       0.107991
4415   H       2.139415       1.075352      -1.441349
4416   H       1.111298       2.335820      -0.741319
4417   H       0.413215       1.102318      -1.783897
4418 Rotational constants (GHz):   3.4577100      1.0502500      0.9739700
4419 Vibrational harmonic frequencies (cm-1):
4420      27.8590          56.3095          95.1152
4421     130.4504         229.9982         233.0775

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4422      279.8611      281.8680      379.0604
4423      390.0224      473.3075      569.5506
4424      599.1604      808.7278      835.2397
4425      901.7905      959.8911     1022.4905
4426     1052.1236     1073.0370     1076.6099
4427     1189.3981     1207.2794     1234.9150
4428     1275.3578     1297.3689     1306.2990
4429     1383.6717     1387.5146     1402.9185
4430     1432.2372     1469.4858     1490.7696
4431     1493.0623     1509.5911     1800.9719
4432     3046.6909     3049.0555     3088.0839
4433     3097.1853     3103.7458     3144.0555
4434     3161.8549     3181.6663     3920.9978
4435 Zero-point correction (Hartree): 0.139309
4436
4437 HOCHCCH3CH2CH2OO.Eltmc
4438 ~~~~~
4439 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45164869
4440 Electronic state : 2-A
4441 Cartesian coordinates (Angs):
4442      C      1.811935      -0.907621      0.071422
4443      C      1.027333      0.151265      0.247118
4444      C     -0.414545     -0.040563      0.622740
4445      C     -1.339242      0.420047     -0.492300
4446      O     -2.719465      0.331750     -0.081247
4447      O     -3.113306     -0.903396     -0.014655
4448      O      3.119974     -0.898855     -0.294994
4449      H      1.454965     -1.917711      0.221781
4450      C      1.516665      1.562881      0.063181
4451      H     -0.625008     -1.089135      0.831386
4452      H     -0.651596      0.533489      1.523087
4453      H     -1.198815      1.472892     -0.733562
4454      H     -1.219188     -0.188641     -1.387452
4455      H      3.407718      0.001017     -0.472667
4456      H      1.385050      1.918785     -0.961790
4457      H      2.571892      1.675366      0.319359
4458      H      0.964490      2.241889      0.714062
4459 Rotational constants (GHz):      4.7964600      0.8767900      0.7807500
4460 Vibrational harmonic frequencies (cm-1):
4461      53.7285      71.7147      89.4977
4462     116.3588     155.1504     271.1468
4463     307.8924     327.9762     383.8881
4464     406.1160     510.9140     539.2368
4465     656.5248     795.4961     837.0464
4466     933.8506     968.3074    1016.5065
4467    1043.4275    1069.7756    1081.4272
4468    1183.6477    1220.7490    1236.2731
4469    1280.1390    1307.8771    1322.0944
4470    1335.7953    1400.0742    1409.7012
4471    1425.2233    1482.0790    1491.9171
4472    1499.1111    1505.3858    1772.0821
4473    3043.5621    3050.7344    3091.7159
4474    3098.1917    3117.5938    3121.3765
4475    3154.5905    3218.4321    3871.8645
4476 Zero-point correction (Hartree): 0.139597
4477
4478 HOCHCCH3CH2CH2OO.Eltmt
4479 ~~~~~
4480 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45146190
4481 Electronic state : 2-A
4482 Cartesian coordinates (Angs):
4483      C      1.808449     -0.870946      0.073997
4484      C      1.022126      0.185896      0.234148
4485      C     -0.415721     -0.007658      0.623098
4486      C     -1.359154      0.443369     -0.480086
4487      O     -2.733501      0.297045     -0.063681
4488      O     -3.085753     -0.951642     -0.027514
4489      O      3.119356     -0.754994     -0.294526
4490      H      1.443150     -1.880050      0.228246
4491      C      1.518328      1.587994      0.035525
4492      H     -0.622997     -1.056074      0.837927
4493      H     -0.642754      0.569183      1.524220

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4494      H      -1.258428      1.504409      -0.700972
4495      H      -1.223508      -0.143918      -1.387232
4496      H      3.537838      -1.616751      -0.290378
4497      H      1.112418      2.031524      -0.876723
4498      H      2.602370      1.614041      -0.037457
4499      H      1.206935      2.222439      0.868047
4500      Rotational constants (GHz):      4.787660      0.8777500      0.7801800
4501      Vibrational harmonic frequencies (cm-1):
4502          56.3337          61.5398          111.1569
4503          118.4974          170.4625          240.0409
4504          267.4307          321.2406          359.2031
4505          385.4776          485.3416          538.0905
4506          660.2330          793.0924          844.5286
4507          900.1542          966.8000          1014.9355
4508          1050.6590          1070.5620          1086.7521
4509          1194.8091          1209.8170          1236.0224
4510          1283.4324          1293.5699          1325.9942
4511          1339.2963          1393.4718          1406.7887
4512          1430.5021          1480.0410          1492.3605
4513          1497.0516          1499.6333          1795.6914
4514          3049.6415          3051.3162          3094.9246
4515          3099.0336          3116.9742          3159.8308
4516          3162.0614          3183.4444          3918.9380
4517      Zero-point correction (Hartree): 0.139463
4518
4519      HOCHCCH3CH2CH2OO.Eltpc
4520      ~~~~~
4521      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45201182
4522      Electronic state : 2-A
4523      Cartesian coordinates (Angs):
4524      C      -2.007490      -0.766543      -0.158771
4525      C      -1.003670      0.103506      -0.211088
4526      C      0.386922      -0.368660      -0.524399
4527      C      1.307083      -0.192810      0.672840
4528      O      2.663592      -0.544892      0.329885
4529      O      3.209099      0.359872      -0.424121
4530      O      -3.304263      -0.488022      0.135709
4531      H      -1.870260      -1.819530      -0.365650
4532      C      -1.199234      1.573372      0.052831
4533      H      0.380775      -1.418458      -0.818898
4534      H      0.807641      0.209533      -1.351093
4535      H      1.321144      0.836694      1.029090
4536      H      1.041753      -0.866617      1.485571
4537      H      -3.399346      0.442897      0.356862
4538      H      -1.153800      1.815574      1.117656
4539      H      -2.155303      1.937117      -0.329843
4540      H      -0.421692      2.153930      -0.443958
4541      Rotational constants (GHz):      5.5881300      0.8426200      0.7822800
4542      Vibrational harmonic frequencies (cm-1):
4543          53.0781          68.9128          92.6832
4544          134.5309          153.8551          269.6361
4545          308.6222          336.0594          387.3273
4546          408.3134          514.1855          543.1282
4547          658.1054          792.9716          836.2138
4548          926.7746          973.8020          1018.9343
4549          1043.2789          1062.5763          1082.5295
4550          1183.7005          1225.6114          1233.7287
4551          1283.3615          1305.6221          1327.7582
4552          1335.9956          1398.4848          1407.9966
4553          1424.1372          1481.3396          1492.3829
4554          1498.2498          1507.0122          1770.7074
4555          3041.9336          3058.3081          3092.2916
4556          3095.3268          3114.2838          3122.0515
4557          3156.0048          3216.5067          3868.2763
4558      Zero-point correction (Hartree): 0.139667
4559
4560      HOCHCCH3CH2CH2OO.Eltpc
4561      ~~~~~
4562      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45145415
4563      Electronic state : 2-A
4564      Cartesian coordinates (Angs):
4565      C      -2.001604      -0.742327      -0.143488

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4566	C	-1.003878	0.131352	-0.193096		
4567	C	0.388943	-0.341258	-0.495733		
4568	C	1.325429	-0.112698	0.679639		
4569	O	2.660431	-0.553504	0.354349		
4570	O	3.240376	0.263637	-0.470784		
4571	O	-3.284177	-0.367272	0.143806		
4572	H	-1.843266	-1.799209	-0.327038		
4573	C	-1.215763	1.598121	0.043935		
4574	H	0.390938	-1.403170	-0.745496		
4575	H	0.796207	0.204117	-1.351080		
4576	H	1.390356	0.938782	0.954426		
4577	H	1.039528	-0.710211	1.543648		
4578	H	-3.874869	-1.114517	0.041352		
4579	H	-0.835668	1.906024	1.020700		
4580	H	-2.271803	1.852258	0.004772		
4581	H	-0.683224	2.183896	-0.707787		
4582	Rotational constants (GHz):		5.6476000	0.8348200	0.7774800	
4583	Vibrational harmonic frequencies (cm-1):					
4584		49.7688	62.1260		111.8830	
4585		127.3880	172.9634		210.4648	
4586		261.2065	320.6001		362.4027	
4587		382.3184	485.9407		542.2492	
4588		657.6454	793.1815		842.6844	
4589		892.9237	971.7160		1015.6927	
4590		1050.5671	1064.3973		1088.9214	
4591		1195.4017	1206.0764		1235.3924	
4592		1278.4451	1296.7273		1326.6436	
4593		1338.9397	1392.0899		1404.1120	
4594		1429.8617	1479.4113		1492.5962	
4595		1497.1967	1499.5171		1794.2645	
4596		3052.0717	3056.5095		3095.4248	
4597		3101.9954	3108.8201		3158.4228	
4598		3161.4501	3179.2350		3920.3404	
4599	Zero-point correction (Hartree):		0.139351			
4600						
4601	HOCHCCH3CH2CH2OO.Elttc					
4602	~~~~~					
4603	E(UM062X/Aug-CC-pVTZ) (Hartree):		-421.45091885			
4604	Electronic state :		2-A			
4605	Cartesian coordinates (Angs):					
4606	C	2.019457	-0.817672	0.008327		
4607	C	1.098313	0.106194	0.263784		
4608	C	-0.265828	-0.308594	0.739631		
4609	C	-1.331637	0.046086	-0.278635		
4610	O	-2.612365	-0.306310	0.287546		
4611	O	-3.586183	-0.017001	-0.518699		
4612	O	3.280374	-0.604705	-0.449534		
4613	H	1.832634	-1.872400	0.160319		
4614	C	1.352064	1.578443	0.081059		
4615	H	-0.294439	-1.382104	0.927499		
4616	H	-0.506575	0.195948	1.679682		
4617	H	-1.359513	1.112952	-0.500090		
4618	H	-1.213321	-0.513727	-1.205893		
4619	H	3.413792	0.330153	-0.629580		
4620	H	1.084613	1.925417	-0.920047		
4621	H	2.395599	1.846085	0.257166		
4622	H	0.758393	2.155065	0.791451		
4623	Rotational constants (GHz):		5.6123100	0.7832700	0.7367300	
4624	Vibrational harmonic frequencies (cm-1):					
4625		53.8263	72.5390		95.9165	
4626		114.0774	128.2612		270.0024	
4627		279.2909	331.3963		381.0101	
4628		385.4593	495.6250		548.1192	
4629		637.7717	787.1260		832.2222	
4630		931.2207	1006.1629		1023.5025	
4631		1047.5933	1065.7010		1104.9684	
4632		1179.5446	1217.2770		1228.0802	
4633		1292.8911	1306.1027		1310.3396	
4634		1333.4085	1402.8581		1413.8348	
4635		1426.4010	1485.5788		1492.6064	
4636		1504.5213	1508.5126		1772.3846	
4637		3044.6967	3051.5936		3084.0365	

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4638          3099.7247          3110.5957          3118.4691
4639          3143.5100          3214.7052          3871.4970
4640 Zero-point correction (Hartree): 0.139435
4641
4642 HOCHCCH3CH2CH2OO.El1ttt
4643 ~~~~~
4644 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45055503
4645 Electronic state : 2-A
4646 Cartesian coordinates (Angs):
4647   C      2.019747      -0.786239      0.012765
4648   C      1.092870      0.133198      0.249446
4649   C     -0.268522     -0.285052      0.729399
4650   C     -1.347484      0.078620     -0.271565
4651   O     -2.613552     -0.338726      0.285451
4652   O     -3.600278     -0.055760     -0.507019
4653   O      3.268503     -0.461379     -0.437772
4654   H      1.826796     -1.842387      0.164177
4655   C      1.353458      1.598099      0.055223
4656   H     -0.298640     -1.360915      0.906120
4657   H     -0.498650      0.209545      1.677373
4658   H     -1.411543      1.151424     -0.448613
4659   H     -1.217059     -0.439965     -1.220983
4660   H      3.818674     -1.244931     -0.472194
4661   H      0.843713      1.981548     -0.831597
4662   H      2.415948      1.794482     -0.062124
4663   H      0.982964      2.166359      0.910953
4664 Rotational constants (GHz): 5.7031700      0.7796800      0.7330400
4665 Vibrational harmonic frequencies (cm-1):
4666   49.4497          85.7927          94.1556
4667   109.3073         155.9037         223.1140
4668   264.6973         296.5680         353.0401
4669   371.2835         465.2999         545.6444
4670   640.9286         785.9895         840.5879
4671   895.2056         1002.6418        1021.9917
4672   1055.0963        1069.6735        1106.7878
4673   1189.2775        1208.1309        1226.7501
4674   1292.2113        1296.0405        1310.2441
4675   1338.0122        1392.7459        1413.1792
4676   1430.7267        1482.9877        1493.2188
4677   1498.6237        1508.4037        1795.6003
4678   3050.3658        3052.0386        3087.7339
4679   3100.1541        3106.2284        3147.3929
4680   3162.0558        3180.1953        3919.4495
4681 Zero-point correction (Hartree): 0.139230
4682
4683
4684 TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Ec
4685 ~~~~~
4686 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82495066
4687 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74993036
4688 T1 diagnostic: 0.027178
4689 E(MP2/Aug-CC-pVTZ) (Hartree): -420.69194733
4690 E(MP3/Aug-CC-pVTZ) (Hartree): -420.73018644
4691 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.70966304
4692 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74344876
4693 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15893222
4694 E(UHF/Aug-CC-pVTZ) (Hartree): -419.13843132
4695 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.43069294
4696 Electronic state : 2-A
4697 Cartesian coordinates (Angs):
4698   C      0.897061      -0.546190      0.623516
4699   C      0.499806      0.751999      0.364265
4700   C     -0.899828      1.100331      0.734933
4701   C     -1.862983      0.349260     -0.214481
4702   O     -1.608941     -1.029261     -0.103469
4703   O     -0.379546     -1.295814     -0.660220
4704   O      2.063821     -1.066021      0.210856
4705   H      0.465226     -1.110783      1.437486
4706   C      1.222207      1.567402     -0.659583
4707   H     -1.133763      0.784748      1.752116
4708   H     -1.076472      2.173656      0.656888
4709   H     -2.901957      0.490788      0.082090

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4710      H      -1.719342      0.671026      -1.248151
4711      H      2.398259      -0.574510      -0.546052
4712      H      1.015811      1.199817      -1.672535
4713      H      2.304179      1.548632      -0.511108
4714      H      0.907815      2.608579      -0.619976
4715 Rotational constants (GHz):      2.9232700      1.9578100      1.4160100
4716 Vibrational harmonic frequencies (cm-1):
4717      i584.5270      104.0146      131.1446
4718      152.9753      280.3153      301.1201
4719      328.3390      384.9481      405.1223
4720      438.5013      509.0466      585.3565
4721      622.4213      804.3175      876.8799
4722      933.8620      966.4459      987.6532
4723      1013.3413      1029.7845      1074.4238
4724      1089.5739      1180.5453      1223.0220
4725      1246.1206      1264.0096      1324.3687
4726      1343.1694      1375.3321      1386.2243
4727      1413.1340      1480.3285      1482.9774
4728      1490.9019      1502.0566      1565.9389
4729      3013.5153      3063.7344      3073.1651
4730      3083.0540      3122.8568      3133.5583
4731      3139.1511      3225.4811      3857.2312
4732 Zero-point correction (Hartree): 0.138990
4733
4734 TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Et
4735 ~~~~~
4736 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82644110
4737 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.75168260
4738 T1 diagnostic: 0.027377
4739 E(MP2/Aug-CC-pVTZ) (Hartree): -420.69320422
4740 E(MP3/Aug-CC-pVTZ) (Hartree): -420.73169845
4741 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.71075959
4742 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74484390
4743 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.16124987
4744 E(UHF/Aug-CC-pVTZ) (Hartree): -419.14094997
4745 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.43224778
4746 Electronic state : 2-A
4747 Cartesian coordinates (Angs):
4748      C      0.901440      -0.521479      0.586849
4749      C      0.502829      0.769096      0.333071
4750      C     -0.894366      1.109763      0.725147
4751      C     -1.864531      0.326386      -0.190794
4752      O     -1.591884      -1.049777      -0.073455
4753      O     -0.384427      -1.307941      -0.683039
4754      O      2.095071      -0.960328      0.136906
4755      H      0.439773      -1.087856      1.386068
4756      C      1.212414      1.628625      -0.655606
4757      H     -1.109120      0.822969      1.754911
4758      H     -1.083272      2.178781      0.618222
4759      H     -2.898699      0.457600      0.126698
4760      H     -1.748306      0.635648      -1.231358
4761      H      2.156168      -1.910354      0.265310
4762      H      1.301757      2.650040      -0.281367
4763      H      0.641760      1.676875      -1.589447
4764      H      2.203139      1.246316      -0.884335
4765 Rotational constants (GHz):      2.8787500      1.9716900      1.3999900
4766 Vibrational harmonic frequencies (cm-1):
4767      i553.2027      109.9272      129.4570
4768      161.2925      272.9190      293.9918
4769      335.0045      356.8991      383.6058
4770      430.7677      499.5686      584.3038
4771      625.0749      816.1024      874.9959
4772      937.0347      964.9763      987.8429
4773      1010.4461      1035.3106      1075.9675
4774      1087.1538      1189.3977      1224.8218
4775      1245.0144      1264.3001      1303.5546
4776      1334.5962      1374.3540      1390.3968
4777      1422.9022      1477.8849      1482.0055
4778      1488.2023      1492.0330      1602.7358
4779      3031.4077      3066.6412      3072.5900
4780      3092.3654      3121.7575      3134.3623
4781      3168.0763      3189.7552      3887.1174

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4782 Zero-point correction (Hartree): 0.139034
4783
4784
4785 TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Ec
4786 ~~~~~
4787 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.80543099
4788 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.73000039
4789 T1 diagnostic: 0.024966
4790 E(MP2/Aug-CC-pVTZ) (Hartree): -420.67733307
4791 E(MP3/Aug-CC-pVTZ) (Hartree): -420.71333383
4792 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.69231131
4793 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.72403263
4794 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.12957042
4795 E(UHF/Aug-CC-pVTZ) (Hartree): -419.11164555
4796 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41459562
4797 Electronic state : 2-A
4798 Cartesian coordinates (Angs):
4799 O 1.611663 -1.284114 -0.619711
4800 H 0.570609 -1.436504 0.047100
4801 C -0.397947 -1.100677 0.836472
4802 O 2.231586 -0.228477 0.005948
4803 C -0.728993 0.240864 0.373594
4804 C 1.585033 0.992460 -0.352959
4805 C 0.358900 1.279457 0.506288
4806 H 0.156254 -1.138816 1.772511
4807 H -1.154259 -1.878237 0.771877
4808 C -1.881294 0.561876 -0.234616
4809 O -2.930091 -0.252592 -0.482316
4810 H -2.076507 1.567403 -0.583044
4811 H 2.343442 1.759914 -0.195592
4812 H 1.326531 0.944954 -1.412172
4813 H -0.024832 2.261609 0.223290
4814 H 0.680104 1.342327 1.549750
4815 H -2.740806 -1.145064 -0.177763
4816 Rotational constants (GHz): 3.7713900 1.2756300 1.0917400
4817 Vibrational harmonic frequencies (cm-1):
4818 i2187.2165 79.1229 145.5697
4819 202.8478 290.9588 295.2709
4820 344.0117 403.4398 455.9409
4821 495.2855 550.5102 563.2053
4822 629.2395 656.4428 815.4285
4823 873.4114 917.9509 956.2470
4824 990.7497 1016.8466 1060.0645
4825 1081.7357 1118.5491 1190.0307
4826 1204.8801 1238.1535 1253.3422
4827 1299.2440 1329.1686 1375.6154
4828 1396.7598 1416.0353 1465.7503
4829 1478.7994 1485.3532 1530.7273
4830 1702.6711 3050.4029 3069.6122
4831 3098.1448 3102.9731 3128.3971
4832 3176.8308 3215.6662 3865.5866
4833 Zero-point correction (Hartree): 0.134451
4834
4835 TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Et
4836 ~~~~~
4837 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41378992
4838 Electronic state : 2-A
4839 Cartesian coordinates (Angs):
4840 O 1.601501 -1.290271 -0.618535
4841 H 0.561291 -1.438259 0.056889
4842 C -0.401768 -1.097574 0.847814
4843 O 2.232270 -0.235626 0.001025
4844 C -0.713173 0.247279 0.381248
4845 C 1.594707 0.986734 -0.362118
4846 C 0.371862 1.287446 0.498634
4847 H 0.154954 -1.145404 1.781839
4848 H -1.189898 -1.835589 0.756039
4849 C -1.868947 0.544929 -0.223165
4850 O -2.847699 -0.382535 -0.401426
4851 H -2.078130 1.543523 -0.589924
4852 H 2.358378 1.750500 -0.211240
4853 H 1.332110 0.935967 -1.420313

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4854      H      -0.010168      2.268012      0.206377
4855      H      0.697337      1.359552      1.540003
4856      H      -3.610527      0.016269      -0.822647
4857 Rotational constants (GHz):      3.7784100      1.2856200      1.0982000
4858 Vibrational harmonic frequencies (cm-1):
4859      i2126.1464      82.8438      145.7752
4860      213.6238      269.8116      277.2568
4861      325.9406      373.3494      448.8572
4862      472.1455      554.2206      568.7976
4863      633.4221      661.9724      823.5970
4864      875.3510      878.8346      957.0137
4865      1001.7419      1015.9198      1062.1319
4866      1082.5804      1119.0508      1198.9166
4867      1199.9316      1231.2216      1252.2669
4868      1295.3559      1318.6255      1377.5621
4869      1397.1068      1404.6352      1462.3339
4870      1478.6047      1479.7281      1516.7170
4871      1730.1079      3050.1858      3067.5503
4872      3099.5063      3107.3536      3126.1656
4873      3182.5087      3211.7110      3914.6619
4874 Zero-point correction (Hartree): 0.134291
4875
4876 TS.HOHCCH3CH2CH2OO.1-6Hshift.b.Ec
4877 ~~~~~
4878 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41342897
4879 Electronic state : 2-A
4880 Cartesian coordinates (Angs):
4881      O      -1.809153      1.189157      -0.280637
4882      H      -0.693200      1.491482      0.191782
4883      C      0.459690      1.311138      0.776573
4884      O      -1.506597      0.067604      -1.009623
4885      C      0.653638      -0.107794      0.532762
4886      C      -1.543084      -1.075315      -0.157669
4887      C      -0.494299      -0.994585      0.960701
4888      H      0.164990      1.569807      1.791662
4889      H      1.170044      2.019741      0.358664
4890      C      1.682250      -0.631587      -0.156204
4891      O      2.736439      0.031551      -0.672135
4892      H      1.754807      -1.694854      -0.345186
4893      H      -2.553466      -1.197939      0.236613
4894      H      -1.317258      -1.896094      -0.838222
4895      H      -0.152773      -2.001917      1.198934
4896      H      -0.942200      -0.582073      1.864560
4897      H      2.654362      0.974213      -0.496627
4898 Rotational constants (GHz):      3.3187200      1.4055600      1.2662400
4899 Vibrational harmonic frequencies (cm-1):
4900      i2094.4757      79.0026      123.8287
4901      232.6307      277.1059      301.8495
4902      371.7860      378.3727      434.8235
4903      486.2273      537.4493      568.2219
4904      625.1325      708.2326      807.3081
4905      858.3569      921.8416      954.5784
4906      1018.9063      1030.5444      1058.5716
4907      1082.5619      1126.5080      1200.3832
4908      1219.9226      1253.2084      1266.0461
4909      1287.5495      1327.3345      1364.0460
4910      1396.2710      1414.5928      1482.8872
4911      1488.3685      1498.0181      1501.1903
4912      1689.9085      3068.2305      3082.1468
4913      3098.4667      3116.4651      3135.8086
4914      3174.3543      3212.3579      3857.4644
4915 Zero-point correction (Hartree): 0.134683
4916
4917 TS.HOHCCH3CH2CH2OO.1-6Hshift.b.Et
4918 ~~~~~
4919 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41202505
4920 Electronic state : 2-A
4921 Cartesian coordinates (Angs):
4922      O      -1.801016      1.194880      -0.292037
4923      H      -0.680972      1.494659      0.182105
4924      C      0.458122      1.309432      0.788425
4925      O      -1.505795      0.067479      -1.018020

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4926 C 0.640213 -0.110418 0.546060
4927 C -1.555137 -1.071067 -0.163841
4928 C -0.505830 -1.004294 0.957098
4929 H 0.137967 1.569895 1.795354
4930 H 1.204489 1.976818 0.373802
4931 C 1.677405 -0.607886 -0.141367
4932 O 2.680110 0.183750 -0.600182
4933 H 1.766000 -1.668997 -0.347278
4934 H -2.566519 -1.181391 0.231818
4935 H -1.340686 -1.896938 -0.842239
4936 H -0.165710 -2.015214 1.183006
4937 H -0.955428 -0.603189 1.865159
4938 H 3.325829 -0.339119 -1.078065
4939 Rotational constants (GHz): 3.3264600 1.4097200 1.2706800
4940 Vibrational harmonic frequencies (cm-1):
4941 i2051.6284 80.8964 118.0649
4942 234.7208 253.7706 296.7965
4943 327.8990 367.3283 412.4711
4944 463.3578 542.0591 565.4153
4945 629.6163 708.5276 808.9682
4946 856.5643 886.7265 954.9900
4947 1018.2313 1030.5736 1064.8990
4948 1082.5759 1127.6163 1207.4368
4949 1210.8433 1252.4923 1264.9906
4950 1289.6721 1309.7406 1357.9237
4951 1397.5991 1405.8849 1478.3326
4952 1482.6085 1488.6295 1499.8821
4953 1716.0912 3066.0063 3080.8514
4954 3108.1941 3113.8368 3133.5914
4955 3180.4327 3210.1388 3913.5482
4956 Zero-point correction (Hartree): 0.134414
4957
4958
4959 #####
4960 Z-HOCH=C(CH3)CH2CH2OO ring closure and H-shift
4961 #####
4962
4963 HOCHCCH3CH2CH2OO.Zcpmm
4964 ~~~~~
4965 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44926728
4966 Electronic state : 2-A
4967 Cartesian coordinates (Angs):
4968 C 1.130828 1.189643 0.118372
4969 C 1.238603 -0.132009 -0.010035
4970 C 0.223458 -1.204350 0.298823
4971 C -1.174937 -0.855596 0.776147
4972 O -2.076071 -0.621963 -0.337399
4973 O -1.939195 0.550472 -0.866455
4974 O 0.048799 1.933320 0.470619
4975 H 2.005167 1.806843 -0.055894
4976 C 2.555327 -0.707592 -0.455973
4977 H 0.121413 -1.869420 -0.565394
4978 H 0.663012 -1.830250 1.083227
4979 H -1.627782 -1.712607 1.269338
4980 H -1.213156 0.009725 1.433576
4981 H -0.745437 1.559668 0.057560
4982 H 3.299289 0.071191 -0.610861
4983 H 2.443891 -1.258622 -1.393007
4984 H 2.945669 -1.411728 0.283331
4985 Rotational constants (GHz): 2.8902200 1.5369100 1.1689500
4986 Vibrational harmonic frequencies (cm-1):
4987 24.0365 77.6570 189.7251
4988 198.5005 212.4232 301.1457
4989 319.7088 342.3071 426.8330
4990 433.3245 555.5785 612.1342
4991 683.9066 774.3618 863.0769
4992 915.0358 972.8046 1009.5127
4993 1050.9749 1071.7262 1096.5676
4994 1181.8355 1220.7331 1247.8945
4995 1277.4254 1332.8511 1356.0380
4996 1407.6980 1409.2349 1419.2418
4997 1438.9876 1461.5529 1484.0105

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4998      1501.8632          1507.0806          1769.4280
4999      3030.3042          3041.7617          3055.8862
5000      3088.3897          3111.8810          3143.4802
5001      3168.9225          3179.4980          3648.0915
5002 Zero-point correction (Hartree): 0.140370
5003
5004 HOCHCCH3CH2CH2OO.Zcppc
5005 ~~~~~
5006 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44991842
5007 Electronic state : 2-A
5008 Cartesian coordinates (Angs):
5009   C      1.302368      1.134243      -0.052999
5010   C      1.292066      -0.197500      -0.038492
5011   C      0.113401      -1.112402      0.187562
5012   C     -1.101218      -0.564118      0.907252
5013   O     -1.906118      0.273034      0.035929
5014   O     -2.522093      -0.422441      -0.870935
5015   O      0.278841      2.017500      0.086638
5016   H      2.242014      1.657752      -0.178460
5017   C      2.581383      -0.932962      -0.282837
5018   H     -0.224491      -1.555842      -0.754835
5019   H      0.469624      -1.953295      0.789785
5020   H     -1.753771      -1.364950      1.247106
5021   H     -0.836395      0.090558      1.735721
5022   H     -0.571467      1.619975      -0.129949
5023   H      3.407289      -0.247262      -0.461502
5024   H      2.495186      -1.588545      -1.153039
5025   H      2.838972      -1.566692      0.569206
5026 Rotational constants (GHz):   3.0876200      1.3938000      1.0892800
5027 Vibrational harmonic frequencies (cm-1):
5028      41.4157          88.8959          158.4002
5029     203.7030         214.9268         267.4457
5030     306.5270         349.4743         426.3144
5031     468.9643         540.3332         555.0457
5032     616.7284         783.5881         848.6957
5033     920.2684         977.4469        1010.4465
5034    1023.8451        1070.5587        1118.5778
5035    1177.7980        1205.3420        1226.1172
5036    1285.3179        1308.7509        1328.8084
5037    1396.5434        1402.0385        1419.5250
5038    1434.5639        1466.7983        1484.7455
5039    1489.9621        1503.0773        1770.8431
5040    3041.0376        3043.7765        3071.5466
5041    3088.6966        3103.7687        3142.8778
5042    3164.1479        3197.6601        3816.3222
5043 Zero-point correction (Hartree): 0.140248
5044
5045 HOCHCCH3CH2CH2OO.Zcptt
5046 ~~~~~
5047 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44798473
5048 Electronic state : 2-A
5049 Cartesian coordinates (Angs):
5050   C      1.111782      1.202708      -0.048985
5051   C      1.321607      -0.106468      0.000181
5052   C      0.372817      -1.143483      0.544186
5053   C     -1.082610      -0.764033      0.699462
5054   O     -1.584852      -0.416972      -0.610449
5055   O     -2.785048      0.066786      -0.547755
5056   O     -0.001108      1.821837      0.451410
5057   H      1.860828      1.861847      -0.473951
5058   C      2.623586      -0.662260      -0.501470
5059   H      0.429102      -2.020392      -0.107435
5060   H      0.730553      -1.483099      1.521683
5061   H     -1.670436      -1.612639      1.049149
5062   H     -1.242637      0.091413      1.346309
5063   H     -0.106376      2.684059      0.045726
5064   H      3.140249      -1.213026      0.288487
5065   H      3.289287      0.123328      -0.854380
5066   H      2.454407      -1.363486      -1.321472
5067 Rotational constants (GHz):   3.1846200      1.3743500      1.1036000
5068 Vibrational harmonic frequencies (cm-1):
5069      41.7350          54.6761          136.9906

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5070      196.3076      224.8723      256.5599
5071      272.2639      309.1968      342.1811
5072      389.1014      449.4868      541.9392
5073      634.2976      783.3691      838.9369
5074      888.2290      1005.2984      1008.2993
5075      1044.5282      1077.3965      1102.6649
5076      1177.8265      1204.1175      1242.1809
5077      1276.9776      1294.3337      1304.8379
5078      1384.4248      1413.3817      1421.5673
5079      1433.4271      1466.7757      1483.4140
5080      1500.1768      1504.6908      1800.8913
5081      3040.9819      3045.7174      3070.2552
5082      3094.2460      3095.3060      3140.4667
5083      3175.4861      3184.9905      3907.3554
5084 Zero-point correction (Hartree): 0.139565
5085
5086 HOCHCCH3CH2CH2OO.Zctpc
5087 ~~~~~
5088 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44515262
5089 Electronic state : 2-A
5090 Cartesian coordinates (Angs):
5091 C      -1.954737      0.702111      -0.066637
5092 C      -1.292319      -0.449834      -0.007600
5093 C      0.197765      -0.675928      0.038772
5094 C      1.099300      0.522071      0.262716
5095 O      2.448422      0.069257      0.503280
5096 O      3.004518      -0.353378      -0.590800
5097 O      -1.493168      1.984059      -0.122603
5098 H      -3.036633      0.701284      -0.068602
5099 C      -2.079754      -1.732002      0.012289
5100 H      0.399791      -1.381335      0.850752
5101 H      0.521164      -1.176700      -0.878264
5102 H      1.155607      1.183685      -0.603865
5103 H      0.836007      1.076985      1.162625
5104 H      -0.546872      2.014117      -0.268205
5105 H      -3.150674      -1.546910      -0.040197
5106 H      -1.874075      -2.301120      0.921577
5107 H      -1.804015      -2.368020      -0.832066
5108 Rotational constants (GHz):      3.2170000      1.1150700      0.8728000
5109 Vibrational harmonic frequencies (cm-1):
5110      25.4172      78.3647      123.7774
5111      170.7876      196.9246      227.9818
5112      287.8662      320.1712      343.9952
5113      406.9443      474.0316      574.1455
5114      604.6082      791.2435      883.9768
5115      921.8576      975.5759      1005.4773
5116      1051.2166      1083.7976      1123.9663
5117      1173.5548      1183.5992      1246.7477
5118      1278.9744      1303.1522      1346.0534
5119      1355.9993      1411.8816      1419.2780
5120      1434.4271      1483.0102      1487.6386
5121      1504.0531      1515.7753      1779.0413
5122      3042.4192      3047.0036      3065.3448
5123      3076.6750      3095.3128      3140.2386
5124      3146.0393      3213.1117      3925.5280
5125 Zero-point correction (Hartree): 0.139759
5126
5127 HOCHCCH3CH2CH2OO.Zctpt
5128 ~~~~~
5129 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44961874
5130 Electronic state : 2-A
5131 Cartesian coordinates (Angs):
5132 C      -1.910461      0.687968      -0.132568
5133 C      -1.279218      -0.468402      0.020212
5134 C      0.193008      -0.658194      0.265105
5135 C      1.080153      0.569106      0.189292
5136 O      2.452055      0.165698      0.416055
5137 O      2.935128      -0.475134      -0.603425
5138 O      -1.293149      1.911294      -0.076811
5139 H      -2.980286      0.712591      -0.304352
5140 C      -2.063894      -1.748177      -0.033569
5141 H      0.327699      -1.125570      1.246155

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5142      H      0.572150      -1.379256      -0.464639
5143      H      1.037631      1.055505      -0.781581
5144      H      0.876641      1.290249      0.974713
5145      H     -1.926284      2.602984      -0.272360
5146      H     -3.124880     -1.566021     -0.195353
5147      H     -1.952764     -2.308170      0.897707
5148      H     -1.699699     -2.390990     -0.837673
5149      Rotational constants (GHz):   3.1892200      1.1588400      0.8959600
5150      Vibrational harmonic frequencies (cm-1):
5151          34.7291          89.3545          133.3168
5152          169.8388          185.6689          216.9190
5153          265.2060          311.7155          345.4390
5154          397.6089          456.9792          567.6594
5155          604.5898          790.8203          878.8482
5156          888.6487          966.6599          1004.5028
5157          1046.3952          1088.0718          1117.8057
5158          1174.1608          1201.1280          1238.9297
5159          1268.2535          1294.4717          1332.8919
5160          1353.3483          1407.4306          1422.2608
5161          1431.8591          1481.9638          1483.7375
5162          1493.8845          1504.6745          1803.5656
5163          3037.9988          3048.1738          3074.2592
5164          3098.3665          3123.7778          3140.1703
5165          3183.9106          3189.7624          3920.7129
5166      Zero-point correction (Hartree): 0.139584
5167
5168      HOCHCCH3CH2CH2OO.Zgmmc
5169      ~~~~~
5170      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45072057
5171      Electronic state : 2-A
5172      Cartesian coordinates (Angs):
5173      C      1.989804      0.208706      -0.313793
5174      C      0.826097      0.596713      0.196926
5175      C     -0.065618     -0.359934      0.947609
5176      C     -0.945036     -1.198469      0.032037
5177      O     -1.823393     -0.354934     -0.746128
5178      O     -2.718326      0.210818      0.003761
5179      O      2.543784     -1.034946     -0.234980
5180      H      2.629282      0.883352     -0.866545
5181      C      0.339780      2.005975      0.026131
5182      H      0.509180     -1.048789      1.575217
5183      H     -0.716760      0.191344      1.626975
5184      H     -0.361834     -1.730557     -0.718451
5185      H     -1.574360     -1.891379      0.589167
5186      H      2.003592     -1.606928      0.316729
5187      H     -0.624440      2.029662     -0.484220
5188      H      1.047187      2.600169     -0.550200
5189      H      0.201475      2.487689      0.996649
5190      Rotational constants (GHz):   3.3559600      1.2984200      1.0556100
5191      Vibrational harmonic frequencies (cm-1):
5192          40.9393          66.7204          142.3623
5193          169.4739          193.3883          289.2887
5194          302.5363          332.5190          387.9733
5195          421.2621          534.2735          570.9138
5196          613.4048          790.2132          848.8792
5197          917.2383          948.1353          1009.7677
5198          1031.0112          1071.8344          1097.2237
5199          1177.1280          1189.8680          1239.8074
5200          1266.6471          1299.3519          1313.3219
5201          1364.8695          1399.9540          1410.5359
5202          1423.9707          1481.6530          1488.0521
5203          1493.7835          1504.0293          1772.4866
5204          3041.5945          3051.1800          3087.2260
5205          3106.0248          3108.3076          3140.4678
5206          3149.7913          3219.9452          3871.8849
5207      Zero-point correction (Hartree): 0.139837
5208
5209      HOCHCCH3CH2CH2OO.Zgmmt
5210      ~~~~~
5211      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45252662
5212      Electronic state : 2-A
5213      Cartesian coordinates (Angs):

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5214	C	1.937512	-0.188903	-0.323205		
5215	C	0.805674	-0.633427	0.203909		
5216	C	-0.070602	0.296764	1.002205		
5217	C	-0.912154	1.199539	0.117663		
5218	O	-1.770587	0.420154	-0.748972		
5219	O	-2.692514	-0.194761	-0.074327		
5220	O	2.332130	1.115667	-0.158502		
5221	H	2.592745	-0.818658	-0.913257		
5222	C	0.345735	-2.044789	0.001752		
5223	H	-0.736259	-0.273491	1.650451		
5224	H	0.540127	0.946490	1.631171		
5225	H	-1.556161	1.858637	0.698149		
5226	H	-0.290957	1.773311	-0.566664		
5227	H	3.207424	1.243071	-0.526465		
5228	H	0.236027	-2.554879	0.961179		
5229	H	1.048398	-2.611123	-0.608111		
5230	H	-0.630563	-2.066941	-0.485989		
5231	Rotational constants (GHz):			3.2226000	1.3598600	1.0889800
5232	Vibrational harmonic frequencies (cm-1):					
5233		42.8964	65.6193		142.7389	
5234		167.1418	189.3145		227.3757	
5235		288.6729	320.2290		354.3743	
5236		391.2909	531.7092		574.5252	
5237		617.5566	798.6739		848.1971	
5238		878.3959	950.0970		1009.2751	
5239		1028.4883	1072.7596		1100.3847	
5240		1182.1118	1197.7530		1226.2701	
5241		1262.8379	1299.1358		1318.7714	
5242		1362.3503	1390.7542		1407.4201	
5243		1423.0941	1474.4708		1481.9141	
5244		1491.8754	1503.0181		1794.6668	
5245		3050.6164	3075.4455		3095.1329	
5246		3105.4278	3124.1288		3136.8179	
5247		3163.0238	3188.8317		3919.8657	
5248	Zero-point correction (Hartree):			0.139596		
5249						
5250	HOCHCCH3CH2CH2OO.Zgmpc					
5251	~~~~~					
5252	E(UM062X/Aug-CC-pVTZ) (Hartree):			-421.44933493		
5253	Electronic state : 2-A					
5254	Cartesian coordinates (Angs):					
5255	C	1.782933	0.110969	-0.461481		
5256	C	0.787914	0.564110	0.293452		
5257	C	-0.004858	-0.353506	1.188551		
5258	C	-1.119576	-1.100004	0.464262		
5259	O	-2.097280	-0.166343	-0.034011		
5260	O	-1.863617	0.176104	-1.265665		
5261	O	2.230116	-1.173930	-0.541764		
5262	H	2.351128	0.759979	-1.113582		
5263	C	0.402348	2.013945	0.272419		
5264	H	0.633315	-1.104711	1.666413		
5265	H	-0.447622	0.220846	2.003959		
5266	H	-0.752162	-1.663208	-0.392318		
5267	H	-1.670244	-1.749300	1.143820		
5268	H	1.742706	-1.737215	0.064959		
5269	H	1.019339	2.575114	-0.427427		
5270	H	0.518723	2.460585	1.262732		
5271	H	-0.641492	2.138175	-0.020258		
5272	Rotational constants (GHz):			2.7294700	1.4523500	1.2564800
5273	Vibrational harmonic frequencies (cm-1):					
5274		48.7034	88.8848		105.7465	
5275		169.7326	194.4482		263.3324	
5276		294.1944	342.2144		378.2690	
5277		420.1903	528.8116		569.2579	
5278		604.0069	779.9811		872.6524	
5279		918.2761	938.0512		1019.9914	
5280		1036.1814	1069.0318		1087.0051	
5281		1177.5739	1191.8773		1236.3051	
5282		1258.3935	1300.3856		1329.8438	
5283		1370.3998	1391.7892		1410.7006	
5284		1423.2240	1481.1253		1483.1346	
5285		1491.9566	1502.5607		1774.5235	

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5286      3036.0261              3048.8346              3086.6194
5287      3098.1440              3104.4574              3141.0885
5288      3151.2493              3221.7205              3877.9113
5289 Zero-point correction (Hartree): 0.139695
5290
5291 HOCHCCH3CH2CH2OO.Zgmp
5292 ~~~~~
5293 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45143242
5294 Electronic state : 2-A
5295 Cartesian coordinates (Angs):
5296   C      1.737121      0.063987      -0.456171
5297   C      0.779185      0.601911      0.284741
5298   C     -0.011417     -0.262962      1.230502
5299   C     -1.095726     -1.067273      0.528296
5300   O     -2.080353     -0.182475     -0.047689
5301   O     -1.816170      0.105465     -1.286838
5302   O      2.025882     -1.274731     -0.377320
5303   H      2.322426      0.642226     -1.160931
5304   C      0.431283      2.055253      0.184803
5305   H      0.645789     -0.982963      1.721704
5306   H     -0.471362      0.351282      2.006168
5307   H     -0.687958     -1.672298     -0.278096
5308   H     -1.653186     -1.683368      1.232423
5309   H      2.762741     -1.485878     -0.951833
5310   H      1.056551      2.565317     -0.546653
5311   H      0.559200      2.551269      1.149607
5312   H     -0.611754      2.182851     -0.110643
5313 Rotational constants (GHz):      2.6594900      1.5166600      1.2947300
5314 Vibrational harmonic frequencies (cm-1):
5315      45.6868              87.5472              103.4694
5316     176.4799             193.2789             234.0679
5317     281.1618             330.6672             348.3348
5318     397.9300             526.6332             570.6983
5319     607.3737             787.0443             870.6459
5320     876.5100             939.9320            1016.1217
5321    1035.2074            1070.4997            1088.9494
5322    1183.0382            1198.2857            1234.1057
5323    1242.8935            1310.5007            1325.2313
5324    1366.3777            1382.6238            1408.4118
5325    1421.3718            1472.8623            1481.4155
5326    1485.9827            1501.6823            1796.0196
5327    3048.6422            3067.6456            3095.2545
5328    3103.2459            3114.5449            3137.1026
5329    3164.9746            3192.3371            3920.0508
5330 Zero-point correction (Hartree): 0.139521
5331
5332 HOCHCCH3CH2CH2OO.Zgmtc
5333 ~~~~~
5334 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44965828
5335 Electronic state : 2-A
5336 Cartesian coordinates (Angs):
5337   C      1.939070      -0.129593      -0.510460
5338   C      1.011908      0.552033      0.154141
5339   C      0.089828     -0.124896      1.137626
5340   C     -1.102311     -0.796531      0.478876
5341   O     -1.901160      0.241346     -0.129589
5342   O     -2.928763     -0.251629     -0.747865
5343   O      2.204870     -1.462661     -0.411107
5344   H      2.596994      0.343679     -1.226528
5345   C      0.832012      2.025207     -0.065783
5346   H      0.613282     -0.886342      1.724394
5347   H     -0.277367      0.604850      1.861275
5348   H     -0.805748     -1.479880     -0.317169
5349   H     -1.739491     -1.315071      1.194778
5350   H      1.645233     -1.868477      0.256231
5351   H     -0.181116      2.248067     -0.403871
5352   H      1.532750      2.401156     -0.809499
5353   H      0.992846      2.578250      0.862484
5354 Rotational constants (GHz):      3.0103600      1.2180800      1.0238900
5355 Vibrational harmonic frequencies (cm-1):
5356      41.4082              75.5142              119.9922
5357     173.6373             195.7565             273.3382

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5358      284.5693      314.9211      381.6568
5359      392.4674      489.2844      577.5848
5360      622.5919      786.1280      841.5853
5361      921.7769      977.9475     1025.9881
5362     1049.6434     1070.3287     1087.9050
5363     1176.7408     1196.4185     1244.8787
5364     1276.7479     1294.6012     1306.7742
5365     1367.8364     1402.7677     1410.5180
5366     1422.6055     1481.9338     1491.9293
5367     1499.3863     1505.2994     1775.1273
5368     3043.9052     3050.1255     3078.3368
5369     3098.5812     3105.7877     3137.3926
5370     3141.1266     3219.1818     3876.0556
5371 Zero-point correction (Hartree): 0.139670
5372
5373 HOCHCCH3CH2CH2OO.Zgmtt
5374 ~~~~~
5375 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45153725
5376 Electronic state : 2-A
5377 Cartesian coordinates (Angs):
5378      C      1.880460      -0.188728      -0.506354
5379      C      1.011983      0.572220      0.144584
5380      C      0.096187      -0.044062      1.170887
5381      C     -1.088956      -0.750130      0.542855
5382      O     -1.874325      0.247915      -0.150741
5383      O     -2.889016      -0.281038      -0.759924
5384      O      1.966358      -1.535761      -0.260800
5385      H      2.549319      0.206647      -1.261521
5386      C      0.889736      2.038765      -0.135028
5387      H      0.635776      -0.789604      1.756667
5388      H     -0.265876      0.721474      1.859021
5389      H     -0.775125      -1.488032      -0.193238
5390      H     -1.741217      -1.213280      1.282420
5391      H      2.681224      -1.918254      -0.771152
5392      H     -0.121915      2.284581      -0.462218
5393      H      1.588769      2.357583      -0.907021
5394      H      1.088445      2.621573      0.767096
5395 Rotational constants (GHz):      2.9146800      1.2701200      1.0549900
5396 Vibrational harmonic frequencies (cm-1):
5397      42.7504      72.7486      117.7732
5398      178.3161      198.3964      245.1979
5399      285.7025      300.6185      347.4777
5400      375.8057      479.9849      582.0684
5401      623.8398      794.2295      840.9293
5402      877.0195      983.2028     1025.2759
5403     1042.4252     1075.1355     1088.8214
5404     1181.7763     1199.4183     1228.8308
5405     1269.4839     1298.6573     1317.1769
5406     1362.1365     1396.8202     1406.5667
5407     1421.5974     1473.6656     1482.2938
5408     1502.4534     1505.0698     1794.8735
5409     3050.0418     3071.5608     3089.2414
5410     3105.2245     3118.0648     3137.4365
5411     3152.1171     3190.2015     3919.1491
5412 Zero-point correction (Hartree): 0.139541
5413
5414 HOCHCCH3CH2CH2OO.Zgpmc
5415 ~~~~~
5416 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45240759
5417 Electronic state : 2-A
5418 Cartesian coordinates (Angs):
5419      C      1.224405      1.071636      0.115225
5420      C      1.093779      -0.235051     -0.098039
5421      C      0.100153      -0.780139     -1.085588
5422      C     -1.252678     -1.100586     -0.463721
5423      O     -1.846708      0.122595      0.018775
5424      O     -1.626316      0.305916      1.289588
5425      O      0.501693      2.068096     -0.462038
5426      H      1.972419      1.462813      0.792974
5427      C      1.914167     -1.228647      0.668231
5428      H     -0.054263     -0.084383     -1.913673
5429      H      0.486521     -1.704024     -1.522661

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5430	H	-1.953299	-1.490637	-1.200553		
5431	H	-1.174329	-1.775711	0.385619		
5432	H	-0.359671	1.738532	-0.737933		
5433	H	1.276658	-1.891783	1.259108		
5434	H	2.597727	-0.732283	1.354866		
5435	H	2.499926	-1.858654	-0.004990		
5436	Rotational constants (GHz):		2.4124700	1.7738900	1.3808600	
5437	Vibrational harmonic frequencies (cm-1):					
5438		53.2250	92.8312		110.8594	
5439		190.7603	202.6129		259.5484	
5440		307.3685	344.1491		378.7662	
5441		437.9692	526.9002		582.3746	
5442		602.7792	774.7668		862.8993	
5443		918.0243	979.9982		993.6932	
5444		1030.2699	1066.0743		1084.6708	
5445		1184.8261	1199.6995		1224.5053	
5446		1269.9523	1306.9516		1323.5696	
5447		1366.7961	1384.1554		1411.7458	
5448		1422.4428	1479.2083		1487.6470	
5449		1488.9137	1500.8396		1764.8020	
5450		3040.9682	3056.5544		3088.9997	
5451		3091.9236	3100.8731		3138.8295	
5452		3159.6501	3206.2195		3848.4104	
5453	Zero-point correction (Hartree): 0.139763					
5454						
5455	HOCHCCH3CH2CH2O.O.Zgppc					
5456	~~~~~					
5457	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.84631979					
5458	E(CCSD/Aug-CC-pVTZ) (Hartree): -420.77536686					
5459	T1 diagnostic: 0.021002					
5460	E(MP2/Aug-CC-pVTZ) (Hartree): -420.72348730					
5461	E(MP3/Aug-CC-pVTZ) (Hartree): -420.76218978					
5462	E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72673939					
5463	E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76408756					
5464	E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18016550					
5465	E(UHF/Aug-CC-pVTZ) (Hartree): -419.17484935					
5466	E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45480404					
5467	Electronic state : 2-A					
5468	Cartesian coordinates (Angs):					
5469	C	-1.212494	1.178878	-0.172259		
5470	C	-1.161420	-0.120390	0.111263		
5471	C	-0.063202	-0.717029	0.948967		
5472	C	1.038780	-1.369346	0.134278		
5473	O	1.696511	-0.421967	-0.746504		
5474	O	2.167644	0.596960	-0.102567		
5475	O	-0.325313	2.138965	0.186655		
5476	H	-2.036973	1.595904	-0.737046		
5477	C	-2.216824	-1.058983	-0.394807		
5478	H	0.382627	0.021461	1.615150		
5479	H	-0.480267	-1.497923	1.590496		
5480	H	1.813810	-1.800446	0.767521		
5481	H	0.656562	-2.124151	-0.549973		
5482	H	0.523487	1.748654	0.428011		
5483	H	-2.961550	-0.533786	-0.990435		
5484	H	-2.729056	-1.555064	0.433194		
5485	H	-1.788407	-1.845085	-1.022259		
5486	Rotational constants (GHz):		2.6040800	1.7509900	1.2063500	
5487	Vibrational harmonic frequencies (cm-1):					
5488		44.7648	126.1924		134.7356	
5489		191.5450	199.3966		275.1822	
5490		313.8253	352.8731		395.9432	
5491		453.1138	531.0890		580.7217	
5492		633.5081	769.4751		848.0543	
5493		928.5450	971.3108		982.7232	
5494		1032.1058	1072.3501		1091.7482	
5495		1189.0619	1205.0560		1249.2238	
5496		1274.8693	1304.4794		1327.1191	
5497		1372.8944	1403.2116		1416.6370	
5498		1424.7850	1480.5896		1492.7890	
5499		1495.1440	1502.5296		1770.9465	
5500		3040.2241	3062.2873		3085.6176	
5501		3092.1114	3115.3914		3138.1233	

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5502          3155.0114          3201.6968          3806.0569
5503 Zero-point correction (Hartree): 0.140187
5504
5505 HOCHCCH3CH2CH2OO.Zgppt
5506 ~~~~~
5507 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45053934
5508 Electronic state : 2-A
5509 Cartesian coordinates (Angs):
5510 C      -1.451259      0.979163      -0.222332
5511 C      -1.140884      -0.268690      0.103488
5512 C       0.033012      -0.571021      0.992191
5513 C       1.204235      -1.175474      0.235921
5514 O       1.720483      -0.246319      -0.742162
5515 O       2.350518      0.735054      -0.172919
5516 O      -0.750905      2.051340      0.251475
5517 H      -2.292076      1.204611      -0.869038
5518 C      -1.948873      -1.422287      -0.410435
5519 H       0.381536      0.331125      1.491996
5520 H      -0.260136      -1.289196      1.763415
5521 H       2.025859      -1.431021      0.902989
5522 H       0.917013      -2.045772      -0.351916
5523 H      -1.030789      2.852096      -0.193360
5524 H      -2.767359      -1.083959      -1.044064
5525 H      -2.374184      -1.998170      0.415019
5526 H      -1.338005      -2.110464      -0.999191
5527 Rotational constants (GHz): 2.5793500      1.6307200      1.1579300
5528 Vibrational harmonic frequencies (cm-1):
5529      23.6969      58.4108      132.3345
5530      164.5839      199.0826      216.6921
5531      280.8366      320.5261      381.6193
5532      386.6381      528.8669      572.3737
5533      614.8579      776.2974      854.9305
5534      893.9685      973.2870      992.2028
5535      1030.1971      1072.2597      1095.1143
5536      1184.1722      1200.4864      1231.9331
5537      1262.4902      1303.4023      1328.5719
5538      1356.8879      1397.4897      1415.4413
5539      1423.4672      1472.9296      1483.7819
5540      1495.5237      1502.2582      1800.5278
5541      3044.4417      3056.4649      3090.8389
5542      3096.1945      3134.4264      3134.7851
5543      3154.8935      3177.6820      3922.3740
5544 Zero-point correction (Hartree): 0.139516
5545
5546 HOCHCCH3CH2CH2OO.Zgpptc
5547 ~~~~~
5548 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45306200
5549 Electronic state : 2-A
5550 Cartesian coordinates (Angs):
5551 C      -1.371459      1.110287      -0.212460
5552 C      -1.279054      -0.192751      0.039897
5553 C      -0.238619      -0.760398      0.970525
5554 C       1.076458      -1.083310      0.289359
5555 O       1.692400      0.187561      -0.031864
5556 O       2.794303      0.047624      -0.699848
5557 O      -0.565969      2.095075      0.262908
5558 H      -2.159874      1.507199      -0.839848
5559 C      -2.218373      -1.170693      -0.601847
5560 H      -0.038244      -0.078086      1.801032
5561 H      -0.616913      -1.684079      1.412400
5562 H       1.770432      -1.617850      0.936960
5563 H       0.946632      -1.624807      -0.646736
5564 H       0.302756      1.738926      0.479120
5565 H      -2.920348      -0.670727      -1.267018
5566 H      -2.789432      -1.717126      0.152526
5567 H      -1.674596      -1.914337      -1.190851
5568 Rotational constants (GHz): 2.8029500      1.4171900      1.0897600
5569 Vibrational harmonic frequencies (cm-1):
5570      57.3231      80.2590      130.1165
5571      196.3217      214.8427      249.4889
5572      312.0548      331.1202      379.1148
5573      419.9506      492.9681      589.0586

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5574      621.0146      776.7252      853.3318
5575      924.1319      978.4966      1023.9317
5576      1044.5439     1072.3649     1089.5633
5577      1187.7336     1201.8755     1242.6615
5578      1288.0289     1295.5147     1324.7652
5579      1375.5354     1395.8599     1414.3787
5580      1424.0857     1480.8590     1485.3804
5581      1499.6902     1502.5269     1768.9913
5582      3039.1369     3057.5259     3085.6433
5583      3086.1935     3104.6398     3138.6926
5584      3146.6525     3200.4163     3835.2996
5585 Zero-point correction (Hartree): 0.139922
5586
5587 HOCHCCH3CH2CH2OO.Zgtmp
5588 ~~~~~
5589 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45141848
5590 Electronic state : 2-A
5591 Cartesian coordinates (Angs):
5592   C      1.910795      0.759196      0.121764
5593   C      1.289882     -0.377677     -0.163657
5594   C     -0.151579     -0.373830     -0.595839
5595   C     -1.058966     -0.353502      0.623931
5596   O     -2.443031     -0.497986      0.240163
5597   O     -2.891044      0.578278     -0.330829
5598   O      1.269773      1.963812      0.025290
5599   H      2.943778      0.787010      0.449125
5600   C      1.978439     -1.700807     -0.021869
5601   H     -0.376871      0.502971     -1.201488
5602   H     -0.368963     -1.266471     -1.184824
5603   H     -0.873423     -1.199722      1.283912
5604   H     -0.959773      0.582450      1.170849
5605   H      1.885295      2.681120      0.181772
5606   H      2.995821     -1.587669      0.349828
5607   H      2.019433     -2.220512     -0.981357
5608   H      1.437702     -2.352289      0.669216
5609 Rotational constants (GHz):      3.1249400      1.1802200      0.9183300
5610 Vibrational harmonic frequencies (cm-1):
5611      43.1009      58.2287      115.8739
5612      165.0305      197.0364      238.2868
5613      252.7400      310.3572      332.7529
5614      401.3085      536.1713      573.7785
5615      594.5100      790.6777      875.4494
5616      885.5576      963.3209     1008.2226
5617     1055.7709     1071.9139     1084.4082
5618     1192.6253     1201.1349     1234.1893
5619     1271.0156     1303.6814     1323.4556
5620     1342.5573     1394.4848     1404.8444
5621     1422.0094     1481.0544     1484.2054
5622     1496.6169     1504.6700     1794.8701
5623     3045.1051     3073.9297     3094.3677
5624     3096.8570     3130.5898     3137.3229
5625     3160.9014     3185.7677     3918.9888
5626 Zero-point correction (Hartree): 0.139537
5627
5628 HOCHCCH3CH2CH2OO.Zgtpc
5629 ~~~~~
5630 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45153269
5631 Electronic state : 2-A
5632 Cartesian coordinates (Angs):
5633   C     -2.172461     -0.321246      0.095284
5634   C     -1.165908      0.518131     -0.127722
5635   C      0.187291      0.041686     -0.584998
5636   C      1.068171     -0.279022      0.612972
5637   O      2.385520     -0.687902      0.189328
5638   O      3.064743      0.317159     -0.272783
5639   O     -2.164945     -1.672241     -0.066668
5640   H     -3.137976      0.022345      0.441649
5641   C     -1.322705      1.991198      0.109069
5642   H      0.126622     -0.838889     -1.230495
5643   H      0.680113      0.819819     -1.169329
5644   H      1.185360      0.584699      1.265590
5645   H      0.686718     -1.124351      1.183673

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5646      H      -1.320539      -1.962562      -0.423113
5647      H      -2.308195      2.227326      0.506967
5648      H      -1.184559      2.550868      -0.818376
5649      H      -0.576415      2.360131      0.816786
5650      Rotational constants (GHz):      3.3818200      1.0889300      0.8774500
5651      Vibrational harmonic frequencies (cm-1):
5652      47.0904      59.3591      123.6889
5653      170.7596      199.3611      262.7582
5654      289.7434      348.5679      378.5753
5655      401.8149      542.5799      582.9100
5656      584.9880      790.7431      859.8135
5657      922.9408      969.4043      1012.0313
5658      1055.9308      1070.7385      1080.7951
5659      1181.8975      1203.1236      1241.7774
5660      1275.1277      1291.2127      1326.6449
5661      1338.6892      1396.8576      1407.5070
5662      1424.5132      1482.0798      1488.2826
5663      1500.1410      1517.0705      1774.5180
5664      3046.0285      3051.1932      3094.0154
5665      3095.2825      3107.2019      3139.8687
5666      3155.7517      3215.6197      3868.0294
5667      Zero-point correction (Hartree): 0.139827
5668
5669      HOCHCCH3CH2CH2OO.Zgtpt
5670      ~~~~~
5671      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45212613
5672      Electronic state : 2-A
5673      Cartesian coordinates (Angs):
5674      C      2.127603      -0.341528      -0.095140
5675      C      1.165326      0.542943      0.129471
5676      C      -0.187364      0.093080      0.611583
5677      C      -1.043209      -0.328801      -0.571457
5678      O      -2.372897      -0.693155      -0.141944
5679      O      -3.062456      0.351967      0.198994
5680      O      1.924794      -1.681023      0.107142
5681      H      3.108102      -0.051935      -0.454980
5682      C      1.367680      2.004129      -0.131708
5683      H      -0.093737      -0.750153      1.295365
5684      H      -0.694026      0.907621      1.130262
5685      H      -1.146821      0.470655      -1.304120
5686      H      -0.647740      -1.226149      -1.042759
5687      H      2.747212      -2.160115      -0.002551
5688      H      2.358161      2.207788      -0.536103
5689      H      1.245541      2.581101      0.787141
5690      H      0.627563      2.379937      -0.842295
5691      Rotational constants (GHz):      3.3237100      1.1223700      0.8913600
5692      Vibrational harmonic frequencies (cm-1):
5693      44.5717      62.7876      124.9787
5694      165.7322      198.6336      247.3023
5695      251.3303      323.5266      341.8888
5696      388.0639      534.2879      585.8553
5697      590.3510      792.7493      869.2410
5698      883.3122      966.9106      1011.3992
5699      1053.3917      1076.6941      1081.4453
5700      1191.2637      1199.1809      1233.0549
5701      1281.3985      1292.1512      1332.3943
5702      1337.5528      1393.4216      1403.6697
5703      1422.3264      1480.7076      1484.0234
5704      1495.7953      1503.7741      1794.3768
5705      3046.1018      3078.2855      3095.8321
5706      3096.8492      3128.8474      3136.0435
5707      3162.9429      3187.1175      3917.9089
5708      Zero-point correction (Hartree): 0.139628
5709
5710      HOCHCCH3CH2CH2OO.Zgttc
5711      ~~~~~
5712      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45042784
5713      Electronic state : 2-A
5714      Cartesian coordinates (Angs):
5715      C      2.104641      -0.568463      -0.240010
5716      C      1.312290      0.440597      0.107703
5717      C      -0.027993      0.218210      0.760028

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5718 C -1.112626 0.082160 -0.291915
5719 O -2.377396 -0.051830 0.392218
5720 O -3.360089 -0.181256 -0.444657
5721 O 1.870417 -1.896168 -0.060880
5722 H 3.059988 -0.404822 -0.720364
5723 C 1.705336 1.861328 -0.170639
5724 H -0.036159 -0.666473 1.402354
5725 H -0.266928 1.063845 1.407142
5726 H -1.175497 0.961918 -0.931327
5727 H -0.976950 -0.802550 -0.913781
5728 H 1.034099 -2.032532 0.393316
5729 H 2.655471 1.914321 -0.699395
5730 H 1.798883 2.428605 0.757942
5731 H 0.953749 2.368736 -0.780328
5732 Rotational constants (GHz): 3.3294000 1.0160900 0.8374500
5733 Vibrational harmonic frequencies (cm-1):
5734 38.7932 77.6442 94.8878
5735 139.8178 200.9508 250.4780
5736 290.2145 327.8353 372.3155
5737 417.0661 482.9092 583.9397
5738 592.0907 785.2912 855.9910
5739 925.0215 1001.1203 1021.6723
5740 1060.4102 1069.2113 1106.8713
5741 1179.7885 1189.0477 1240.3022
5742 1286.7704 1294.3287 1310.4366
5743 1338.5068 1401.1275 1410.1341
5744 1425.0838 1483.4063 1498.2418
5745 1503.4465 1519.3107 1774.2744
5746 3045.0797 3053.4774 3085.9181
5747 3093.3019 3098.8228 3140.5612
5748 3143.5995 3217.9271 3868.9362
5749 Zero-point correction (Hartree): 0.139643
5750
5751 HOCHCCH3CH2CH2OO.Zgttt
5752 ~~~~~
5753 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45104760
5754 Electronic state : 2-A
5755 Cartesian coordinates (Angs):
5756 C -2.053189 0.599099 -0.225343
5757 C -1.317933 -0.453371 0.106343
5758 C 0.021659 -0.269816 0.769411
5759 C 1.093315 -0.063957 -0.283016
5760 O 2.369121 0.010541 0.392306
5761 O 3.344002 0.172234 -0.447333
5762 O -1.626086 1.874716 0.028101
5763 H -3.014937 0.501082 -0.715376
5764 C -1.764448 -1.849604 -0.202493
5765 H 0.006837 0.594417 1.432625
5766 H 0.267704 -1.151374 1.363568
5767 H 1.148329 -0.892628 -0.988741
5768 H 0.949566 0.869895 -0.824176
5769 H -2.309986 2.504765 -0.202678
5770 H -2.716664 -1.859774 -0.730790
5771 H -1.874359 -2.432432 0.714363
5772 H -1.029221 -2.367983 -0.822790
5773 Rotational constants (GHz): 3.3026200 1.0414100 0.8528300
5774 Vibrational harmonic frequencies (cm-1):
5775 35.2380 76.3247 96.6421
5776 134.4576 191.2049 232.7439
5777 239.3380 307.2442 337.3690
5778 392.6337 476.7409 587.3282
5779 593.6222 784.7065 865.6428
5780 884.6411 1000.0943 1019.4168
5781 1061.7149 1066.9938 1109.0101
5782 1185.1855 1197.6959 1224.3470
5783 1291.9015 1296.4355 1313.5955
5784 1338.5135 1394.3958 1409.3311
5785 1422.4374 1481.1256 1490.5724
5786 1501.6101 1505.9176 1795.8774
5787 3045.8563 3073.8538 3087.7664
5788 3095.3978 3123.9218 3137.3848
5789 3150.5048 3187.7628 3918.4496

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5790 Zero-point correction (Hartree): 0.139339
5791
5792 HOCHCCH3CH2CH2OO.Zlpmt
5793 ~~~~~
5794 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45151641
5795 Electronic state : 2-A
5796 Cartesian coordinates (Angs):
5797 C 1.709130 -0.226743 -0.323255
5798 C 0.795301 0.611124 0.149026
5799 C -0.135776 0.198069 1.251049
5800 C -1.593007 0.117408 0.813127
5801 O -1.758911 -0.884811 -0.205799
5802 O -1.500924 -0.409033 -1.388435
5803 O 1.864615 -1.493909 0.166624
5804 H 2.384572 0.062005 -1.120454
5805 C 0.651378 1.990819 -0.417397
5806 H 0.163263 -0.765875 1.658631
5807 H -0.093554 0.929779 2.064129
5808 H -2.229950 -0.209878 1.632958
5809 H -1.960679 1.057390 0.405589
5810 H 2.506297 -1.971295 -0.360311
5811 H -0.318260 2.112806 -0.904269
5812 H 1.422064 2.196291 -1.158778
5813 H 0.725858 2.746742 0.368080
5814 Rotational constants (GHz): 2.4927700 1.5844300 1.3619900
5815 Vibrational harmonic frequencies (cm-1):
5816 38.5354 95.0414 105.8187
5817 171.9951 201.3511 235.2032
5818 277.7503 319.9738 379.0078
5819 387.2898 530.7926 560.7205
5820 611.0331 778.5857 863.2415
5821 888.8703 973.1139 999.1345
5822 1033.8970 1072.5724 1078.9874
5823 1185.7482 1204.4895 1233.3178
5824 1243.8367 1315.2524 1326.5390
5825 1359.1635 1393.7535 1416.5175
5826 1419.5859 1471.0735 1483.8980
5827 1491.5533 1505.6461 1794.0954
5828 3046.5267 3048.6438 3096.0378
5829 3101.3892 3132.5287 3136.3074
5830 3157.4578 3183.7466 3922.8972
5831 Zero-point correction (Hartree): 0.139590
5832
5833 HOCHCCH3CH2CH2OO.Zlppt
5834 ~~~~~
5835 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45063142
5836 Electronic state : 2-A
5837 Cartesian coordinates (Angs):
5838 C 1.819552 -0.330908 -0.295792
5839 C 0.907450 0.556593 0.077349
5840 C -0.151373 0.204237 1.084539
5841 C -1.554601 0.556428 0.624112
5842 O -1.857585 -0.056339 -0.648478
5843 O -1.921103 -1.348537 -0.548453
5844 O 1.866143 -1.596525 0.219269
5845 H 2.588540 -0.082635 -1.018835
5846 C 0.908945 1.941423 -0.497872
5847 H -0.110448 -0.857348 1.317768
5848 H 0.020190 0.753581 2.016356
5849 H -2.305341 0.217826 1.336218
5850 H -1.677583 1.621621 0.436252
5851 H 2.486993 -2.129793 -0.278425
5852 H 1.785546 2.109178 -1.121442
5853 H 0.908141 2.695031 0.293948
5854 H 0.024480 2.117110 -1.114549
5855 Rotational constants (GHz): 2.5875400 1.5287200 1.1667400
5856 Vibrational harmonic frequencies (cm-1):
5857 25.7644 49.2800 143.5286
5858 167.0971 194.1854 236.4249
5859 278.4320 313.8739 362.1245
5860 405.1788 512.5127 567.3335
5861 624.1476 775.2516 848.2362

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5862      891.7903          976.0122          984.2137
5863      1030.8415         1070.1423         1099.5314
5864      1187.0526         1205.5319         1235.7481
5865      1259.3822         1295.7444         1330.1128
5866      1357.1006         1401.9563         1418.2209
5867      1421.4405         1472.1631         1484.9152
5868      1492.4410         1509.2736         1800.8498
5869      3041.9735         3043.3968         3091.0038
5870      3098.1414         3136.7252         3141.4738
5871      3157.9596         3179.4653         3920.8526
5872 Zero-point correction (Hartree): 0.139512
5873
5874 HOCHCCH3CH2CH2OO.Zlptt
5875 ~~~~~
5876 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45028605
5877 Electronic state : 2-A
5878 Cartesian coordinates (Angs):
5879 C      -1.999039      0.048185      -0.452034
5880 C      -0.949007     -0.534742      0.109762
5881 C      -0.098358      0.197613      1.112093
5882 C      1.387094      0.049875      0.860514
5883 O      1.669237      0.580826     -0.453851
5884 O      2.902767      0.373239     -0.795236
5885 O     -2.371765      1.330853     -0.154412
5886 H     -2.623033     -0.474901     -1.167680
5887 C     -0.587990     -1.950106     -0.229491
5888 H     -0.365097      1.252916      1.129000
5889 H     -0.285842     -0.197648      2.115933
5890 H      1.981323      0.618614      1.574282
5891 H      1.718042     -0.987696      0.863734
5892 H     -3.072826      1.612212     -0.743375
5893 H     -1.339358     -2.404120     -0.873313
5894 H     -0.502860     -2.560579      0.673214
5895 H      0.371533     -2.003091     -0.748869
5896 Rotational constants (GHz):      3.1424900      1.1632600      1.0333300
5897 Vibrational harmonic frequencies (cm-1):
5898      31.1387          57.4874          108.7861
5899      193.6568         213.3292         241.8764
5900      280.4807         312.9197         337.6982
5901      395.8865         470.8439         561.6418
5902      628.8962         777.3126         841.8577
5903      886.3631         973.2580        1014.9300
5904      1045.7805        1075.9053        1095.4822
5905      1182.3439        1204.6011        1236.3738
5906      1270.4945        1298.6339        1322.9877
5907      1356.8018        1401.3671        1418.2395
5908      1424.0884        1470.8202        1485.0320
5909      1497.3576        1514.2876        1801.0893
5910      3043.5390        3045.9127        3091.0014
5911      3095.0292        3129.7364        3138.1720
5912      3148.3095        3183.1646        3920.9824
5913 Zero-point correction (Hartree): 0.139483
5914
5915 HOCHCCH3CH2CH2OO.Zpmtc
5916 ~~~~~
5917 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44892315
5918 Electronic state : 2-A
5919 Cartesian coordinates (Angs):
5920 C      1.225893      1.208723      0.077346
5921 C      1.410632     -0.105668     -0.028430
5922 C      0.343809     -1.167296     -0.161927
5923 C     -1.005756     -0.923354      0.481733
5924 O     -1.808500     -0.110126     -0.414995
5925 O     -3.030709      0.014428      0.005569
5926 O      0.073591      1.925072      0.060217
5927 H      2.079423      1.862132      0.207285
5928 C      2.814589     -0.644409     -0.047855
5929 H      0.183558     -1.430688     -1.213029
5930 H      0.736846     -2.074807      0.302965
5931 H     -1.558074     -1.849666      0.622762
5932 H     -0.932562     -0.385217      1.426376
5933 H     -0.657800      1.417526     -0.308304

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5934      H      3.551357      0.153489      0.021877
5935      H      3.006202      -1.197355     -0.971065
5936      H      2.980993      -1.338376     0.779600
5937 Rotational constants (GHz):      3.6361300      1.2623400      0.9796100
5938 Vibrational harmonic frequencies (cm-1):
5939      19.6519      76.2984      145.2685
5940      207.5452      220.5482      267.3857
5941      294.9970      345.4938      349.8160
5942      448.9702      518.0648      563.8675
5943      624.1732      787.7658      832.0384
5944      925.1017      1004.3463     1016.8289
5945      1036.8728     1075.0445     1108.9520
5946      1184.7616     1207.4077     1234.1039
5947      1280.7706     1305.7384     1323.5230
5948      1391.9311     1412.2769     1419.7006
5949      1431.2856     1463.8643     1485.3120
5950      1500.8632     1503.7261     1772.1061
5951      3039.4061     3041.9396     3077.8754
5952      3087.7320     3096.2801     3142.7642
5953      3155.4912     3200.5034     3814.3305
5954 Zero-point correction (Hartree): 0.139977
5955
5956 HOCHCCH3CH2CH2OO.Zptpc
5957 ~~~~~
5958 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45311898
5959 Electronic state : 2-A
5960 Cartesian coordinates (Angs):
5961      C      -1.337776      1.167113      0.144008
5962      C      -1.356078      -0.137348     -0.121298
5963      C      -0.086233      -0.827402     -0.549217
5964      C      0.933326      -0.932568     0.592911
5965      O      2.279812      -0.698882     0.113257
5966      O      2.414009      0.523274     -0.297511
5967      O      -0.265061      1.992419     0.069056
5968      H      -2.225219      1.700550     0.458868
5969      C      -2.610523      -0.947993     0.004703
5970      H      -0.305186      -1.817407     -0.945692
5971      H      0.390244      -0.264818     -1.356330
5972      H      0.747120      -0.187308     1.364677
5973      H      0.975110      -1.922479     1.039906
5974      H      0.546981      1.524914     -0.173442
5975      H      -2.881161      -1.403777     -0.950454
5976      H      -3.446566     -0.332927     0.334061
5977      H      -2.487689     -1.762045     0.723351
5978 Rotational constants (GHz):      3.2290800      1.3886100      1.0409300
5979 Vibrational harmonic frequencies (cm-1):
5980      70.9878      75.4034      181.5667
5981      196.5113      214.0703      295.3972
5982      296.6820      349.5854      401.9228
5983      527.4069      567.3644      592.9057
5984      606.8148      804.7100      871.8093
5985      930.0972      964.8976     1014.9382
5986      1033.8493     1073.4721     1075.2889
5987      1200.6918     1213.1969     1246.7772
5988      1288.4881     1302.6108     1325.8487
5989      1368.4561     1398.8044     1406.8098
5990      1423.7255     1482.5153     1494.0460
5991      1503.4373     1508.8030     1762.0564
5992      3042.6950     3059.0856     3090.0887
5993      3100.2097     3121.8062     3137.0446
5994      3166.2918     3210.1517     3747.9121
5995 Zero-point correction (Hartree): 0.140671
5996
5997
5998 TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Zh
5999 ~~~~~
6000 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82290136
6001 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74780200
6002 T1 diagnostic: 0.027632
6003 E(MP2/Aug-CC-pVTZ) (Hartree): -420.68959699
6004 E(MP3/Aug-CC-pVTZ) (Hartree): -420.72757334
6005 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.70732238

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6006 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74089315
6007 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15569713
6008 E(UHF/Aug-CC-pVTZ) (Hartree): -419.13522923
6009 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.42867123
6010 Electronic state : 2-A
6011 Cartesian coordinates (Angs):
6012 C -0.225486 1.261185 -0.046634
6013 C -1.014997 0.183361 0.288575
6014 C -0.363531 -0.892676 1.084760
6015 C 0.671914 -1.572693 0.150479
6016 O 1.553838 -0.605444 -0.371589
6017 O 0.868505 0.186239 -1.267089
6018 O 0.726247 1.683063 0.817033
6019 H -0.561307 1.977356 -0.789752
6020 C -2.230068 -0.138468 -0.510283
6021 H 0.163980 -0.494518 1.949035
6022 H -1.084801 -1.640822 1.415571
6023 H 1.293669 -2.278879 0.700038
6024 H 0.165493 -2.081734 -0.672729
6025 H 1.456220 2.067705 0.320778
6026 H -2.071248 -1.044599 -1.103181
6027 H -2.493173 0.669297 -1.190938
6028 H -3.084554 -0.328926 0.142964
6029 Rotational constants (GHz): 2.5274700 2.1855300 1.6981700
6030 Vibrational harmonic frequencies (cm-1):
6031 i607.7865 138.5662 158.4735
6032 173.2502 238.6210 275.5832
6033 323.6091 378.7176 434.5920
6034 442.6917 493.6161 596.9295
6035 629.7035 804.2215 874.7583
6036 916.7996 979.4077 996.0024
6037 1008.2363 1035.3478 1071.6900
6038 1083.2220 1187.9358 1218.4413
6039 1238.7452 1263.3048 1313.8985
6040 1321.9079 1364.1076 1396.5419
6041 1416.4615 1474.0568 1476.2740
6042 1485.8078 1494.4816 1580.6759
6043 3035.2683 3061.8629 3082.5547
6044 3086.4816 3128.0387 3140.5013
6045 3146.2336 3165.6929 3852.5523
6046 Zero-point correction (Hartree): 0.138936
6047
6048 TS.HOCHCCH3CH2CH2O0.cycHOCHCCH3CH2CH2O0.Zp
6049 ~~~~~
6050 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82459295
6051 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74901814
6052 T1 diagnostic: 0.026545
6053 E(MP2/Aug-CC-pVTZ) (Hartree): -420.69314458
6054 E(MP3/Aug-CC-pVTZ) (Hartree): -420.73006351
6055 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.71010883
6056 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74269577
6057 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15379424
6058 E(UHF/Aug-CC-pVTZ) (Hartree): -419.13410207
6059 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.42980062
6060 Electronic state : 2-A
6061 Cartesian coordinates (Angs):
6062 C 0.264881 1.272855 -0.006594
6063 C 1.007221 0.142348 -0.318909
6064 C 0.312532 -0.947264 -1.060958
6065 C -0.752520 -1.543270 -0.111180
6066 O -1.543094 -0.494526 0.416411
6067 O -0.761392 0.238666 1.298738
6068 O -0.752451 1.742482 -0.753384
6069 H 0.698749 2.032966 0.632045
6070 C 2.234549 -0.182764 0.460105
6071 H -0.185913 -0.568288 -1.954860
6072 H 1.007489 -1.731098 -1.362977
6073 H -1.439278 -2.204613 -0.639172
6074 H -0.278491 -2.076997 0.713862
6075 H -1.414245 1.040369 -0.847075
6076 H 2.049751 -1.019782 1.140764
6077 H 2.570915 0.664760 1.054642

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6078      H          3.046541      -0.481714      -0.206128
6079 Rotational constants (GHz):      2.5474400      2.2040800      1.7088700
6080 Vibrational harmonic frequencies (cm-1):
6081      i589.2412      148.4698      166.7360
6082      186.3656      244.1548      319.1700
6083      376.0619      425.6069      442.8246
6084      467.7017      500.0235      595.2845
6085      636.0796      795.4367      881.5022
6086      903.5941      973.4984      995.5179
6087      1005.8630      1031.3427      1069.6499
6088      1073.5617      1184.2861      1214.3732
6089      1262.1894      1269.6616      1312.8932
6090      1340.3680      1369.4256      1395.9655
6091      1416.7420      1475.8834      1481.4894
6092      1487.0234      1499.0715      1554.8259
6093      3035.0817      3069.2795      3071.9588
6094      3088.6041      3120.4220      3135.5229
6095      3141.8760      3197.3187      3731.1289
6096 Zero-point correction (Hartree): 0.139182
6097
6098
6099 TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Zc
6100 ~~~~~
6101 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41388538
6102 Electronic state : 2-A
6103 Cartesian coordinates (Angs):
6104      O      -1.953200      0.709729      -0.843874
6105      H      -1.081665      1.382104      -0.240421
6106      C      -0.088042      1.598713      0.548536
6107      O      -2.176009      -0.349107      0.009137
6108      C      0.726041      0.401034      0.371658
6109      C      -1.110227      -1.286587      -0.097239
6110      C      0.083660      -0.903718      0.775320
6111      H      -0.639485      1.655303      1.485836
6112      H      0.370484      2.537415      0.253653
6113      C      1.930202      0.489202      -0.211689
6114      O      2.779922      -0.520931      -0.504577
6115      H      2.344672      1.445286      -0.502068
6116      H      -1.537182      -2.229748      0.245099
6117      H      -0.827718      -1.372330      -1.147986
6118      H      0.790085      -1.738092      0.760909
6119      H      -0.266085      -0.821483      1.807747
6120      H      2.391381      -1.367842      -0.267779
6121 Rotational constants (GHz):      3.5653900      1.3311700      1.1269500
6122 Vibrational harmonic frequencies (cm-1):
6123      i2089.6467      73.3864      144.2458
6124      252.2848      254.3888      295.2603
6125      348.6658      402.9211      446.4342
6126      498.5905      580.1781      589.5122
6127      631.7255      644.0132      781.6250
6128      877.4454      914.9174      957.1782
6129      1014.4730      1019.6854      1050.7670
6130      1089.1779      1119.6484      1187.5560
6131      1205.4486      1238.3923      1283.2037
6132      1302.1902      1329.7816      1360.7501
6133      1395.0488      1421.0353      1461.2732
6134      1480.4697      1489.5087      1522.7000
6135      1708.9601      3049.8736      3067.4395
6136      3089.7423      3096.8584      3127.0348
6137      3191.0539      3217.8402      3869.7027
6138 Zero-point correction (Hartree): 0.134600
6139
6140 TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Zt
6141 ~~~~~
6142 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.80534605
6143 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.73022356
6144 T1 diagnostic: 0.025215
6145 E(MP2/Aug-CC-pVTZ) (Hartree): -420.67701734
6146 E(MP3/Aug-CC-pVTZ) (Hartree): -420.71328940
6147 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.69250327
6148 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.72444558
6149 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.13115853

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6150 E(UHF/Aug-CC-pVTZ) (Hartree): -419.11271414
6151 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41444056
6152 Electronic state : 2-A
6153 Cartesian coordinates (Angs):
6154 O -1.958174 0.689970 -0.852131
6155 H -1.100700 1.371563 -0.255314
6156 C -0.107906 1.612556 0.537761
6157 O -2.173687 -0.365790 0.004806
6158 C 0.708535 0.416080 0.378459
6159 C -1.093869 -1.293638 -0.088837
6160 C 0.092307 -0.898487 0.784797
6161 H -0.666306 1.675348 1.470149
6162 H 0.342921 2.551728 0.231718
6163 C 1.910845 0.483199 -0.203602
6164 O 2.663257 -0.627244 -0.435099
6165 H 2.336862 1.429326 -0.517010
6166 H -1.514879 -2.238742 0.254936
6167 H -0.805100 -1.382272 -1.137196
6168 H 0.835255 -1.693932 0.735464
6169 H -0.255891 -0.826943 1.818525
6170 H 3.517194 -0.379830 -0.793344
6171 Rotational constants (GHz): 3.5570000 1.3494100 1.1376500
6172 Vibrational harmonic frequencies (cm-1):
6173 i2125.9030 73.8258 144.8234
6174 242.5021 249.7489 277.2143
6175 327.3942 345.9792 434.1601
6176 488.7135 585.1494 591.6852
6177 631.5893 647.1744 787.8479
6178 874.9232 885.4648 959.9891
6179 1010.0703 1018.8154 1048.2654
6180 1086.5471 1119.0282 1196.7306
6181 1207.3084 1240.5505 1248.2845
6182 1297.1116 1342.5440 1356.1230
6183 1389.9385 1421.1517 1460.2205
6184 1479.4794 1483.1757 1522.4986
6185 1730.6236 3059.4946 3072.5546
6186 3098.4729 3125.9796 3131.2908
6187 3185.5875 3190.1089 3913.8734
6188 Zero-point correction (Hartree): 0.134375
6189
6190 TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Zc
6191 ~~~~~
6192 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41379943
6193 Electronic state : 2-A
6194 Cartesian coordinates (Angs):
6195 O -2.172289 0.392037 -0.380920
6196 H -1.317307 1.295368 -0.178889
6197 C -0.206735 1.814036 0.262017
6198 O -1.391242 -0.629704 -0.865925
6199 C 0.611405 0.617457 0.350430
6200 C -0.866227 -1.382095 0.221721
6201 C 0.006509 -0.517110 1.144415
6202 H -0.575528 2.200157 1.210717
6203 H 0.132768 2.587840 -0.419221
6204 C 1.731349 0.477639 -0.376591
6205 O 2.518254 -0.619024 -0.430998
6206 H 2.115330 1.275673 -0.997117
6207 H -1.684337 -1.853060 0.769799
6208 H -0.276027 -2.153903 -0.274322
6209 H 0.755735 -1.145670 1.632699
6210 H -0.605105 -0.096046 1.941020
6211 H 2.158878 -1.316387 0.126103
6212 Rotational constants (GHz): 3.1329900 1.5781800 1.3050800
6213 Vibrational harmonic frequencies (cm-1):
6214 i2020.1929 84.2323 122.3046
6215 255.4016 284.1316 331.6035
6216 358.5807 390.2188 436.0733
6217 500.3482 540.9057 592.0663
6218 625.1512 680.8618 806.0707
6219 858.9725 915.1989 955.7221
6220 1018.3961 1026.9489 1073.6031
6221 1080.3392 1124.4093 1184.5750

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6222      1219.6511      1273.1274      1280.3392
6223      1294.0000      1322.8966      1362.4060
6224      1385.3673      1413.3022      1475.8292
6225      1489.2252      1497.7021      1511.2492
6226      1696.0246      3056.3752      3066.6361
6227      3098.0780      3108.6079      3127.2132
6228      3190.4441      3221.2841      3857.8356
6229 Zero-point correction (Hartree): 0.134853
6230
6231 TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Zt
6232 ~~~~~
6233 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41432079
6234 Electronic state : 2-A
6235 Cartesian coordinates (Angs):
6236 O      -2.168964      0.339083      -0.413326
6237 H      -1.346566      1.264500      -0.213022
6238 C      -0.251609      1.827108      0.230581
6239 O      -1.354748      -0.671518      -0.861320
6240 C      0.581625      0.646906      0.357829
6241 C      -0.820534      -1.388581      0.250952
6242 C      0.004495      -0.482768      1.174198
6243 H      -0.642849      2.226174      1.164337
6244 H      0.078148      2.591364      -0.466420
6245 C      1.697711      0.483597      -0.364566
6246 O      2.402750      -0.677734      -0.310386
6247 H      2.081282      1.259780      -1.015882
6248 H      -1.633378      -1.880493      0.788119
6249 H      -0.184189      -2.137160      -0.219485
6250 H      0.785654      -1.075760      1.647731
6251 H      -0.630097      -0.067457      1.955818
6252 H      3.189563      -0.617176      -0.854909
6253 Rotational constants (GHz):      3.109560      1.615940      1.3292500
6254 Vibrational harmonic frequencies (cm-1):
6255 i2067.2203      80.7269      124.9799
6256      250.6726      266.1617      300.6704
6257      356.4600      362.9145      392.0901
6258      485.5641      539.6044      596.8966
6259      623.0864      686.1959      811.2804
6260      863.2249      869.4587      959.7051
6261      1018.4655      1026.5592      1065.5672
6262      1082.7047      1121.8113      1197.6638
6263      1225.5901      1247.1964      1275.1394
6264      1282.8936      1324.1650      1362.3878
6265      1380.6641      1412.3404      1475.0907
6266      1485.7310      1494.0201      1503.3449
6267      1716.2163      3068.8958      3089.5693
6268      3101.5952      3126.8974      3144.1488
6269      3189.2682      3192.6181      3910.7707
6270 Zero-point correction (Hartree): 0.134619
6271
6272
6273 #####
6274 E-HOCH=CHCH2CH2OO ring closure
6275 #####
6276
6277 HOCHCHCH2CH2OO.Ecpmc
6278 ~~~~~
6279 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13875016
6280 Electronic state : 2-A
6281 Cartesian coordinates (Angs):
6282 C      -1.464605      -0.422977      0.119382
6283 C      -1.214437      0.847892      -0.164136
6284 C      0.132747      1.506700      -0.092726
6285 C      1.242428      0.655855      0.476854
6286 O      1.542377      -0.394003      -0.472187
6287 O      2.422013      -1.221736      -0.000305
6288 O      -2.679471      -1.027466      0.067432
6289 H      -0.700741      -1.127820      0.419328
6290 H      -2.038291      1.479660      -0.483204
6291 H      0.436862      1.853511      -1.084376
6292 H      0.067173      2.402931      0.529284
6293 H      2.158746      1.227493      0.615094

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6294      H      0.967614      0.177698      1.416724
6295      H      -3.347513     -0.392658     -0.208613
6296      Rotational constants (GHz):      4.5202800      1.4779300      1.1717900
6297      Vibrational harmonic frequencies (cm-1):
6298          48.1026          124.2428          131.8012
6299          214.6629          263.0421          302.0468
6300          395.1256          448.3625          524.2222
6301          619.2420          798.5684          872.2430
6302          939.1204          992.9402          1001.4340
6303          1064.1514          1112.3987          1161.7700
6304          1229.2525          1254.3525          1293.3706
6305          1297.0187          1350.5167          1387.6863
6306          1403.8246          1421.8062          1476.3599
6307          1506.1178          1767.7863          3052.5511
6308          3078.7936          3092.3963          3144.1966
6309          3156.9067          3222.3314          3857.5254
6310      Zero-point correction (Hartree): 0.111644
6311
6312      HOCHCHCH2CH2OO.Ecpmt
6313      ~~~~~
6314      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13755268
6315      Electronic state : 2-A
6316      Cartesian coordinates (Angs):
6317      C      -1.459720      -0.380138      0.100018
6318      C      -1.195673      0.890109      -0.161260
6319      C      0.160351      1.527147      -0.087119
6320      C      1.259783      0.656818      0.472133
6321      O      1.538632      -0.395509      -0.482336
6322      O      2.331305      -1.292747      0.015563
6323      O      -2.730887      -0.869703      0.027081
6324      H      -0.695940      -1.096969      0.379060
6325      H      -2.021999      1.524596      -0.459245
6326      H      0.465324      1.880214      -1.076448
6327      H      0.109175      2.419006      0.542606
6328      H      2.186733      1.212246      0.607498
6329      H      0.982718      0.178054      1.410801
6330      H      -2.726850      -1.817098      0.170634
6331      Rotational constants (GHz):      4.4196600      1.5059900      1.1816000
6332      Vibrational harmonic frequencies (cm-1):
6333          42.0257          126.7007          135.7249
6334          206.3338          235.5286          286.2958
6335          312.5589          394.5795          519.4377
6336          621.7216          802.1858          879.4116
6337          933.8539          972.8706          994.0134
6338          1062.5462          1111.2065          1185.9560
6339          1215.4124          1235.8830          1286.2828
6340          1299.1804          1353.5418          1387.9902
6341          1389.6808          1417.4445          1475.1009
6342          1504.8745          1790.0874          3052.1121
6343          3078.1940          3091.5871          3143.5744
6344          3188.7776          3190.6990          3917.2498
6345      Zero-point correction (Hartree): 0.111267
6346
6347      HOCHCHCH2CH2OO.Ecppc
6348      ~~~~~
6349      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13947030
6350      Electronic state : 2-A
6351      Cartesian coordinates (Angs):
6352      C      -1.529484      -0.302489      0.170987
6353      C      -1.034845      0.811980      -0.349991
6354      C      0.374698      1.300939      -0.188853
6355      C      1.232616      0.510313      0.773581
6356      O      1.481866      -0.830752      0.290517
6357      O      2.258116      -0.821903      -0.748450
6358      O      -2.804690      -0.750430      0.033491
6359      H      -0.945277      -0.991818      0.765712
6360      H      -1.686990      1.431986      -0.958476
6361      H      0.886349      1.319515      -1.154593
6362      H      0.364612      2.334302      0.167739
6363      H      2.203798      0.980548      0.914588
6364      H      0.745164      0.362278      1.736279
6365      H      -3.307907      -0.136598      -0.510058

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6366 Rotational constants (GHz): 4.9983100 1.4387300 1.2663800
6367 Vibrational harmonic frequencies (cm-1):
6368 67.8308 117.8662 148.3515
6369 204.1084 269.3890 314.1250
6370 431.1025 446.1421 535.4174
6371 625.5700 811.4498 862.5680
6372 928.0912 984.7397 995.4913
6373 1037.2588 1118.6221 1160.2299
6374 1227.7424 1248.8181 1283.3823
6375 1316.4783 1350.1384 1390.1106
6376 1399.1873 1413.6909 1474.9318
6377 1494.2587 1766.1610 3055.8556
6378 3083.2992 3099.4234 3154.0351
6379 3155.0453 3223.1537 3859.8894
6380 Zero-point correction (Hartree): 0.111753
6381
6382 HOCHCHCH2CH2OO.Ecppt
6383 ~~~~~
6384 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13802000
6385 Electronic state : 2-A
6386 Cartesian coordinates (Angs):
6387 C -1.529449 -0.270471 0.138609
6388 C -1.022385 0.847727 -0.355323
6389 C 0.393919 1.310374 -0.189437
6390 C 1.239116 0.507328 0.773733
6391 O 1.461834 -0.842237 0.299354
6392 O 2.237854 -0.857438 -0.739800
6393 O -2.840301 -0.599535 -0.051762
6394 H -0.944052 -0.982245 0.709316
6395 H -1.680273 1.480772 -0.939231
6396 H 0.906484 1.324864 -1.154913
6397 H 0.399687 2.343160 0.169092
6398 H 2.219956 0.958170 0.911539
6399 H 0.749641 0.373436 1.737641
6400 H -3.013743 -1.474224 0.298727
6401 Rotational constants (GHz): 4.9691000 1.4437000 1.2654800
6402 Vibrational harmonic frequencies (cm-1):
6403 67.3447 120.3136 150.1679
6404 197.9145 232.0141 293.8005
6405 317.3200 440.0979 534.0222
6406 625.9645 814.0036 865.5497
6407 925.5620 971.6286 985.4511
6408 1035.0411 1118.1520 1185.3130
6409 1218.1745 1229.5988 1278.3390
6410 1313.1957 1355.4120 1387.3704
6411 1392.6868 1407.0145 1473.1566
6412 1491.9981 1788.7664 3055.7378
6413 3082.3562 3098.1625 3153.7357
6414 3187.0484 3189.4940 3917.0116
6415 Zero-point correction (Hartree): 0.111400
6416
6417 HOCHCHCH2CH2OO.Ectpc
6418 ~~~~~
6419 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13938546
6420 Electronic state : 2-A
6421 Cartesian coordinates (Angs):
6422 C 1.936312 -0.344147 -0.048058
6423 C 1.221437 0.766858 0.066513
6424 C -0.268783 0.828034 0.220496
6425 C -0.935101 -0.530449 0.227231
6426 O -2.358621 -0.381508 0.409864
6427 O -2.926371 0.085049 -0.659898
6428 O 3.285433 -0.418540 -0.190501
6429 H 1.502893 -1.335730 -0.039989
6430 H 1.740157 1.720866 0.048268
6431 H -0.526798 1.344957 1.148427
6432 H -0.706390 1.411545 -0.592537
6433 H -0.780617 -1.069171 -0.707047
6434 H -0.617071 -1.141356 1.070902
6435 H 3.661109 0.467113 -0.200841
6436 Rotational constants (GHz): 9.8150100 0.9944200 0.9536900
6437 Vibrational harmonic frequencies (cm-1):

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6438      69.9008      110.5973      147.6182
6439      162.2996      271.1103      322.2673
6440      376.4266      438.7931      543.6010
6441      669.5200      774.6993      854.3725
6442      955.3967      987.5271      994.7808
6443      1101.3430      1108.4992      1158.9623
6444      1238.2333      1253.1820      1285.9201
6445      1320.6570      1340.1831      1350.9176
6446      1403.4472      1422.6524      1492.0627
6447      1503.2176      1766.7069      3055.1602
6448      3089.3721      3090.7007      3150.9597
6449      3159.3541      3214.6008      3858.0659
6450 Zero-point correction (Hartree): 0.111728
6451
6452 HOCHCHCH2CH2OO.Ecpt
6453 ~~~~~
6454 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13741398
6455 Electronic state : 2-A
6456 Cartesian coordinates (Angs):
6457 C      1.939941      -0.306288      -0.043998
6458 C      1.212318      0.795109      0.054537
6459 C      -0.277420      0.841180      0.204218
6460 C      -0.931955      -0.522116      0.240755
6461 O      -2.357334      -0.384119      0.418383
6462 O      -2.929968      0.042776      -0.665264
6463 O      3.297206      -0.251505      -0.178406
6464 H      1.511880      -1.302568      -0.024448
6465 H      1.733897      1.744451      0.023800
6466 H      -0.541629      1.377099      1.119589
6467 H      -0.719151      1.403362      -0.621714
6468 H      -0.772293      -1.080333      -0.681255
6469 H      -0.609342      -1.110884      1.098530
6470 H      3.660101      -1.135645      -0.245271
6471 Rotational constants (GHz):      9.8556000      0.9914600      0.9518100
6472 Vibrational harmonic frequencies (cm-1):
6473      68.2076      106.6733      144.7125
6474      160.4354      191.3743      296.9736
6475      323.3690      370.0179      543.0483
6476      668.8520      773.9917      862.0336
6477      949.6565      970.6268      991.1841
6478      1100.9311      1106.9279      1182.2731
6479      1219.8489      1238.4636      1285.5997
6480      1318.8167      1339.1135      1355.0051
6481      1384.0531      1421.4667      1490.5967
6482      1501.8193      1787.9223      3055.0370
6483      3087.8865      3089.4569      3148.9799
6484      3179.5770      3191.1718      3919.9732
6485 Zero-point correction (Hartree): 0.111234
6486
6487 HOCHCHCH2CH2OO.Ecttc
6488 ~~~~~
6489 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13876938
6490 Point group : CS
6491 Electronic state : 2-A"
6492 Cartesian coordinates (Angs):
6493 C      -0.771975      -1.802408      0.000000
6494 C      0.515982      -1.485695      0.000000
6495 C      1.065624      -0.090714      0.000000
6496 C      -0.000000      0.979201      0.000000
6497 O      0.681606      2.250581      0.000000
6498 O      -0.157836      3.238907      0.000000
6499 O      -1.288633      -3.057915      0.000000
6500 H      -1.565508      -1.066926      0.000000
6501 H      1.246994      -2.288398      0.000000
6502 H      1.705699      0.056392      0.873368
6503 H      1.705699      0.056392      -0.873368
6504 H      -0.628043      0.945712      -0.890070
6505 H      -0.628043      0.945712      0.890070
6506 H      -0.575674      -3.703771      0.000000
6507 Rotational constants (GHz):      9.0291200      0.9776300      0.8918700
6508 Vibrational harmonic frequencies (cm-1):
6509      73.9734 ( A")      103.8979 ( A")      122.8267 ( A")

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6510      131.4241 ( A'')      268.2891 ( A'')      288.7826 ( A')
6511      369.1405 ( A')      428.2408 ( A'')      526.8094 ( A')
6512      646.7481 ( A')      765.5339 ( A'')      849.9082 ( A'')
6513      979.3574 ( A')      985.2831 ( A'')      1031.1827 ( A')
6514      1082.6697 ( A'')      1125.1460 ( A')      1161.8411 ( A')
6515      1227.6135 ( A'')      1258.5921 ( A')      1296.4638 ( A')
6516      1307.5496 ( A'')      1331.8992 ( A')      1351.7050 ( A')
6517      1404.0158 ( A')      1431.0892 ( A')      1498.7546 ( A')
6518      1512.6102 ( A')      1765.5679 ( A')      3055.2827 ( A')
6519      3083.1958 ( A')      3084.1565 ( A'')      3140.6048 ( A'')
6520      3162.7702 ( A')      3218.6361 ( A')      3860.5767 ( A')
6521 Zero-point correction (Hartree): 0.111476
6522
6523 HOCHCHCH2CH200.Ecttt
6524 ~~~~~
6525 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13700871
6526 Point group : CS
6527 Electronic state : 2-A''
6528 Cartesian coordinates (Angs):
6529 C      -0.730667      -1.816974      0.000000
6530 C      0.550123      -1.482173      0.000000
6531 C      1.078835      -0.080256      0.000000
6532 C      -0.000000      0.976032      0.000000
6533 O      0.661347      2.258959      0.000000
6534 O      -0.193057      3.234275      0.000000
6535 O      -1.122947      -3.123534      0.000000
6536 H      -1.532954      -1.087177      0.000000
6537 H      1.278914      -2.283852      0.000000
6538 H      1.717525      0.073764      0.873326
6539 H      1.717525      0.073764      -0.873326
6540 H      -0.627193      0.934602      -0.890543
6541 H      -0.627193      0.934602      0.890543
6542 H      -2.079119      -3.183081      0.000000
6543 Rotational constants (GHz):      9.0451300      0.9756500      0.8903900
6544 Vibrational harmonic frequencies (cm-1):
6545      78.1147 ( A'')      105.6336 ( A'')      123.3877 ( A')
6546      141.6512 ( A'')      214.4010 ( A'')      288.1418 ( A')
6547      304.9511 ( A'')      364.9563 ( A')      524.9464 ( A')
6548      646.4276 ( A')      765.6786 ( A'')      858.0770 ( A'')
6549      969.0092 ( A'')      971.9698 ( A')      1029.4277 ( A')
6550      1082.5480 ( A'')      1124.5327 ( A')      1184.5187 ( A')
6551      1224.9998 ( A')      1228.0631 ( A'')      1296.3103 ( A')
6552      1306.9655 ( A'')      1329.6117 ( A')      1356.7021 ( A')
6553      1384.6632 ( A')      1429.1669 ( A')      1497.5473 ( A')
6554      1511.9850 ( A')      1787.3630 ( A')      3054.9617 ( A')
6555      3080.6423 ( A')      3083.6770 ( A'')      3137.9846 ( A'')
6556      3181.5268 ( A')      3193.1579 ( A')      3919.4957 ( A')
6557 Zero-point correction (Hartree): 0.111136
6558
6559 HOCHCHCH2CH200.Egppc
6560 ~~~~~
6561 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59741321
6562 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53562656
6563 T1 diagnostic: 0.021635
6564 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49135115
6565 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52284012
6566 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49450832
6567 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52470252
6568 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13366994
6569 E(UHF/Aug-CC-pVTZ) (Hartree): -380.12852112
6570 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14077322
6571 Electronic state : 2-A
6572 Cartesian coordinates (Angs):
6573 C      1.710511      -0.236631      0.326987
6574 C      0.944346      0.767676      -0.075868
6575 C      -0.364970      1.093381      0.572448
6576 C      -1.559565      0.810304      -0.322689
6577 O      -1.648835      -0.595790      -0.641420
6578 O      -1.913557      -1.302412      0.413399
6579 O      2.897580      -0.615656      -0.206873
6580 H      1.435802      -0.870144      1.161279
6581 H      1.254587      1.369726      -0.925861

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6582      H      -0.486348      0.518270      1.490682
6583      H      -0.411223      2.150053      0.846885
6584      H      -2.497548      1.093650      0.152897
6585      H      -1.469744      1.294969      -1.293789
6586      H      3.111038      -0.054046      -0.958204
6587 Rotational constants (GHz):      4.8942000      1.4051200      1.2198500
6588 Vibrational harmonic frequencies (cm-1):
6589      48.4327      73.9465      138.6868
6590      203.0000      282.0698      338.0806
6591      432.5349      464.7401      534.2373
6592      576.6960      817.7682      871.9379
6593      917.7207      978.5767      989.2948
6594      1056.1982      1130.6006      1160.8082
6595      1215.2377      1261.8162      1278.7131
6596      1308.6740      1341.0988      1362.0063
6597      1399.2443      1409.4212      1476.6644
6598      1490.7193      1764.6782      3063.6467
6599      3091.5359      3117.6738      3151.0787
6600      3153.2238      3205.8634      3858.7646
6601 Zero-point correction (Hartree): 0.111551
6602
6603 HOCHCHCH2CH200.Egppt
6604 ~~~~~
6605 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13943708
6606 Electronic state : 2-A
6607 Cartesian coordinates (Angs):
6608      C      1.687236      -0.201097      0.290896
6609      C      0.928303      0.817527      -0.079823
6610      C      -0.388725      1.111221      0.566132
6611      C      -1.573046      0.788725      -0.329917
6612      O      -1.625150      -0.623845      -0.632210
6613      O      -1.858347      -1.327385      0.431741
6614      O      2.875457      -0.478173      -0.312634
6615      H      1.391623      -0.864289      1.097960
6616      H      1.258737      1.441503      -0.902645
6617      H      -0.499833      0.540022      1.488258
6618      H      -0.463606      2.168069      0.832364
6619      H      -2.520100      1.052277      0.139199
6620      H      -1.491630      1.262981      -1.306601
6621      H      3.266520      -1.263601      0.072556
6622 Rotational constants (GHz):      4.8400900      1.4303100      1.2324500
6623 Vibrational harmonic frequencies (cm-1):
6624      47.9251      75.1564      145.3360
6625      199.4227      255.2148      299.2435
6626      337.1138      454.6666      532.7269
6627      576.7199      824.7387      880.4943
6628      914.9683      965.1112      979.4742
6629      1051.9435      1134.6384      1179.6874
6630      1207.3830      1246.9137      1270.9962
6631      1304.0541      1339.5274      1365.6406
6632      1395.8855      1399.3995      1477.7779
6633      1490.5910      1787.2229      3065.8359
6634      3092.1485      3116.9292      3153.6702
6635      3169.3150      3183.6903      3915.4862
6636 Zero-point correction (Hartree): 0.111259
6637
6638 HOCHCHCH2CH200.Egppt
6639 ~~~~~
6640 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13810416
6641 Electronic state : 2-A
6642 Cartesian coordinates (Angs):
6643      C      1.871289      -0.153176      0.329989
6644      C      1.054218      0.635267      -0.348775
6645      C      -0.127526      1.310639      0.274269
6646      C      -1.450685      0.761239      -0.222213
6647      O      -1.582532      -0.580829      0.295585
6648      O      -2.656826      -1.158544      -0.143306
6649      O      2.936654      -0.767166      -0.254017
6650      H      1.728227      -0.344927      1.388712
6651      H      1.232642      0.780890      -1.408353
6652      H      -0.094393      1.210822      1.360925
6653      H      -0.117389      2.380612      0.054960

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6654      H      -2.303019      1.331426      0.145625
6655      H      -1.494215      0.695959     -1.308917
6656      H      3.386003      -1.326284      0.381331
6657 Rotational constants (GHz):      5.3088800      1.2317300      1.0613900
6658 Vibrational harmonic frequencies (cm-1):
6659      44.1585      72.5962      110.5274
6660      188.9176      240.8283      278.9011
6661      332.8114      396.6938      537.4121
6662      566.3702      818.6533      871.5105
6663      917.0749      963.8968      1031.6287
6664      1067.3404      1123.0761      1179.5649
6665      1205.2590      1250.2644      1276.6812
6666      1299.0977      1337.7871      1364.5492
6667      1392.9945      1406.0468      1473.0211
6668      1500.3771      1790.1720      3062.0313
6669      3083.9850      3105.3708      3142.0309
6670      3170.7630      3183.3007      3917.6972
6671 Zero-point correction (Hartree): 0.110954
6672
6673 HOCHCHCH2CH200.Elmmc
6674 ~~~~~
6675 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -381.59783370
6676 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -381.53613947
6677 T1 diagnostic: 0.021613
6678 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49167334
6679 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52332066
6680 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49483364
6681 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52518461
6682 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13467350
6683 E(UHF/Aug-CC-pVTZ) (Hartree): -380.12952628
6684 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14119558
6685 Electronic state : 2-A
6686 Cartesian coordinates (Angs):
6687      C      2.124153      0.276916     -0.042485
6688      C      0.874173     -0.099991     -0.272337
6689      C     -0.241856      0.871925     -0.502115
6690      C     -1.331538      0.777029      0.551962
6691      O     -1.920688     -0.543726      0.557753
6692      O     -2.625917     -0.751207     -0.511793
6693      O      3.188259     -0.535457      0.177972
6694      H      2.419325      1.318728     -0.015007
6695      H      0.628268     -1.157591     -0.294153
6696      H      0.142333      1.893574     -0.495348
6697      H     -0.708634      0.706852     -1.475186
6698      H     -0.933191      0.894050      1.558058
6699      H     -2.137311      1.487177      0.372899
6700      H      2.906379     -1.454950      0.147128
6701 Rotational constants (GHz):      7.1870100      1.0976100      1.0399700
6702 Vibrational harmonic frequencies (cm-1):
6703      56.8155      83.9327      145.6926
6704      184.7958      282.8152      330.2073
6705      441.3317      475.5827      532.5543
6706      584.2154      819.8312      856.1046
6707      908.1255      989.8147      997.8385
6708      1093.6706      1120.4717      1158.1126
6709      1207.1273      1245.8661      1294.7724
6710      1306.4289      1340.7014      1365.5644
6711      1394.4322      1413.1006      1474.5714
6712      1489.2539      1763.9730      3068.0372
6713      3093.6743      3112.8341      3158.6898
6714      3163.9251      3203.8754      3858.7945
6715 Zero-point correction (Hartree): 0.111670
6716
6717 HOCHCHCH2CH200.Elmmt
6718 ~~~~~
6719 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13870637
6720 Electronic state : 2-A
6721 Cartesian coordinates (Angs):
6722      C      2.125235      0.248322     -0.058651
6723      C      0.872717     -0.128232     -0.259321
6724      C     -0.238762      0.845137     -0.498006
6725      C     -1.328976      0.766348      0.557172

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6726 O -1.950491 -0.538911 0.551717
6727 O -2.674554 -0.711942 -0.511242
6728 O 3.126265 -0.649485 0.162286
6729 H 2.416229 1.294412 -0.065456
6730 H 0.636743 -1.185922 -0.247669
6731 H 0.146936 1.866620 -0.504487
6732 H -0.709261 0.670049 -1.467856
6733 H -0.927013 0.865361 1.563809
6734 H -2.117523 1.497240 0.384897
6735 H 3.962841 -0.194512 0.267517
6736 Rotational constants (GHz): 7.4165000 1.0823000 1.0299300
6737 Vibrational harmonic frequencies (cm-1):
6738 58.1094 83.5004 145.1692
6739 179.0405 261.2688 283.6740
6740 343.9772 473.3522 529.3861
6741 579.8470 819.7825 865.7344
6742 908.1426 967.9874 997.4035
6743 1095.1717 1120.2871 1176.8371
6744 1197.1457 1237.6120 1272.9478
6745 1306.9577 1339.9534 1366.4940
6746 1393.0371 1401.3962 1474.2716
6747 1488.3671 1786.6412 3064.6038
6748 3092.0681 3109.0438 3157.2482
6749 3166.1291 3193.1663 3917.7310
6750 Zero-point correction (Hartree): 0.111296
6751
6752 HOCHCHCH2CH2OO.Elmpc
6753 ~~~~~
6754 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14045498
6755 Electronic state : 2-A
6756 Cartesian coordinates (Angs):
6757 C 1.990995 0.290723 0.147957
6758 C 0.783071 0.146789 -0.378955
6759 C -0.267488 1.210011 -0.300446
6760 C -1.511384 0.771514 0.459024
6761 O -2.173244 -0.296686 -0.251029
6762 O -1.760532 -1.467795 0.130963
6763 O 2.994221 -0.622237 0.132025
6764 H 2.297937 1.195879 0.657647
6765 H 0.524123 -0.780504 -0.880382
6766 H 0.132568 2.092020 0.204050
6767 H -0.576875 1.525457 -1.299715
6768 H -1.276596 0.401779 1.454863
6769 H -2.249624 1.570606 0.506442
6770 H 2.693745 -1.425720 -0.304047
6771 Rotational constants (GHz): 5.3864800 1.3147700 1.1153500
6772 Vibrational harmonic frequencies (cm-1):
6773 63.8294 89.1137 132.6084
6774 185.0105 288.9820 340.3975
6775 444.6962 474.8875 529.9831
6776 562.1000 845.9667 860.7239
6777 884.3868 990.1286 1016.3122
6778 1084.0668 1116.5833 1160.1911
6779 1213.2703 1237.8761 1291.0053
6780 1322.3524 1344.0177 1370.2374
6781 1386.2854 1415.5074 1472.7173
6782 1485.0646 1763.5710 3057.6900
6783 3092.6181 3104.3023 3161.1612
6784 3167.6961 3201.1436 3857.5971
6785 Zero-point correction (Hartree): 0.111662
6786
6787 HOCHCHCH2CH2OO.Elmp
6788 ~~~~~
6789 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13752742
6790 Electronic state : 2-A
6791 Cartesian coordinates (Angs):
6792 C 1.989507 0.262297 0.130044
6793 C 0.777124 0.125563 -0.382394
6794 C -0.261349 1.198630 -0.291182
6795 C -1.508613 0.770590 0.468626
6796 O -2.193658 -0.275300 -0.251268
6797 O -1.812128 -1.459012 0.124798

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6798      O      2.930095      -0.719142      0.038424
6799      H      2.295569      1.168905      0.643384
6800      H      0.522343      -0.800812      -0.883005
6801      H      0.147817      2.075144      0.216406
6802      H      -0.571089      1.522324      -1.287893
6803      H      -1.275494      0.383278      1.458211
6804      H      -2.231510      1.582752      0.531264
6805      H      3.737879      -0.446456      0.475440
6806      Rotational constants (GHz):      5.4572000      1.2998800      1.1070100
6807      Vibrational harmonic frequencies (cm-1):
6808      64.2559      86.3268      130.5274
6809      178.1882      258.9797      287.9710
6810      353.5359      474.4244      526.6953
6811      558.9309      844.4467      871.0567
6812      882.9824      970.8423      1018.2529
6813      1084.6321      1117.4167      1179.0426
6814      1201.6086      1237.9409      1264.4799
6815      1319.0775      1345.9730      1370.6756
6816      1385.7920      1403.8346      1472.6167
6817      1484.7002      1785.9588      3055.0045
6818      3090.6026      3101.1149      3159.7897
6819      3162.9384      3196.9708      3918.7962
6820      Zero-point correction (Hartree): 0.111280
6821
6822      HOCHCHCH2CH2OO.Elmtc
6823      ~~~~~
6824      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14044555
6825      Electronic state : 2-A
6826      Cartesian coordinates (Angs):
6827      C      2.175963      0.186009      0.179724
6828      C      0.978214      0.057207      -0.373761
6829      C      -0.069240      1.126498      -0.303036
6830      C      -1.324123      0.674537      0.417155
6831      O      -1.901820      -0.397832      -0.361864
6832      O      -2.954285      -0.892729      0.211247
6833      O      3.175990      -0.730064      0.170248
6834      H      2.475424      1.081714      0.710223
6835      H      0.723648      -0.859065      -0.897583
6836      H      0.322422      1.997960      0.224062
6837      H      -0.351103      1.458940      -1.304999
6838      H      -1.111008      0.276191      1.408134
6839      H      -2.073764      1.462124      0.484559
6840      H      2.890411      -1.518371      -0.301936
6841      Rotational constants (GHz):      7.0870600      1.0463600      0.9597700
6842      Vibrational harmonic frequencies (cm-1):
6843      49.5994      90.3886      116.2541
6844      189.2059      270.1401      329.0272
6845      396.3809      452.8971      546.4457
6846      570.7131      812.1939      856.0773
6847      929.8350      991.5934      1033.3265
6848      1078.2671      1125.6248      1160.3652
6849      1217.0645      1246.0738      1296.9406
6850      1298.3373      1341.4574      1365.5075
6851      1398.7018      1414.1608      1472.0318
6852      1501.0744      1763.3001      3060.7044
6853      3085.6154      3109.2440      3146.6216
6854      3165.8735      3201.7740      3857.2177
6855      Zero-point correction (Hartree): 0.111494
6856
6857      HOCHCHCH2CH2OO.Elmtt
6858      ~~~~~
6859      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13798496
6860      Electronic state : 2-A
6861      Cartesian coordinates (Angs):
6862      C      2.173117      0.167424      0.157258
6863      C      0.970963      0.041464      -0.381228
6864      C      -0.072376      1.111851      -0.290724
6865      C      -1.324757      0.656602      0.432221
6866      O      -1.926112      -0.388564      -0.364734
6867      O      -2.984436      -0.874250      0.205234
6868      O      3.112428      -0.815310      0.071604
6869      H      2.470110      1.065938      0.689801

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6870	H	0.724771	-0.874854	-0.904278	
6871	H	0.322664	1.978532	0.242455	
6872	H	-0.361053	1.454522	-1.287458	
6873	H	-1.105852	0.232019	1.411023	
6874	H	-2.063330	1.451864	0.527200	
6875	H	3.915968	-0.547075	0.519265	
6876	Rotational constants (GHz):			7.2581100	1.0369700 0.9544000
6877	Vibrational harmonic frequencies (cm-1):				
6878		51.3622	91.4555		114.8537
6879		180.4182	259.3054		273.7506
6880		340.7793	398.9651		541.7653
6881		570.7578	811.9286		867.1642
6882		927.9807	970.4569		1033.7417
6883		1079.4163	1128.4707		1178.0868
6884		1206.8534	1237.1343		1279.3676
6885		1297.4922	1339.9602		1367.0724
6886		1398.1003	1403.2247		1471.8138
6887		1500.6779	1786.2808		3058.6410
6888		3085.1347	3105.6017		3145.9876
6889		3164.0356	3195.5698		3917.2662
6890	Zero-point correction (Hartree): 0.111131				
6891					
6892	HOCHCHCH2CH2OO.Elpmc				
6893	~~~~~				
6894	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14031527				
6895	Electronic state : 2-A				
6896	Cartesian coordinates (Angs):				
6897	C	-1.716898	0.146092	-0.385021	
6898	C	-0.768732	0.610804	0.416624	
6899	C	0.428961	1.348511	-0.088900	
6900	C	1.742575	0.638342	0.211557	
6901	O	1.802244	-0.622303	-0.477781	
6902	O	1.259329	-1.577483	0.218050	
6903	O	-2.823031	-0.544588	-0.015065	
6904	H	-1.686140	0.288376	-1.458048	
6905	H	-0.834430	0.427859	1.485386	
6906	H	0.348477	1.499505	-1.166609	
6907	H	0.496962	2.339651	0.368448	
6908	H	2.593005	1.204843	-0.164387	
6909	H	1.864156	0.433781	1.274056	
6910	H	-2.805809	-0.701510	0.933953	
6911	Rotational constants (GHz):			4.6279400	1.5523400 1.2629400
6912	Vibrational harmonic frequencies (cm-1):				
6913		62.2880	96.0757		108.9101
6914		193.1536	290.6709		350.8344
6915		422.9886	466.9158		540.3184
6916		553.9728	824.1871		861.6162
6917		942.6393	983.8111		993.8037
6918		1040.3522	1132.5951		1164.1930
6919		1225.5704	1237.3195		1280.0041
6920		1318.0575	1343.4109		1360.5222
6921		1394.6357	1413.1371		1473.5582
6922		1485.7583	1764.5370		3051.7259
6923		3091.9388	3105.8278		3154.9038
6924		3159.3070	3207.7406		3860.3590
6925	Zero-point correction (Hartree): 0.111534				
6926					
6927	HOCHCHCH2CH2OO.Elpmc				
6928	~~~~~				
6929	E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13829904				
6930	Electronic state : 2-A				
6931	Cartesian coordinates (Angs):				
6932	C	1.679246	0.110683	0.354616	
6933	C	0.765612	0.682938	-0.412719	
6934	C	-0.448739	1.353033	0.142140	
6935	C	-1.743553	0.626339	-0.199469	
6936	O	-1.783544	-0.650949	0.461241	
6937	O	-1.236397	-1.586352	-0.258257	
6938	O	2.781777	-0.496873	-0.162806	
6939	H	1.592392	0.106015	1.436620	
6940	H	0.886845	0.636445	-1.488836	
6941	H	-0.374506	1.436458	1.227989	

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6942      H      -0.541797      2.369393      -0.249760
6943      H      -2.611147      1.164789      0.178867
6944      H      -1.844907      0.444686      -1.267936
6945      H      3.283043      -0.922361      0.534221
6946      Rotational constants (GHz):      4.5792500      1.5738300      1.2710500
6947      Vibrational harmonic frequencies (cm-1):
6948          56.7528          97.4223          108.0751
6949          185.1658          241.9628          299.6491
6950          352.1428          462.0451          539.3009
6951          549.7923          828.6190          865.8652
6952          946.9980          961.6997          986.9639
6953          1038.2792          1136.0127          1180.7630
6954          1211.3605          1235.3846          1257.8402
6955          1313.9456          1340.3052          1361.4416
6956          1392.6747          1399.1790          1473.5968
6957          1484.3704          1787.1973          3054.9106
6958          3091.7525          3103.3339          3155.9447
6959          3170.1119          3189.6327          3917.6516
6960      Zero-point correction (Hartree): 0.111125
6961
6962      HOCHCHCH2CH200.Elptc
6963      ~~~~~
6964      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13968393
6965      Electronic state : 2-A
6966      Cartesian coordinates (Angs):
6967      C      -1.897069      -0.144664      -0.371056
6968      C      -1.056654      0.583217      0.350585
6969      C      0.114627      1.304085      -0.242630
6970      C      1.447573      0.762783      0.234917
6971      O      1.597683      -0.567063      -0.306902
6972      O      2.675606      -1.139922      0.129742
6973      O      -2.970820      -0.834603      0.085399
6974      H      -1.789832      -0.253802      -1.443022
6975      H      -1.197984      0.654553      1.425816
6976      H      0.080097      1.244268      -1.331847
6977      H      0.085634      2.364985      0.016705
6978      H      2.288937      1.353669      -0.125466
6979      H      1.498795      0.678604      1.320216
6980      H      -3.036259      -0.742095      1.040786
6981      Rotational constants (GHz):      5.3681500      1.2172800      1.0551600
6982      Vibrational harmonic frequencies (cm-1):
6983          47.1882          74.8600          110.7871
6984          204.1682          265.0175          334.2196
6985          391.4892          446.2482          540.5382
6986          567.6268          814.9271          863.6201
6987          917.8374          988.6263          1035.2476
6988          1069.2262          1122.3981          1159.4625
6989          1215.5601          1267.2054          1288.0298
6990          1298.6105          1341.6350          1362.4937
6991          1398.3535          1414.8400          1472.9430
6992          1500.9427          1766.3020          3062.0597
6993          3082.9820          3106.9162          3140.2931
6994          3153.5250          3208.4551          3860.2757
6995      Zero-point correction (Hartree): 0.111391
6996
6997      HOCHCHCH2CH200.Eltmc
6998      ~~~~~
6999      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59757712
7000      E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53594843
7001      T1 diagnostic: 0.021541
7002      E(MP2/Aug-CC-pVTZ) (Hartree): -381.49136426
7003      E(MP3/Aug-CC-pVTZ) (Hartree): -381.52330142
7004      E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49452390
7005      E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52516264
7006      E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13519483
7007      E(UHF/Aug-CC-pVTZ) (Hartree): -380.13005206
7008      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14085582
7009      Electronic state : 2-A
7010      Cartesian coordinates (Angs):
7011      C      -2.116996      0.458740      0.023049
7012      C      -1.201545      -0.458753      0.304944
7013      C      0.215959      -0.116171      0.646310

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7014      C      1.167619      -0.590526      -0.439314
7015      O      2.539002      -0.357420      -0.056058
7016      O      2.828865      0.907518      -0.091009
7017      O      -3.413943      0.237036      -0.302756
7018      H      -1.893836      1.518356      0.037417
7019      H      -1.476744      -1.509855      0.279228
7020      H      0.330920      0.961839      0.759748
7021      H      0.510763      -0.579923      1.590163
7022      H      1.107798      -1.667516      -0.590321
7023      H      0.992433      -0.071408      -1.380229
7024      H      -3.592948      -0.708296      -0.307352
7025      Rotational constants (GHz): 10.0368700      0.9316200      0.9000000
7026      Vibrational harmonic frequencies (cm-1):
7027      62.6193      86.0716      114.6904
7028      178.5780      307.7151      321.7048
7029      372.5639      446.0057      522.6093
7030      624.6712      795.8463      850.8975
7031      958.7976      991.0461      1019.8069
7032      1068.2658      1129.2750      1160.1231
7033      1220.7535      1266.9190      1283.4531
7034      1312.2745      1329.5215      1347.5466
7035      1395.5665      1412.2663      1485.2413
7036      1499.6656      1761.8549      3064.9628
7037      3093.7449      3118.4546      3151.9409
7038      3157.1601      3205.8173      3858.7043
7039      Zero-point correction (Hartree): 0.111578
7040
7041      HOCHCHCH2CH200.Eltmt
7042      ~~~~~
7043      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13929131
7044      Electronic state : 2-A
7045      Cartesian coordinates (Angs):
7046      C      -2.116572      0.416829      0.046261
7047      C      -1.191134      -0.498223      0.288145
7048      C      0.220217      -0.150112      0.644152
7049      C      1.178600      -0.580618      -0.453727
7050      O      2.546494      -0.334731      -0.064552
7051      O      2.817275      0.934757      -0.071963
7052      O      -3.393009      0.084359      -0.290855
7053      H      -1.898587      1.478277      0.110791
7054      H      -1.466099      -1.544455      0.212146
7055      H      0.326348      0.924914      0.792302
7056      H      0.517839      -0.642064      1.572851
7057      H      1.135422      -1.653914      -0.632830
7058      H      0.995182      -0.039785      -1.380697
7059      H      -3.922847      0.874692      -0.404589
7060      Rotational constants (GHz): 10.0574900      0.9318000      0.9003200
7061      Vibrational harmonic frequencies (cm-1):
7062      62.7043      88.0215      115.2441
7063      181.9248      265.8166      316.5343
7064      323.3749      385.1449      520.7013
7065      621.7596      796.6855      865.7763
7066      956.6579      970.6860      1017.8475
7067      1067.6172      1133.8664      1179.0186
7068      1212.3615      1246.3360      1283.4095
7069      1299.5434      1330.5167      1356.9055
7070      1382.7914      1407.6503      1484.8791
7071      1499.8352      1785.0922      3063.0106
7072      3094.1621      3115.4457      3156.4935
7073      3171.1139      3181.9716      3915.6844
7074      Zero-point correction (Hartree): 0.111303
7075
7076      HOCHCHCH2CH200.Eltpc
7077      ~~~~~
7078      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.59774833
7079      E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53608544
7080      T1 diagnostic: 0.021615
7081      E(MP2/Aug-CC-pVTZ) (Hartree): -381.49148884
7082      E(MP3/Aug-CC-pVTZ) (Hartree): -381.52339626
7083      E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49466624
7084      E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52527544
7085      E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13522254

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7086 E(UHF/Aug-CC-pVTZ) (Hartree): -380.13007016
7087 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14108463
7088 Electronic state : 2-A
7089 Cartesian coordinates (Angs):
7090 C 2.234338 0.135592 -0.357583
7091 C 1.152266 -0.409745 0.181764
7092 C -0.208548 -0.304048 -0.433368
7093 C -1.139220 0.517425 0.443306
7094 O -2.467277 0.557499 -0.118814
7095 O -3.071055 -0.583770 0.015422
7096 O 3.496844 0.090426 0.134221
7097 H 2.198969 0.685380 -1.290008
7098 H 1.240777 -0.954326 1.118051
7099 H -0.143183 0.158791 -1.418965
7100 H -0.656921 -1.291129 -0.560283
7101 H -1.221690 0.101001 1.446713
7102 H -0.828505 1.559128 0.495662
7103 H 3.509436 -0.407433 0.957481
7104 Rotational constants (GHz): 13.1446600 0.8826300 0.8713100
7105 Vibrational harmonic frequencies (cm-1):
7106 67.8392 71.8809 132.1719
7107 170.9503 293.7329 332.8483
7108 372.3254 440.9682 536.2726
7109 616.7591 789.1311 849.8083
7110 973.1622 989.9596 1014.5884
7111 1068.2345 1126.4066 1158.0426
7112 1225.3138 1255.7702 1293.0913
7113 1309.0186 1331.2088 1346.1744
7114 1393.1945 1412.4869 1483.8683
7115 1498.2063 1764.3313 3068.2706
7116 3092.7231 3113.9544 3151.3558
7117 3158.2694 3205.3995 3859.9303
7118 Zero-point correction (Hartree): 0.111557
7119
7120 HOCHCHCH2CH2OO.Eltpt
7121 ~~~~~
7122 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13930049
7123 Electronic state : 2-A
7124 Cartesian coordinates (Angs):
7125 C -2.230972 0.064200 0.344730
7126 C -1.142923 -0.387317 -0.259035
7127 C 0.211479 -0.361046 0.375652
7128 C 1.147173 0.565479 -0.382958
7129 O 2.467725 0.545511 0.198395
7130 O 3.082314 -0.567691 -0.062484
7131 O -3.453504 0.041539 -0.254464
7132 H -2.198295 0.469898 1.351149
7133 H -1.236164 -0.785712 -1.263260
7134 H 0.141500 -0.028243 1.412508
7135 H 0.660147 -1.356295 0.376634
7136 H 1.244648 0.273692 -1.427997
7137 H 0.830008 1.604246 -0.313275
7138 H -4.122658 0.379656 0.342337
7139 Rotational constants (GHz): 13.3164800 0.8817100 0.8703500
7140 Vibrational harmonic frequencies (cm-1):
7141 68.0919 72.1152 131.6989
7142 167.9317 240.6208 305.5826
7143 330.2599 384.9810 534.3830
7144 612.6315 793.2149 862.2344
7145 970.0369 973.8711 1011.7579
7146 1068.5068 1129.8299 1178.0602
7147 1214.5548 1242.4344 1280.3932
7148 1305.1409 1331.0117 1354.6634
7149 1382.6060 1408.1982 1484.8761
7150 1499.3454 1785.4662 3065.4744
7151 3093.5087 3110.7624 3157.8435
7152 3168.6656 3184.8947 3916.5030
7153 Zero-point correction (Hartree): 0.111225
7154
7155 HOCHCHCH2CH2OO.Elttc
7156 ~~~~~
7157 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14004222

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7158 Electronic state : 2-A
7159 Cartesian coordinates (Angs):
7160 C -2.275809 0.148690 -0.367891
7161 C -1.260724 0.112279 0.484643
7162 C 0.071423 0.733498 0.193929
7163 C 1.150763 -0.325924 0.094412
7164 O 2.412869 0.349900 -0.093776
7165 O 3.395681 -0.491871 -0.180792
7166 O -3.506287 -0.390315 -0.187617
7167 H -2.204780 0.644611 -1.328060
7168 H -1.382734 -0.396042 1.437314
7169 H 0.028218 1.293552 -0.740915
7170 H 0.348530 1.438096 0.981051
7171 H 1.231526 -0.919900 1.004892
7172 H 0.998327 -0.988116 -0.756826
7173 H -3.551102 -0.825174 0.669474
7174 Rotational constants (GHz): 13.6874400 0.8329600 0.8191700
7175 Vibrational harmonic frequencies (cm-1):
7176 60.8092 90.3699 93.3198
7177 165.2775 280.7597 313.8347
7178 355.1919 453.9746 528.9095
7179 593.7630 785.7557 851.2485
7180 989.6390 993.0427 1029.7627
7181 1104.1590 1122.0018 1159.0048
7182 1206.0828 1269.0806 1294.2590
7183 1309.3283 1318.2802 1346.6675
7184 1397.3583 1419.6101 1490.8330
7185 1507.2386 1765.0976 3063.5670
7186 3084.8968 3108.9567 3144.2032
7187 3154.2420 3207.2976 3859.5147
7188 Zero-point correction (Hartree): 0.111442
7189
7190 HOCHCHCH2CH2OO.Elttt
7191 ~~~~~
7192 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13833875
7193 Electronic state : 2-A
7194 Cartesian coordinates (Angs):
7195 C -2.273429 0.105513 -0.345910
7196 C -1.250519 0.154109 0.492492
7197 C 0.075477 0.744656 0.126087
7198 C 1.158404 -0.315660 0.135892
7199 O 2.416046 0.340116 -0.137218
7200 O 3.400500 -0.503981 -0.153931
7201 O -3.469088 -0.443689 0.003341
7202 H -2.206311 0.507793 -1.351936
7203 H -1.375714 -0.260890 1.486384
7204 H 0.027645 1.201252 -0.863577
7205 H 0.354735 1.529938 0.832104
7206 H 1.248309 -0.804624 1.105828
7207 H 1.003251 -1.068940 -0.635313
7208 H -4.091178 -0.375805 -0.722381
7209 Rotational constants (GHz): 13.8484500 0.8326000 0.8185100
7210 Vibrational harmonic frequencies (cm-1):
7211 57.7469 90.3574 103.0039
7212 158.1623 229.2563 299.1034
7213 314.3737 359.8705 526.9658
7214 590.0482 784.7093 863.0777
7215 967.4995 986.9136 1029.3380
7216 1103.2365 1124.1121 1179.2551
7217 1199.0412 1244.0592 1293.4717
7218 1302.6613 1312.7888 1355.5095
7219 1382.0788 1415.5474 1491.3168
7220 1507.2022 1788.3995 3061.7607
7221 3086.0660 3106.1688 3145.2990
7222 3169.8118 3184.8758 3916.9350
7223 Zero-point correction (Hartree): 0.111015
7224
7225
7226 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Ec.b
7227 ~~~~~
7228 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.10724016
7229 Electronic state : 2-A

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7230 Cartesian coordinates (Angs):
7231 C 1.217486 0.279742 0.364305
7232 C 0.341773 1.097742 -0.320596
7233 C -1.027092 1.246613 0.229747
7234 C -1.844235 -0.064593 -0.045476
7235 O -0.992753 -1.095210 -0.485394
7236 O 0.005605 -1.255843 0.439528
7237 O 2.391428 -0.139894 -0.136307
7238 H 1.213890 0.247341 1.445253
7239 H 0.518331 1.286381 -1.373712
7240 H -0.974047 1.394725 1.307886
7241 H -1.549034 2.096788 -0.204608
7242 H -2.361650 -0.370132 0.865237
7243 H -2.563582 0.066706 -0.852405
7244 H 2.354263 -0.151259 -1.098142
7245 Rotational constants (GHz): 4.7724200 2.2768000 1.7445200
7246 Vibrational harmonic frequencies (cm-1):
7247 1685.0331 79.5739 248.9258
7248 266.7727 368.0530 402.7393
7249 421.1075 441.7393 542.8748
7250 651.4000 781.5885 819.2272
7251 891.5753 903.7398 977.2995
7252 1039.4828 1100.8839 1133.4693
7253 1159.3361 1225.4296 1268.0599
7254 1279.5097 1296.2485 1321.3174
7255 1371.2509 1405.3781 1487.8162
7256 1504.3742 1563.6009 3068.4393
7257 3087.8182 3127.3766 3146.3952
7258 3173.8162 3211.4429 3854.2426
7259 Zero-point correction (Hartree): 0.110770
7260
7261 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Ec
7262 ~~~~~
7263 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.57644612
7264 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.50999223
7265 T1 diagnostic: 0.028421
7266 E(MP2/Aug-CC-pVTZ) (Hartree): -381.46077651
7267 E(MP3/Aug-CC-pVTZ) (Hartree): -381.49072084
7268 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47834524
7269 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50387730
7270 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.10921509
7271 E(UHF/Aug-CC-pVTZ) (Hartree): -380.08883155
7272 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11687402
7273 Electronic state : 2-A
7274 Cartesian coordinates (Angs):
7275 C 1.155879 0.174702 0.396882
7276 C 0.378016 1.143937 -0.200909
7277 C -1.050426 1.263609 0.187134
7278 C -1.791931 -0.024462 -0.246750
7279 O -1.122666 -1.127408 0.316294
7280 O 0.084327 -1.281446 -0.319510
7281 O 2.404324 -0.122337 0.004603
7282 H 0.959046 -0.158255 1.406366
7283 H 0.705464 1.550892 -1.151471
7284 H -1.160467 1.353572 1.268525
7285 H -1.521335 2.128324 -0.278811
7286 H -2.806017 -0.050121 0.151243
7287 H -1.807149 -0.117482 -1.333491
7288 H 2.553350 0.195881 -0.891592
7289 Rotational constants (GHz): 4.8099700 2.3018300 1.7081900
7290 Vibrational harmonic frequencies (cm-1):
7291 1612.2148 155.8931 259.5245
7292 308.9601 339.9696 400.6085
7293 432.1901 440.3496 541.4172
7294 590.7723 747.5627 862.9943
7295 933.5439 972.9901 987.3404
7296 1024.8407 1090.4612 1128.1823
7297 1165.3542 1214.9112 1262.3010
7298 1277.6477 1318.6330 1327.6199
7299 1367.9829 1403.7461 1484.0993
7300 1488.6522 1571.1142 3073.6098
7301 3076.3357 3128.1857 3139.6010

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7302          3172.6958          3222.8911          3853.6386
7303 Zero-point correction (Hartree): 0.111099
7304
7305 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Et.b
7306 ~~~~~
7307 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.10677807
7308 Electronic state : 2-A
7309 Cartesian coordinates (Angs):
7310   C      1.214263      0.289700      0.332681
7311   C      0.326195      1.114648     -0.316324
7312   C     -1.033088      1.235463      0.261697
7313   C     -1.845033     -0.070021     -0.053565
7314   O     -0.991057     -1.100931     -0.491333
7315   O      0.004584     -1.260867      0.433509
7316   O      2.353683     -0.063418     -0.294347
7317   H      1.212212      0.218401      1.414086
7318   H      0.498114      1.324250     -1.363766
7319   H     -0.967915      1.341177      1.344097
7320   H     -1.571161      2.095330     -0.132183
7321   H     -2.385987     -0.385297      0.840440
7322   H     -2.544451      0.076333     -0.875285
7323   H      2.847487     -0.687210      0.243044
7324 Rotational constants (GHz):  4.7508600      2.2809700      1.7416400
7325 Vibrational harmonic frequencies (cm-1):
7326   i672.3229          91.4225          248.4742
7327   275.6830          318.7083          368.7678
7328   416.8751          431.7870          540.0841
7329   655.4871          795.1183          823.1929
7330   885.9184          903.5206          972.9894
7331   1036.2457         1094.7108         1133.0696
7332   1177.5571         1217.2911         1251.4219
7333   1276.5256         1297.2793         1318.4758
7334   1357.5098         1390.8892         1487.3773
7335   1503.7334         1588.4282         3065.0986
7336   3087.2872         3126.5789         3145.9153
7337   3174.3288         3205.5509         3893.7939
7338 Zero-point correction (Hartree): 0.110621
7339
7340 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Et
7341 ~~~~~
7342 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.57685956
7343 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.51053770
7344 T1 diagnostic: 0.028927
7345 E(MP2/Aug-CC-pVTZ) (Hartree): -381.46051972
7346 E(MP3/Aug-CC-pVTZ) (Hartree): -381.49081210
7347 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47833678
7348 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50423593
7349 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.11048561
7350 E(UHF/Aug-CC-pVTZ) (Hartree): -380.08990202
7351 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11743003
7352 Electronic state : 2-A
7353 Cartesian coordinates (Angs):
7354   C      1.147043      0.214569      0.362170
7355   C      0.350660      1.166516     -0.223427
7356   C     -1.071962      1.255057      0.192903
7357   C     -1.791056     -0.052670     -0.223763
7358   O     -1.091404     -1.144407      0.327652
7359   O      0.098491     -1.285160     -0.343113
7360   O      2.388067      0.005591     -0.115672
7361   H      0.939296     -0.138660      1.365124
7362   H      0.673943      1.583833     -1.167781
7363   H     -1.167356      1.347532      1.275518
7364   H     -1.573728      2.104419     -0.268728
7365   H     -2.797301     -0.098079      0.192044
7366   H     -1.822870     -0.148961     -1.309517
7367   H      2.778671     -0.759101      0.315106
7368 Rotational constants (GHz):  4.7651800      2.3156100      1.7036200
7369 Vibrational harmonic frequencies (cm-1):
7370   i590.6847          159.4186          269.6552
7371   294.5891          342.8123          374.2063
7372   399.9901          435.6672          538.4892
7373   595.4815          773.5039          860.5234

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7374      934.0770      971.0382      982.5272
7375      1020.8763     1084.1233     1128.2875
7376      1182.8838     1208.9500     1256.2854
7377      1265.7570     1319.9350     1332.9792
7378      1358.1819     1384.0530     1483.8822
7379      1488.5767     1600.3175     3075.6803
7380      3076.1514     3129.3890     3140.5615
7381      3185.3172     3208.4006     3884.7204
7382      Zero-point correction (Hartree): 0.111054
7383
7384
7385      #####
7386      Z-HOCH=CHCH2CH2OO ring closure
7387      #####
7388
7389      HOCHCHCH2CH2OO.Zcptt
7390      ~~~~~
7391      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13711336
7392      Electronic state : 2-A
7393      Cartesian coordinates (Angs):
7394      C      -1.776794      -0.554659      -0.256263
7395      C      -1.493800      0.732244      -0.393931
7396      C      -0.341202      1.507229      0.179422
7397      C      0.865022      0.702094      0.611509
7398      O      1.362636      0.001504      -0.550034
7399      O      2.306136      -0.829333      -0.236274
7400      O      -1.045956      -1.415474      0.509502
7401      H      -2.641959      -0.983117      -0.748092
7402      H      -2.189973      1.293835      -1.001782
7403      H      -0.017457      2.242074      -0.560669
7404      H      -0.672659      2.085016      1.047217
7405      H      1.667247      1.352616      0.959066
7406      H      0.637097      -0.043564      1.366069
7407      H      -1.284185      -2.321888      0.308221
7408      Rotational constants (GHz):      3.9278800      2.0404800      1.5310900
7409      Vibrational harmonic frequencies (cm-1):
7410      45.9236      64.9179      135.0800
7411      247.0910      265.4998      269.3807
7412      385.3755      449.8302      535.0364
7413      742.0012      759.3706      851.3365
7414      877.4570      975.0962      1014.7206
7415      1055.0647      1080.1995      1130.9052
7416      1232.4978      1259.8112      1284.3392
7417      1303.6282      1317.0023      1385.4671
7418      1420.2666      1446.4422      1472.3424
7419      1505.9929      1788.8382      3052.2248
7420      3086.2696      3096.1607      3178.5278
7421      3182.7917      3214.4693      3910.7664
7422      Zero-point correction (Hartree): 0.111681
7423
7424      HOCHCHCH2CH2OO.Zcptt
7425      ~~~~~
7426      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13858979
7427      Electronic state : 2-A
7428      Cartesian coordinates (Angs):
7429      C      2.258555      0.186620      -0.159502
7430      C      1.324382      1.115087      -0.020896
7431      C      -0.138910      0.947789      0.264829
7432      C      -0.670348      -0.470054      0.176316
7433      O      -2.097451      -0.455162      0.413555
7434      O      -2.742614      0.049252      -0.592871
7435      O      2.019007      -1.155385      -0.046563
7436      H      3.284895      0.462810      -0.367898
7437      H      1.671553      2.134578      -0.122294
7438      H      -0.365199      1.344959      1.258467
7439      H      -0.708414      1.553057      -0.443552
7440      H      -0.503577      -0.913031      -0.802703
7441      H      -0.273150      -1.120533      0.949555
7442      H      2.820279      -1.648133      -0.229019
7443      Rotational constants (GHz):      6.2539000      1.3314300      1.1658700
7444      Vibrational harmonic frequencies (cm-1):
7445      21.5428      88.9392      136.3872

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7446      180.6831      222.3307      282.7500
7447      372.7885      454.7840      567.1876
7448      745.0536      765.6149      806.7722
7449      929.2624      975.1060      977.1411
7450     1054.0019     1098.4514     1128.5862
7451     1236.7695     1247.2451     1290.1310
7452     1310.8892     1328.5947     1348.8740
7453     1422.8371     1441.6560     1484.8573
7454     1496.2722     1791.5757     3050.7558
7455     3091.2172     3117.6643     3185.2642
7456     3187.6863     3213.3065     3917.4230
7457 Zero-point correction (Hartree): 0.111563
7458
7459 HOCHCHCH2CH200.Zcttc
7460 ~~~~~
7461 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13442233
7462 Point group : CS
7463 Electronic state : 2-A''
7464 Cartesian coordinates (Angs):
7465 C      -0.377205      -2.307271      0.000000
7466 C       0.796415      -1.684238      0.000000
7467 C       1.154718      -0.224566      0.000000
7468 C      -0.000000      0.750786      0.000000
7469 O       0.571304      2.076013      0.000000
7470 O      -0.349166      2.989418      0.000000
7471 O      -1.641430      -1.809192      0.000000
7472 H      -0.408505      -3.388123      0.000000
7473 H       1.648626      -2.350758      0.000000
7474 H       1.777089      -0.010247      0.872495
7475 H       1.777089      -0.010247     -0.872495
7476 H      -0.617134      0.675760     -0.897332
7477 H      -0.617134      0.675760      0.897332
7478 H      -1.649264      -0.850327      0.000000
7479 Rotational constants (GHz):      5.8449000      1.2754700      1.0608800
7480 Vibrational harmonic frequencies (cm-1):
7481      43.1149 ( A'' )      81.4073 ( A'' )      129.0539 ( A' )
7482      149.1265 ( A'' )      268.3374 ( A' )      311.4776 ( A'' )
7483      379.5594 ( A' )      482.1220 ( A'' )      508.2954 ( A' )
7484      751.1183 ( A'' )      767.0594 ( A' )      814.7686 ( A'' )
7485      913.8562 ( A' )      1003.6698 ( A'' )      1031.8930 ( A' )
7486     1073.4671 ( A' )      1088.9370 ( A'' )      1145.5511 ( A' )
7487     1230.7542 ( A' )      1253.1947 ( A'' )      1290.3416 ( A' )
7488     1317.5934 ( A'' )      1342.4242 ( A' )      1362.1290 ( A' )
7489     1427.3542 ( A' )      1444.3698 ( A' )      1497.6006 ( A' )
7490     1532.5811 ( A' )      1767.2677 ( A' )      3052.1786 ( A' )
7491     3061.3874 ( A' )      3082.0577 ( A'' )      3121.4614 ( A'' )
7492     3196.9164 ( A' )      3224.9995 ( A' )      3910.9139 ( A' )
7493 Zero-point correction (Hartree): 0.111763
7494
7495 HOCHCHCH2CH200.Zcttt
7496 ~~~~~
7497 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13769930
7498 Point group : CS
7499 Electronic state : 2-A''
7500 Cartesian coordinates (Angs):
7501 C      -0.410643      -2.264632      0.000000
7502 C       0.790060      -1.705198      0.000000
7503 C       1.158136      -0.250913      0.000000
7504 C      0.000000      0.723795      0.000000
7505 O       0.595745      2.042813      0.000000
7506 O      -0.306243      2.973965      0.000000
7507 O      -1.579759      -1.557348      0.000000
7508 H      -0.514846      -3.342783      0.000000
7509 H       1.619897      -2.399009      0.000000
7510 H       1.783976      -0.042358      0.871782
7511 H       1.783976      -0.042358     -0.871782
7512 H      -0.624334      0.644558     -0.886550
7513 H      -0.624334      0.644558      0.886550
7514 H      -2.327588      -2.156356      0.000000
7515 Rotational constants (GHz):      5.8453500      1.3275400      1.0964700
7516 Vibrational harmonic frequencies (cm-1):
7517      17.2363 ( A'' )      78.2270 ( A'' )      128.1975 ( A'' )

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7518      138.3477 ( A')          253.4598 ( A')          270.7581 ( A'')
7519      380.3751 ( A')          456.1568 ( A'')          510.4761 ( A')
7520      745.6136 ( A'')          770.0082 ( A')          803.5707 ( A'')
7521      930.3358 ( A')          978.1798 ( A'')          1016.3361 ( A')
7522      1069.1464 ( A')          1076.6634 ( A'')          1144.0290 ( A')
7523      1221.3629 ( A'')          1252.0845 ( A')          1299.7341 ( A')
7524      1314.2764 ( A')          1315.9130 ( A'')          1340.0882 ( A')
7525      1428.7474 ( A')          1443.9492 ( A')          1493.9967 ( A')
7526      1503.7163 ( A')          1792.5665 ( A')          3051.8416 ( A')
7527      3079.8236 ( A'')          3111.9295 ( A')          3171.9629 ( A'')
7528      3187.6752 ( A')          3213.1564 ( A')          3916.7245 ( A')
7529      Zero-point correction (Hartree): 0.111418
7530
7531      HOCHCHCH2CH200.Zgpmc
7532      ~~~~~
7533      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14139996
7534      Electronic state : 2-A
7535      Cartesian coordinates (Angs):
7536      C      -1.737468      -0.146900      0.370704
7537      C      -0.997116      0.936025      0.587248
7538      C      0.077260      1.427802      -0.337557
7539      C      1.434514      0.783067      -0.094846
7540      O      1.333949      -0.627424      -0.393721
7541      O      1.297258      -1.365867      0.677108
7542      O      -1.644538      -0.999462      -0.676321
7543      H      -2.531448      -0.435613      1.045857
7544      H      -1.192722      1.491430      1.493099
7545      H      -0.201334      1.255270      -1.380993
7546      H      0.200699      2.505915      -0.228546
7547      H      2.192512      1.171852      -0.773936
7548      H      1.761229      0.867044      0.938717
7549      H      -0.785432      -0.913843      -1.104020
7550      Rotational constants (GHz): 3.6140200      2.2889700      1.7079300
7551      Vibrational harmonic frequencies (cm-1):
7552      58.2574      93.1132      123.1605
7553      232.3401      265.0035      361.0549
7554      456.4881      524.6469      582.7744
7555      657.9690      761.3718      837.5371
7556      919.5851      981.6888      992.3137
7557      1035.9988      1083.2694      1141.7043
7558      1223.1119      1228.6007      1276.7832
7559      1312.6929      1350.0219      1370.6682
7560      1383.0603      1438.3066      1483.6831
7561      1488.0368      1742.8540      3054.4239
7562      3091.7480      3110.0397      3163.6564
7563      3210.9156      3231.1092      3838.7502
7564      Zero-point correction (Hartree): 0.111873
7565
7566      HOCHCHCH2CH200.Zgppt
7567      ~~~~~
7568      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13954204
7569      Electronic state : 2-A
7570      Cartesian coordinates (Angs):
7571      C      1.914859      0.090571      -0.431387
7572      C      0.985666      1.025018      -0.298066
7573      C      -0.116046      0.973688      0.714388
7574      C      -1.485281      0.843125      0.071006
7575      O      -1.596557      -0.397079      -0.661614
7576      O      -1.635879      -1.415766      0.141001
7577      O      1.969504      -0.998001      0.385586
7578      H      2.684108      0.156570      -1.191408
7579      H      1.022074      1.860050      -0.985306
7580      H      0.028552      0.133836      1.392152
7581      H      -0.126916      1.885411      1.316826
7582      H      -2.284305      0.853205      0.810695
7583      H      -1.659541      1.610620      -0.682013
7584      H      2.644287      -1.607334      0.083620
7585      Rotational constants (GHz): 4.1422700      1.8180600      1.4550000
7586      Vibrational harmonic frequencies (cm-1):
7587      28.3230      59.2797      144.7891
7588      214.5535      252.6226      295.0937
7589      378.7974      519.7864      568.4510

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7590      668.2856      766.4669      861.6718
7591      890.9170      973.7082      995.9278
7592      1047.5808     1076.0585     1148.4667
7593      1215.0584     1257.7825     1277.3019
7594      1296.0053     1313.5432     1357.1520
7595      1398.7465     1444.7125     1481.0926
7596      1490.7725     1785.2217     3064.5679
7597      3089.8000     3132.9715     3151.1366
7598      3184.5111     3210.8037     3919.8909
7599 Zero-point correction (Hartree): 0.111543
7600
7601 HOCHCHCH2CH200.Zgpctc
7602 ~~~~~
7603 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14241976
7604 Electronic state : 2-A
7605 Cartesian coordinates (Angs):
7606 C      1.897914      -0.385648      -0.365766
7607 C      1.383603      0.840262      -0.401496
7608 C      0.264452      1.332044      0.474141
7609 C     -1.122747      0.977069      -0.024651
7610 O     -1.262451     -0.455486      0.137606
7611 O     -2.386318     -0.899974     -0.330991
7612 O      1.496806     -1.417339      0.410545
7613 H      2.743478     -0.659416     -0.982587
7614 H      1.826601      1.532954     -1.102642
7615 H      0.369226      0.941970      1.491084
7616 H      0.315083      2.417337      0.557387
7617 H     -1.913850      1.441070      0.563359
7618 H     -1.261010      1.196692     -1.081776
7619 H      0.596840     -1.270578      0.724538
7620 Rotational constants (GHz): 4.0906500      1.8775300      1.4146100
7621 Vibrational harmonic frequencies (cm-1):
7622      68.9838      87.6903      136.6126
7623      229.9296      265.9066      335.7055
7624      440.9411      503.4870      609.9387
7625      656.8277      765.8418      844.7707
7626      899.0257      994.9890     1024.7678
7627      1053.7330     1087.6190     1138.3086
7628      1222.6732     1254.0154     1290.0043
7629      1295.5010     1353.6839     1378.2692
7630      1396.6054     1439.7699     1481.4740
7631      1500.2293     1746.2514     3053.1188
7632      3087.8198     3118.3686     3150.7968
7633      3205.2596     3225.7012     3823.1965
7634 Zero-point correction (Hartree): 0.112013
7635
7636 HOCHCHCH2CH200.Zgmtt
7637 ~~~~~
7638 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14019926
7639 Electronic state : 2-A
7640 Cartesian coordinates (Angs):
7641 C      2.270326      -0.081809      0.116109
7642 C      1.368345     -1.008545     -0.173754
7643 C     -0.033049     -0.679805     -0.596835
7644 C     -0.912228     -0.443690      0.621475
7645 O     -2.280375     -0.204704      0.228308
7646 O     -2.418909      0.964599     -0.318224
7647 O      1.972686      1.245837      0.034722
7648 H      3.276542     -0.331255      0.429921
7649 H      1.665202     -2.041996     -0.067885
7650 H     -0.047455      0.226657     -1.201609
7651 H     -0.455768     -1.491488     -1.188285
7652 H     -0.964202     -1.321549      1.263055
7653 H     -0.572122      0.420624      1.189408
7654 H      2.750225      1.776249      0.214973
7655 Rotational constants (GHz): 5.5989900      1.3520200      1.1808600
7656 Vibrational harmonic frequencies (cm-1):
7657      43.3704      65.7348      120.2632
7658      202.9634      257.3635      286.3124
7659      355.0370      527.0481      572.4761
7660      679.5690      764.8308      817.1081
7661      959.4980      972.6762      985.8933

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7662      1066.5337          1079.6370          1137.5424
7663      1223.2900          1259.5267          1290.9339
7664      1294.5599          1306.4462          1335.8659
7665      1399.4687          1434.0395          1485.8825
7666      1502.2942          1772.3973          3082.3660
7667      3098.7856          3130.6060          3162.4014
7668      3191.4227          3226.1186          3915.6145
7669      Zero-point correction (Hartree): 0.111644
7670
7671      HOCHCHCH2CH200.Zgtpc
7672      ~~~~~
7673      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14075752
7674      Electronic state : 2-A
7675      Cartesian coordinates (Angs):
7676      C      -2.374942          0.337594          0.155917
7677      C      -1.213663          0.969303          0.026282
7678      C      0.051787          0.353347          -0.491740
7679      C      0.940906          -0.095044          0.658214
7680      O      2.162758          -0.680760          0.162951
7681      O      2.948064          0.222433          -0.339989
7682      O      -2.645564          -0.950933          -0.168538
7683      H      -3.253375          0.830196          0.548466
7684      H      -1.180539          2.000982          0.346920
7685      H      -0.142237          -0.503852          -1.142065
7686      H      0.609705          1.072998          -1.090594
7687      H      1.211162          0.739468          1.303249
7688      H      0.474510          -0.883184          1.247021
7689      H      -1.865818          -1.373723          -0.540433
7690      Rotational constants (GHz): 7.9091100 1.1060900 1.0406700
7691      Vibrational harmonic frequencies (cm-1):
7692      27.6412          67.0647          124.0091
7693      202.9161          276.6980          353.9663
7694      400.0936          544.5398          578.0624
7695      659.8564          773.9056          803.7664
7696      971.0301          980.5378          995.6468
7697      1062.8364          1078.2751          1139.3897
7698      1219.6081          1248.4100          1274.1562
7699      1303.1465          1327.5545          1348.3426
7700      1397.1146          1436.2636          1488.9787
7701      1512.6791          1754.1465          3055.7317
7702      3094.2064          3114.3684          3156.7534
7703      3212.0556          3233.4812          3862.2667
7704      Zero-point correction (Hartree): 0.111811
7705
7706      HOCHCHCH2CH200.Zgtpt
7707      ~~~~~
7708      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14074793
7709      Electronic state : 2-A
7710      Cartesian coordinates (Angs):
7711      C      -2.324227          0.311436          0.177412
7712      C      -1.219788          1.035274          0.068940
7713      C      0.059043          0.494489          -0.498552
7714      C      0.866340          -0.199202          0.587154
7715      O      2.103565          -0.717299          0.053086
7716      O      2.945104          0.237649          -0.200539
7717      O      -2.363701          -0.988806          -0.234841
7718      H      -3.239998          0.710018          0.596257
7719      H      -1.251137          2.050569          0.437250
7720      H      -0.153083          -0.226551          -1.288160
7721      H      0.664985          1.295553          -0.919357
7722      H      1.120232          0.478128          1.401064
7723      H      0.342422          -1.072435          0.970777
7724      H      -3.251384          -1.339617          -0.149199
7725      Rotational constants (GHz): 7.5430100 1.1750500 1.0826100
7726      Vibrational harmonic frequencies (cm-1):
7727      24.4640          68.1809          125.1362
7728      203.0655          252.2195          270.6904
7729      363.9977          526.6943          578.7486
7730      676.4526          766.1211          809.5074
7731      966.7978          974.4646          988.3892
7732      1065.2591          1078.1403          1135.2163
7733      1225.4347          1262.0164          1288.1527

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7734      1294.5643          1310.5307          1334.8408
7735      1397.7532          1434.8279          1485.8232
7736      1501.1418          1774.3630          3082.8514
7737      3097.4074          3132.3512          3162.7554
7738      3193.8803          3228.2664          3916.4641
7739      Zero-point correction (Hartree): 0.111623
7740
7741      HOCHCHCH2CH200.Zgttc
7742      ~~~~~
7743      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13967776
7744      Electronic state : 2-A
7745      Cartesian coordinates (Angs):
7746      C      2.398795      0.120656      -0.319230
7747      C      1.388901      0.958388      -0.113563
7748      C      0.123169      0.616565      0.617809
7749      C     -0.960737      0.190896      -0.354749
7750      O     -2.151912     -0.090414      0.411191
7751      O     -3.129570     -0.472234     -0.351222
7752      O      2.490714     -1.166102      0.096813
7753      H      3.285422      0.415956     -0.862452
7754      H      1.484300      1.951272     -0.529376
7755      H      0.277657     -0.180984      1.349411
7756      H     -0.228776      1.479200      1.183930
7757      H     -1.203033      0.978332     -1.067333
7758      H     -0.693941     -0.714815     -0.898969
7759      H      1.703757     -1.418004      0.588932
7760      Rotational constants (GHz):      7.1967100      1.0749200      1.0053600
7761      Vibrational harmonic frequencies (cm-1):
7762      27.6140          75.3062          103.2976
7763      164.6930          279.9752          327.4172
7764      409.5551          486.7181          584.7638
7765      659.6895          772.5865          798.5818
7766      963.9454          998.3189          1023.3267
7767      1066.5952          1102.6237          1135.4684
7768      1203.3977          1251.5210          1290.0301
7769      1301.4801          1310.1920          1349.7321
7770      1403.9103          1437.3067          1501.7698
7771      1515.9947          1754.9348          3056.6056
7772      3086.3611          3107.6039          3144.8072
7773      3213.9386          3234.4311          3863.8149
7774      Zero-point correction (Hartree): 0.111649
7775
7776      HOCHCHCH2CH200.Zgttt
7777      ~~~~~
7778      E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13973051
7779      Electronic state : 2-A
7780      Cartesian coordinates (Angs):
7781      C      2.351439      0.076127      -0.312571
7782      C      1.403691      0.990183      -0.166351
7783      C      0.127070      0.732235      0.579489
7784      C     -0.917596      0.150776     -0.353388
7785      O     -2.130330     -0.040952      0.408884
7786      O     -3.082366     -0.527365     -0.325056
7787      O      2.223606     -1.171407      0.223381
7788      H      3.264418      0.272205     -0.861180
7789      H      1.560642      1.950948     -0.635060
7790      H      0.303140      0.027431      1.391986
7791      H     -0.254728      1.656223      1.013054
7792      H     -1.154796      0.818428     -1.180964
7793      H     -0.613335     -0.819983     -0.742173
7794      H      3.019754     -1.683391      0.073604
7795      Rotational constants (GHz):      6.8219700      1.1327600      1.0449100
7796      Vibrational harmonic frequencies (cm-1):
7797      17.7531          75.6068          100.6331
7798      163.6008          251.6023          256.2517
7799      357.1504          470.8270          578.0969
7800      671.1409          764.7380          804.8320
7801      967.3141          972.8733          1022.0913
7802      1068.3820          1103.5542          1130.0493
7803      1208.6234          1269.6215          1292.2993
7804      1293.7736          1312.5331          1316.4638
7805      1403.7061          1435.9979          1494.8269

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7806      1505.7502          1776.5340          3080.9903
7807      3090.6090          3125.2729          3151.1963
7808      3192.8048          3228.0659          3916.2471
7809 Zero-point correction (Hartree): 0.111338
7810
7811 HOCHCHCH2CH2OO.Zlmmc
7812 ~~~~~
7813 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13994056
7814 Electronic state : 2-A
7815 Cartesian coordinates (Angs):
7816   C      2.143768      -0.664679      0.139343
7817   C      0.823500      -0.626813      0.007766
7818   C      0.009027      0.560010     -0.410802
7819   C     -1.165145      0.807557      0.521676
7820   O     -2.073223     -0.316307      0.501905
7821   O     -2.704934     -0.391193     -0.629406
7822   O      3.028093      0.339703     -0.091022
7823   H      2.655945     -1.560534      0.461000
7824   H      0.286885     -1.541015      0.221674
7825   H      0.598678      1.479894     -0.427379
7826   H     -0.393321      0.426727     -1.417786
7827   H     -0.850580      0.878497      1.561091
7828   H     -1.737194      1.687549      0.232840
7829   H      2.573202      1.114817     -0.431159
7830 Rotational constants (GHz): 8.3236200 1.1198900 1.0759200
7831 Vibrational harmonic frequencies (cm-1):
7832      17.6350          67.8239          141.9868
7833      214.7837         252.1685          318.5315
7834      428.7667         524.9213          588.2432
7835      647.9435         778.0323          823.9482
7836      899.4037         997.0807         1004.6641
7837     1043.3525        1106.6705        1128.8582
7838     1219.1224        1238.5768        1279.6884
7839     1305.2664        1337.6068        1369.0230
7840     1397.5003        1441.7449        1472.6402
7841     1491.9527        1760.7025        3057.5479
7842     3090.4578        3101.2578        3159.9774
7843     3209.5933        3231.4405        3876.0568
7844 Zero-point correction (Hartree): 0.111687
7845
7846 HOCHCHCH2CH2OO.Zlmmt
7847 ~~~~~
7848 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14069596
7849 Electronic state : 2-A
7850 Cartesian coordinates (Angs):
7851   C     -2.088309      -0.661230     -0.159614
7852   C     -0.799558     -0.727793      0.137412
7853   C      0.004714      0.427704      0.647944
7854   C      1.058514      0.886017     -0.344729
7855   O      1.993842     -0.180062     -0.630865
7856   O      2.748805     -0.433773      0.393502
7857   O     -2.807425      0.491902     -0.019341
7858   H     -2.635411     -1.519816     -0.529306
7859   H     -0.303212     -1.676494     -0.011978
7860   H     -0.647327      1.274451      0.860453
7861   H      0.514923      0.159490      1.574692
7862   H      0.624742      1.125067     -1.313747
7863   H      1.637611      1.726756      0.033916
7864   H     -3.725278      0.337827     -0.246486
7865 Rotational constants (GHz): 8.0364600 1.1756500 1.1218800
7866 Vibrational harmonic frequencies (cm-1):
7867      23.9377          62.4069          135.4223
7868      205.8432         253.4339         279.2227
7869      389.6089         524.3234         602.4719
7870      656.0122         778.7954         827.2330
7871      890.9544         976.7741         1004.8483
7872     1048.0315        1099.1372        1132.7352
7873     1211.3681        1247.2811        1294.7766
7874     1300.3257        1305.2226        1357.3751
7875     1392.5991        1444.6908        1480.8993
7876     1489.5894        1781.4930        3077.5404
7877     3094.8937        3130.4073        3159.1728

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7878          3191.1439          3224.0324          3920.0462
7879 Zero-point correction (Hartree): 0.111617
7880
7881 HOCHCHCH2CH2OO.Zlmpc
7882 ~~~~~
7883 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13868808
7884 Electronic state : 2-A
7885 Cartesian coordinates (Angs):
7886   C      -1.989705      -0.744530      0.029943
7887   C      -0.720256      -0.485431      0.318009
7888   C      -0.087986      0.872455      0.366130
7889   C       1.236003      0.929434     -0.382633
7890   O       2.209234      0.096137      0.280618
7891   O       2.301386     -1.081886     -0.259005
7892   O      -2.973361      0.146858     -0.259003
7893   H      -2.368788     -1.756248      0.000843
7894   H      -0.087874     -1.335139      0.534889
7895   H      -0.728776      1.638039     -0.079650
7896   H       0.094512      1.182833      1.398414
7897   H       1.147655      0.572355     -1.406187
7898   H       1.661348      1.931503     -0.357447
7899   H      -2.644486      1.046223     -0.180442
7900 Rotational constants (GHz):  6.7689600      1.2445200      1.1083900
7901 Vibrational harmonic frequencies (cm-1):
7902      18.0344          91.5867          105.7143
7903      226.4445          232.0717          322.9611
7904      433.7305          515.3716          568.8543
7905      651.4993          779.4896          844.9060
7906      878.1583          999.1262          1017.5783
7907      1051.9170         1093.4299          1129.7210
7908      1230.1992         1236.6756          1271.0215
7909      1318.5707         1345.2177          1372.6220
7910      1390.8427         1445.6145          1469.7737
7911      1485.7653         1760.8773          3047.9076
7912      3082.0069         3098.8408          3163.8554
7913      3211.9308         3234.1030          3877.2726
7914 Zero-point correction (Hartree): 0.111639
7915
7916 HOCHCHCH2CH2OO.Zlmpc
7917 ~~~~~
7918 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13978773
7919 Electronic state : 2-A
7920 Cartesian coordinates (Angs):
7921   C      -1.922704      -0.708652      0.104527
7922   C      -0.703461      -0.461169      0.557734
7923   C      -0.057498      0.888661      0.521306
7924   C       1.167248      0.936171     -0.379521
7925   O       2.204704      0.079601      0.144661
7926   O       2.144685     -1.121019     -0.347727
7927   O      -2.709907      0.267767     -0.438055
7928   H      -2.355496     -1.700688      0.142598
7929   H      -0.144789     -1.293540      0.961654
7930   H      -0.767207      1.631260      0.156524
7931   H       0.247172      1.192543      1.525260
7932   H       0.948198      0.597554     -1.389685
7933   H       1.610516      1.930687     -0.392956
7934   H      -3.555761     -0.098666     -0.698706
7935 Rotational constants (GHz):  6.1146800      1.3366200      1.2016300
7936 Vibrational harmonic frequencies (cm-1):
7937      27.3716          88.2057          114.5263
7938      221.3444          238.6604          267.6976
7939      403.9375          513.5193          587.8196
7940      654.3555          781.7969          849.4386
7941      877.1053          977.9788          1013.9296
7942      1054.9938         1090.2377          1130.0488
7943      1216.4038         1236.8401          1291.6605
7944      1297.7336         1321.4059          1361.5667
7945      1385.6273         1446.8172          1479.1669
7946      1485.9362         1781.7754          3066.5438
7947      3096.1160         3123.3747          3162.6365
7948      3192.2612         3226.0934          3921.1846
7949 Zero-point correction (Hartree): 0.111599

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7950
7951 HOCHCHCH2CH2OO.Zlmtc
7952 ~~~~~
7953 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13905289
7954 Electronic state : 2-A
7955 Cartesian coordinates (Angs):
7956 C -2.192234 -0.718371 -0.080291
7957 C -0.903735 -0.591983 0.212102
7958 C -0.170168 0.700361 0.418640
7959 C 1.165032 0.721580 -0.299271
7960 O 1.997363 -0.285070 0.318060
7961 O 3.143934 -0.386438 -0.278970
7962 O -3.107001 0.273427 -0.230218
7963 H -2.647185 -1.686944 -0.232436
7964 H -0.333417 -1.505117 0.311545
7965 H -0.739251 1.555554 0.046180
7966 H 0.009899 0.884330 1.481313
7967 H 1.071934 0.464778 -1.353488
7968 H 1.680731 1.674843 -0.191820
7969 H -2.710451 1.127670 -0.039355
7970 Rotational constants (GHz): 9.7604000 1.0288300 0.9728300
7971 Vibrational harmonic frequencies (cm-1):
7972 19.6535 66.5428 120.1996
7973 217.3154 241.8543 313.8582
7974 388.7097 501.0476 578.1024
7975 661.9453 779.6506 823.0225
7976 908.1268 998.9615 1044.1810
7977 1051.8555 1090.0733 1136.9804
7978 1229.3177 1236.2048 1287.8689
7979 1296.4890 1335.1353 1372.6237
7980 1400.6148 1444.0866 1469.3469
7981 1501.9053 1759.4537 3050.8456
7982 3083.3175 3094.3059 3148.6704
7983 3211.1193 3233.2802 3875.4610
7984 Zero-point correction (Hartree): 0.111567
7985
7986 HOCHCHCH2CH2OO.Zlmtt
7987 ~~~~~
7988 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14001114
7989 Electronic state : 2-A
7990 Cartesian coordinates (Angs):
7991 C -2.129890 -0.693101 -0.078516
7992 C -0.912971 -0.635025 0.440602
7993 C -0.162846 0.640650 0.675647
7994 C 1.084324 0.746825 -0.178450
7995 O 1.976008 -0.318638 0.223395
7996 O 3.051639 -0.340873 -0.499865
7997 O -2.819622 0.428371 -0.441076
7998 H -2.637773 -1.636103 -0.239607
7999 H -0.434511 -1.570323 0.694454
8000 H -0.799649 1.494655 0.448190
8001 H 0.129922 0.721365 1.724899
8002 H 0.872470 0.609029 -1.237642
8003 H 1.616475 1.684755 -0.024412
8004 H -3.682831 0.189645 -0.781210
8005 Rotational constants (GHz): 8.1761600 1.0884600 1.0485000
8006 Vibrational harmonic frequencies (cm-1):
8007 23.2548 68.7763 118.9651
8008 204.1627 245.2082 274.0911
8009 350.5013 480.3196 602.0876
8010 655.5972 780.3875 824.4920
8011 907.0490 976.6682 1041.0311
8012 1052.1215 1085.7309 1138.5377
8013 1217.7992 1245.1212 1293.7441
8014 1300.0195 1304.5116 1356.4493
8015 1395.4060 1446.1590 1480.4572
8016 1500.4784 1781.5388 3067.6293
8017 3086.9684 3129.9267 3147.0592
8018 3191.7444 3226.1869 3920.6148
8019 Zero-point correction (Hartree): 0.111450
8020
8021 HOCHCHCH2CH2OO.Zlpmt

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8022 ~~~~~
8023 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13945018
8024 Electronic state : 2-A
8025 Cartesian coordinates (Angs):
8026 C -1.792042 -0.245705 0.497000
8027 C -0.763719 0.514753 0.840462
8028 C 0.080855 1.269692 -0.135131
8029 C 1.532826 0.812047 -0.131362
8030 O 1.629254 -0.554384 -0.573924
8031 O 1.511557 -1.390915 0.414204
8032 O -2.197243 -0.376930 -0.798829
8033 H -2.365981 -0.794326 1.233637
8034 H -0.507953 0.557576 1.890440
8035 H -0.322875 1.165542 -1.141313
8036 H 0.084996 2.336127 0.106554
8037 H 2.127656 1.380476 -0.844490
8038 H 1.979199 0.862095 0.860435
8039 H -2.891109 -1.034385 -0.862684
8040 Rotational constants (GHz): 4.2484800 1.7298900 1.5147800
8041 Vibrational harmonic frequencies (cm-1):
8042 17.9802 96.2996 108.0144
8043 219.1300 246.6748 290.6683
8044 387.2275 523.5856 545.1065
8045 672.0064 766.3136 846.1595
8046 923.9577 971.3979 991.2150
8047 1047.3391 1068.3295 1149.5674
8048 1225.9786 1235.6111 1284.1883
8049 1297.3051 1318.1810 1360.7644
8050 1393.2404 1446.2410 1477.8737
8051 1486.1508 1782.0974 3058.1557
8052 3092.6592 3127.6936 3155.3540
8053 3189.6091 3217.7380 3919.5797
8054 Zero-point correction (Hartree): 0.111492
8055
8056 HOCHCHCH2CH2OO.Zlptt
8057 ~~~~~
8058 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.13906481
8059 Electronic state : 2-A
8060 Cartesian coordinates (Angs):
8061 C -2.005846 -0.189901 0.557402
8062 C -1.055449 0.728700 0.636447
8063 C -0.149303 1.104773 -0.494933
8064 C 1.307147 0.824153 -0.185709
8065 O 1.465252 -0.607883 -0.080592
8066 O 2.673323 -0.927575 0.263857
8067 O -2.267356 -0.865206 -0.597161
8068 H -2.627361 -0.440774 1.408355
8069 H -0.920009 1.219966 1.591008
8070 H -0.434299 0.569448 -1.399886
8071 H -0.232266 2.172840 -0.710148
8072 H 1.972741 1.163634 -0.978403
8073 H 1.622660 1.253347 0.765125
8074 H -2.930518 -1.539498 -0.444117
8075 Rotational constants (GHz): 5.0261900 1.3870900 1.2335400
8076 Vibrational harmonic frequencies (cm-1):
8077 21.3258 66.7347 117.6948
8078 209.2188 235.3191 293.1693
8079 337.7011 470.2339 570.4101
8080 675.2776 764.1390 852.0397
8081 890.5305 971.6337 1039.7919
8082 1062.8667 1072.7564 1140.2453
8083 1216.0551 1265.2629 1288.7033
8084 1296.4313 1299.1031 1356.4039
8085 1399.5920 1448.0565 1478.8844
8086 1502.9722 1786.2420 3066.2634
8087 3082.7260 3125.5137 3141.4267
8088 3187.1186 3213.1129 3920.4763
8089 Zero-point correction (Hartree): 0.111324
8090
8091 HOCHCHCH2CH2OO.Zpmmc
8092 ~~~~~
8093 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.60037010

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8094 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.53772838
8095 T1 diagnostic: 0.022191
8096 E(MP2/Aug-CC-pVTZ) (Hartree): -381.49448818
8097 E(MP3/Aug-CC-pVTZ) (Hartree): -381.52479655
8098 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.49774632
8099 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.52669599
8100 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.13149271
8101 E(UHF/Aug-CC-pVTZ) (Hartree): -380.12616632
8102 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14414641
8103 Electronic state : 2-A
8104 Cartesian coordinates (Angs):
8105 C 1.838020 0.079555 0.342809
8106 C 1.016432 1.117681 0.218070
8107 C -0.200990 1.144807 -0.658951
8108 C -1.489617 0.807122 0.068881
8109 O -1.451380 -0.522535 0.649006
8110 O -1.199537 -1.432397 -0.236220
8111 O 1.729213 -1.129048 -0.251044
8112 H 2.725321 0.135368 0.959152
8113 H 1.258623 2.004009 0.787568
8114 H -0.332366 2.141817 -1.082837
8115 H -0.092628 0.466424 -1.506073
8116 H -1.657397 1.451712 0.929058
8117 H -2.353180 0.834791 -0.595467
8118 H 0.842185 -1.257284 -0.610196
8119 Rotational constants (GHz): 3.8427200 2.2415600 1.6192300
8120 Vibrational harmonic frequencies (cm-1):
8121 53.1930 131.5021 148.7968
8122 214.3796 291.8812 357.7868
8123 466.1477 541.8760 599.5496
8124 667.3210 761.4688 849.8795
8125 886.5390 981.9506 996.2389
8126 1037.1786 1088.8224 1148.0690
8127 1222.6972 1260.3105 1275.4686
8128 1306.3988 1351.2209 1373.7689
8129 1404.3696 1442.6719 1490.4872
8130 1495.2118 1747.8273 3075.1083
8131 3090.8924 3114.1355 3157.0129
8132 3205.6803 3226.0874 3797.6382
8133 Zero-point correction (Hartree): 0.112222
8134
8135 HOCHCHCH2CH200.Zptpc
8136 ~~~~~
8137 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.14299943
8138 Electronic state : 2-A
8139 Cartesian coordinates (Angs):
8140 C 1.990719 -0.256495 0.149012
8141 C 1.485695 0.947781 -0.106531
8142 C 0.056334 1.134753 -0.529354
8143 C -0.937822 0.806510 0.595548
8144 O -2.050788 0.022964 0.099607
8145 O -1.651134 -1.141169 -0.305940
8146 O 1.331854 -1.432158 0.068728
8147 H 3.017806 -0.397564 0.456449
8148 H 2.133420 1.803863 0.003447
8149 H -0.110610 2.147300 -0.887896
8150 H -0.173160 0.466885 -1.364114
8151 H -0.471153 0.216023 1.382390
8152 H -1.404024 1.688816 1.026043
8153 H 0.398713 -1.317709 -0.167528
8154 Rotational constants (GHz): 4.3235600 1.9772300 1.4811700
8155 Vibrational harmonic frequencies (cm-1):
8156 86.7356 102.9580 196.4536
8157 219.3773 324.4331 366.9969
8158 522.0243 568.6202 624.7459
8159 707.6098 753.2826 813.2521
8160 954.6509 992.7960 1003.1022
8161 1032.6939 1079.1186 1135.4807
8162 1230.2006 1263.6910 1287.2719
8163 1308.1613 1339.8173 1375.1774
8164 1399.4617 1431.3431 1493.5697
8165 1509.4091 1733.6295 3059.1022

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8166          3101.0760          3136.5884          3168.4579
8167          3216.8284          3242.0571          3721.9528
8168 Zero-point correction (Hartree): 0.112774
8169
8170
8171 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Zp
8172 ~~~~~
8173 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.57530128
8174 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.50813416
8175 T1 diagnostic: 0.028163
8176 E(MP2/Aug-CC-pVTZ) (Hartree): -381.46065809
8177 E(MP3/Aug-CC-pVTZ) (Hartree): -381.48930848
8178 E(PMP2/Aug-CC-pVTZ) (Hartree): -381.47781124
8179 E(PMP3/Aug-CC-pVTZ) (Hartree): -381.50213210
8180 E(PUHF/Aug-CC-pVTZ) (Hartree): -380.10312287
8181 E(UHF/Aug-CC-pVTZ) (Hartree): -380.08321231
8182 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11528532
8183 Electronic state : 2-A
8184 Cartesian coordinates (Angs):
8185 C -1.313651 0.291233 0.341855
8186 C -0.290224 1.192205 0.597926
8187 C 0.894511 1.228012 -0.296765
8188 C 1.630403 -0.125664 -0.144674
8189 O 0.687093 -1.170389 -0.292135
8190 O -0.130432 -1.179717 0.824619
8191 O -1.677701 -0.116515 -0.885788
8192 H -2.107594 0.163169 1.065677
8193 H -0.202646 1.551906 1.612946
8194 H 0.601424 1.347293 -1.342140
8195 H 1.571932 2.041338 -0.041842
8196 H 2.372267 -0.273285 -0.929519
8197 H 2.096557 -0.203814 0.837668
8198 H -0.889856 -0.408346 -1.366413
8199 Rotational constants (GHz): 3.8895600 2.8846500 2.2593700
8200 Vibrational harmonic frequencies (cm-1):
8201 i623.4638 177.6328 248.3701
8202 280.9721 391.9599 432.6138
8203 452.0873 500.3075 587.6845
8204 663.9523 737.8072 875.1450
8205 919.1406 932.5186 979.4588
8206 1017.9830 1061.3809 1077.5628
8207 1148.8220 1210.9937 1256.2309
8208 1268.3454 1318.6422 1340.3793
8209 1369.6287 1434.1885 1484.4078
8210 1497.9549 1538.4045 3065.6462
8211 3076.6998 3128.7866 3140.1905
8212 3209.6855 3225.6704 3759.1579
8213 Zero-point correction (Hartree): 0.111198
8214
8215 TS.HOCHCHCH2CH2OO.cycHOCHCHCH2CH2OO.Zt
8216 ~~~~~
8217 E(UM062X/Aug-CC-pVTZ) (Hartree): -382.11419635
8218 Electronic state : 2-A
8219 Cartesian coordinates (Angs):
8220 C -1.287511 0.259883 0.386557
8221 C -0.294591 1.181154 0.633815
8222 C 0.851787 1.247950 -0.305377
8223 C 1.636262 -0.084230 -0.149982
8224 O 0.753486 -1.169180 -0.328771
8225 O -0.090769 -1.241275 0.751995
8226 O -1.630822 -0.007392 -0.891770
8227 H -2.019276 0.015380 1.147963
8228 H -0.171789 1.509338 1.655646
8229 H 0.518979 1.326247 -1.338814
8230 H 1.519237 2.078630 -0.080707
8231 H 2.397095 -0.186422 -0.923444
8232 H 2.090673 -0.145555 0.840312
8233 H -2.025769 -0.883393 -0.942661
8234 Rotational constants (GHz): 3.8492700 2.8899600 2.2304200
8235 Vibrational harmonic frequencies (cm-1):
8236 i636.9546 172.7885 237.3710
8237 258.3095 345.3806 425.8914

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8238	446.6402	470.7412	581.9767
8239	665.6133	750.0642	868.5386
8240	930.9654	944.1562	984.0003
8241	1021.3281	1065.7209	1080.7316
8242	1155.5223	1207.5550	1260.3485
8243	1273.2681	1283.4913	1320.2074
8244	1368.5899	1434.2763	1481.3443
8245	1490.0791	1559.9629	3068.6534
8246	3091.3822	3132.4485	3147.5517
8247	3178.7540	3223.6184	3862.1701

8248 Zero-point correction (Hartree): 0.111151

8249
8250
8251 #####
8252 E-HOCH=C(CH3)CH2CH2OO ring closure and H-shift
8253 #####

8254
8255 HOHCCH3CH2CH2OO.Ecppc

8256 ~~~~~

8257 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45033361

8258 Electronic state : 2-A

8259 Cartesian coordinates (Angs):

8260	C	-1.103065	-0.871471	0.191141
8261	C	-0.923169	0.437989	0.049117
8262	C	0.395924	1.105234	0.334463
8263	C	1.491277	0.242106	0.917800
8264	O	1.954620	-0.751298	-0.027162
8265	O	2.592063	-0.202878	-1.014324
8266	O	-2.250252	-1.571520	-0.021246
8267	H	-0.307885	-1.538884	0.491128
8268	C	-1.996493	1.381879	-0.412544
8269	H	0.784451	1.565845	-0.579038
8270	H	0.231319	1.930178	1.035728
8271	H	2.356948	0.841506	1.192988
8272	H	1.153244	-0.338338	1.774789
8273	H	-2.959546	-0.976412	-0.277049
8274	H	-2.282302	2.070261	0.386228
8275	H	-2.903590	0.887905	-0.759677
8276	H	-1.630930	1.989086	-1.243099

8277 Rotational constants (GHz): 3.2229900 1.1959300 1.0071900

8278 Vibrational harmonic frequencies (cm-1):

8279	51.8982	69.8197	73.8428
8280	147.1759	217.6721	261.0593
8281	300.7799	325.5790	340.9710
8282	477.0424	492.8291	545.1056
8283	613.4975	792.7749	844.9085
8284	922.6439	972.1016	990.6421
8285	1022.9268	1055.5205	1118.1250
8286	1179.2911	1217.1855	1231.9348
8287	1277.5549	1296.8105	1317.5123
8288	1396.5873	1402.2311	1423.3292
8289	1438.1956	1472.3417	1478.9286
8290	1496.0521	1505.6938	1781.0266
8291	3038.5655	3048.2013	3068.5338
8292	3098.9307	3100.1948	3124.0822
8293	3154.6785	3232.9326	3881.6709

8294 Zero-point correction (Hartree): 0.139650

8295
8296 HOHCCH3CH2CH2OO.Ecppt

8297 ~~~~~

8298 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45049488

8299 Electronic state : 2-A

8300 Cartesian coordinates (Angs):

8301	C	-1.104756	-0.841832	0.194140
8302	C	-0.917761	0.462519	0.041328
8303	C	0.404086	1.129509	0.303331
8304	C	1.497118	0.278838	0.908852
8305	O	1.943860	-0.756505	0.000620
8306	O	2.585868	-0.256450	-1.009129
8307	O	-2.321172	-1.428384	-0.034035
8308	H	-0.313292	-1.514921	0.498488
8309	C	-2.014262	1.373580	-0.423936

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8310      H      0.789235      1.563549      -0.624469
8311      H      0.244566      1.974288      0.981369
8312      H      2.371537      0.878173      1.155111
8313      H      1.158947      -0.265689      1.789342
8314      H      -2.238138      -2.380469      0.030156
8315      H      -2.237775      2.126436      0.335668
8316      H      -2.924844      0.823720      -0.643640
8317      H      -1.705234      1.909941      -1.323966
8318      Rotational constants (GHz):      3.2608800      1.1933500      1.0065700
8319      Vibrational harmonic frequencies (cm-1):
8320          64.2134          69.7592          128.4212
8321          147.9245          202.7073          220.2890
8322          280.1259          304.5266          309.7661
8323          459.1385          476.7862          545.6244
8324          617.3729          804.5104          838.1869
8325          894.5427          972.8820          987.6513
8326          1020.9739          1061.4689          1119.3137
8327          1187.0261          1200.6626          1231.1333
8328          1279.8442          1304.1932          1315.6101
8329          1387.4788          1398.6469          1409.4114
8330          1438.5514          1469.9868          1491.9479
8331          1493.7130          1495.7324          1800.1772
8332          3041.0298          3049.1693          3070.3455
8333          3095.7183          3097.7090          3153.4042
8334          3168.7181          3202.3506          3921.7865
8335      Zero-point correction (Hartree): 0.139493
8336
8337      HOCHCCH3CH2CH2OO.Ecptc
8338      ~~~~~
8339      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44964409
8340      Electronic state : 2-A
8341      Cartesian coordinates (Angs):
8342      C      0.958460      0.920769      0.176224
8343      C      1.056457      -0.394701      0.011636
8344      C      -0.134754      -1.309029      0.129860
8345      C      -1.439234      -0.683554      0.559397
8346      O      -1.928124      0.141653      -0.523660
8347      O      -3.012965      0.767980      -0.188622
8348      O      1.964580      1.833701      0.114548
8349      H      0.017272      1.414141      0.372494
8350      C      2.341567      -1.103477      -0.306493
8351      H      -0.295534      -1.825626      -0.822258
8352      H      0.096126      -2.096372      0.854757
8353      H      -2.201540      -1.437712      0.748404
8354      H      -1.336795      -0.046262      1.437080
8355      H      2.803597      1.393954      -0.044874
8356      H      2.649076      -1.746589      0.521495
8357      H      3.173599      -0.436166      -0.529254
8358      H      2.211299      -1.746085      -1.179711
8359      Rotational constants (GHz):      3.3065000      1.1620200      0.9115700
8360      Vibrational harmonic frequencies (cm-1):
8361          39.4128          52.5256          72.1304
8362          128.7292          228.7058          257.5636
8363          290.8939          323.7623          338.1896
8364          394.0621          493.4623          563.6174
8365          607.2767          795.5039          831.6187
8366          933.5204          977.2514          1009.9132
8367          1030.1231          1074.5935          1109.3652
8368          1180.0895          1216.7749          1236.2106
8369          1283.9118          1295.7526          1302.1399
8370          1391.7808          1407.0620          1424.9217
8371          1441.9287          1471.4976          1479.7302
8372          1505.3723          1508.0329          1781.5179
8373          3035.6387          3047.6372          3061.6866
8374          3090.1179          3098.7149          3125.4747
8375          3142.3662          3234.4097          3881.7042
8376      Zero-point correction (Hartree): 0.139416
8377
8378      HOCHCCH3CH2CH2OO.Ecptt
8379      ~~~~~
8380      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45008565
8381      Electronic state : 2-A

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8382 Cartesian coordinates (Angs):
8383 C 0.949245 0.896312 0.173511
8384 C 1.049244 -0.416643 0.012924
8385 C -0.135912 -1.337351 0.118120
8386 C -1.445615 -0.719812 0.542801
8387 O -1.925296 0.123323 -0.531726
8388 O -2.955198 0.820810 -0.165589
8389 O 2.041054 1.717938 0.093176
8390 H 0.007111 1.392579 0.368978
8391 C 2.355536 -1.083852 -0.297378
8392 H -0.284575 -1.849886 -0.838045
8393 H 0.095114 -2.126970 0.840052
8394 H -2.210711 -1.475964 0.713060
8395 H -1.351997 -0.094804 1.430111
8396 H 1.762803 2.632521 0.154340
8397 H 2.621025 -1.794855 0.488654
8398 H 3.160225 -0.360887 -0.395257
8399 H 2.281535 -1.650231 -1.228646
8400 Rotational constants (GHz): 3.3040500 1.1760800 0.9184100
8401 Vibrational harmonic frequencies (cm-1):
8402 39.1216 64.6219 128.1937
8403 134.5810 219.8758 237.7368
8404 275.3857 299.8364 306.6485
8405 395.6929 461.5607 564.4930
8406 611.0092 806.0451 825.4997
8407 902.5628 978.5088 1008.2744
8408 1030.0588 1075.5645 1111.3507
8409 1188.2078 1201.5821 1235.4196
8410 1286.3389 1298.9974 1305.7658
8411 1387.2775 1395.9645 1413.2556
8412 1443.2880 1469.1613 1493.2110
8413 1494.0080 1506.8397 1800.8022
8414 3038.4796 3048.6987 3064.8658
8415 3089.6645 3094.9998 3142.0858
8416 3168.8376 3203.8529 3920.8200
8417 Zero-point correction (Hartree): 0.139353
8418
8419 HOCHCCH3CH2CH2OO.Ectpc
8420 ~~~~~
8421 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45041178
8422 Electronic state : 2-A
8423 Cartesian coordinates (Angs):
8424 C 1.572068 -0.848306 -0.035840
8425 C 1.048365 0.370431 0.058022
8426 C -0.430853 0.592940 0.216823
8427 C -1.275230 -0.662205 0.231476
8428 O -2.664912 -0.314663 0.411511
8429 O -3.163533 0.215424 -0.662995
8430 O 2.883973 -1.174345 -0.191749
8431 H 0.970192 -1.745366 0.005025
8432 C 1.858942 1.633757 0.008171
8433 H -0.617029 1.146169 1.142711
8434 H -0.792868 1.228042 -0.596810
8435 H -1.198296 -1.223420 -0.698772
8436 H -1.047709 -1.305710 1.079830
8437 H 3.418857 -0.378750 -0.252772
8438 H 2.936081 1.471320 -0.013281
8439 H 1.647700 2.253607 0.881680
8440 H 1.599093 2.223085 -0.873668
8441 Rotational constants (GHz): 4.4348700 0.9033900 0.7892900
8442 Vibrational harmonic frequencies (cm-1):
8443 53.6282 69.9208 88.4423
8444 135.7319 170.3219 257.5520
8445 290.1776 336.9574 353.7257
8446 404.0617 491.8700 547.3106
8447 647.4542 792.2281 844.8403
8448 918.2831 977.5671 1004.5079
8449 1035.6693 1091.3277 1117.8562
8450 1178.3510 1218.5345 1240.8101
8451 1279.3550 1293.0455 1329.7371
8452 1349.0943 1410.2839 1426.3496
8453 1442.5403 1479.1171 1490.3443

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8454      1503.1670          1506.4381          1778.2516
8455      3040.4836          3052.2854          3075.5687
8456      3093.2477          3105.0726          3127.5160
8457      3154.5866          3227.0072          3881.4336
8458 Zero-point correction (Hartree): 0.139679
8459
8460 HOCHCCH3CH2CH2OO.Ectpt
8461 ~~~~~
8462 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45000645
8463 Electronic state : 2-A
8464 Cartesian coordinates (Angs):
8465 C      1.577852      -0.819250      -0.040591
8466 C      1.039649      0.390526      0.048849
8467 C     -0.439288      0.606583      0.202344
8468 C     -1.275694     -0.652926      0.243520
8469 O     -2.668115     -0.314816      0.420538
8470 O     -3.177044      0.179949     -0.665932
8471 O      2.928480     -1.001619     -0.177833
8472 H      0.988561     -1.727576     -0.009288
8473 C      1.873460      1.636055      0.003073
8474 H     -0.626141      1.177823      1.116948
8475 H     -0.803352      1.224427     -0.623312
8476 H     -1.197913     -1.231149     -0.676395
8477 H     -1.040261     -1.278141      1.103607
8478 H      3.126312     -1.936141     -0.247113
8479 H      2.928756      1.407436     -0.114273
8480 H      1.742175      2.216290      0.919033
8481 H      1.559429      2.272992     -0.826568
8482 Rotational constants (GHz):  4.5430900    0.8957900    0.7869900
8483 Vibrational harmonic frequencies (cm-1):
8484      66.1054          81.8442          118.2333
8485     133.7300         168.4497         211.6414
8486     270.5425         300.3762         340.0182
8487     401.4638         463.2389         548.0668
8488     655.0680         787.2887         856.5622
8489     882.6100         976.6554        1004.0975
8490    1038.8936        1090.5760        1119.9076
8491    1183.3872        1200.1907        1240.4372
8492    1284.8237        1297.3005        1328.9850
8493    1344.8630        1391.9456        1417.1383
8494    1441.1149        1486.2883        1493.8206
8495    1495.3588        1502.2354        1796.0394
8496    3042.9124        3052.9699        3078.1945
8497    3090.6331        3100.8132        3151.6730
8498    3170.4785        3193.7375        3923.0461
8499 Zero-point correction (Hartree): 0.139478
8500
8501 HOCHCCH3CH2CH2OO.Ecttc
8502 ~~~~~
8503 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44977810
8504 Electronic state : 2-A
8505 Cartesian coordinates (Angs):
8506 C      1.488099      -0.916064      -0.005446
8507 C      1.157250      0.372000      -0.004153
8508 C     -0.277382      0.825472     -0.006417
8509 C     -1.301472     -0.284018      0.000130
8510 O     -2.599710      0.348790      0.000616
8511 O     -3.555657     -0.527145      0.004487
8512 O      2.740169     -1.447403      0.002084
8513 H      0.750225     -1.706120     -0.013362
8514 C      2.156681      1.492604      0.004339
8515 H     -0.453841      1.465276      0.863764
8516 H     -0.454740      1.456607     -0.882589
8517 H     -1.248142     -0.912948     -0.888009
8518 H     -1.243594     -0.906166      0.892763
8519 H      3.398381     -0.748000      0.022418
8520 H      3.194147      1.164942     -0.051675
8521 H      2.053967      2.092384      0.911142
8522 H      1.986132      2.160124     -0.842661
8523 Rotational constants (GHz):  4.5196000    0.8584100    0.7311900
8524 Vibrational harmonic frequencies (cm-1):
8525      39.9873          66.4798          104.0525

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8526      118.0175      126.4742      258.2234
8527      277.4712      336.0857      345.7019
8528      356.7540      491.5233      552.7374
8529      628.5252      781.4722      838.9029
8530      916.1860      1004.7024      1027.4762
8531      1032.3684      1102.6472      1113.7519
8532      1180.2951      1219.2221      1231.7335
8533      1285.5998      1297.2377      1310.4639
8534      1346.4920      1411.7788      1429.2141
8535      1447.0180      1479.5478      1495.7512
8536      1506.2214      1512.9631      1778.6707
8537      3041.0038      3052.2032      3069.5630
8538      3084.7357      3103.9782      3128.5020
8539      3142.6828      3227.4756      3881.6338
8540 Zero-point correction (Hartree): 0.139386
8541
8542 HOCHCCH3CH2CH2OO.Ecttt
8543 ~~~~~
8544 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44960190
8545 Electronic state : 2-A
8546 Cartesian coordinates (Angs):
8547 C      1.497402      -0.887783      0.000047
8548 C      1.149149      0.392873      -0.000195
8549 C      -0.286555      0.836909      -0.000243
8550 C      -1.302947      -0.279254      0.000509
8551 O      -2.608087      0.338922      0.000809
8552 O      -3.554154      -0.547667      -0.000566
8553 O      2.808980      -1.279956      0.000127
8554 H      0.772529      -1.692773      0.000239
8555 C      2.167038      1.493856      -0.000459
8556 H      -0.464979      1.472336      0.872425
8557 H      -0.465223      1.471424      -0.873521
8558 H      -1.242267      -0.904675      -0.889847
8559 H      -1.241502      -0.903978      0.891323
8560 H      2.863827      -2.236095      0.000007
8561 H      3.180058      1.102198      -0.000860
8562 H      2.039886      2.130695      0.877666
8563 H      2.039237      2.130865      -0.878364
8564 Rotational constants (GHz): 4.6297500      0.8525500      0.7297200
8565 Vibrational harmonic frequencies (cm-1):
8566      61.1190      98.7035      106.0269
8567      120.7515      124.9046      216.6812
8568      263.0903      301.9858      333.7557
8569      352.6867      461.9462      551.4865
8570      637.3932      777.7230      851.1881
8571      881.7542      1005.5986      1027.6191
8572      1032.6477      1105.6258      1112.9235
8573      1188.1821      1201.6842      1231.4127
8574      1295.4491      1297.7054      1308.7258
8575      1343.6335      1393.4035      1420.2363
8576      1446.5771      1489.3928      1494.3233
8577      1498.0086      1512.2925      1796.4653
8578      3043.6363      3052.7079      3072.4169
8579      3082.2130      3100.2050      3139.7630
8580      3170.4924      3194.7409      3923.5816
8581 Zero-point correction (Hartree): 0.139248
8582
8583 HOCHCCH3CH2CH2OO.Egmpc
8584 ~~~~~
8585 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45079312
8586 Electronic state : 2-A
8587 Cartesian coordinates (Angs):
8588 C      -1.828722      0.593462      -0.318153
8589 C      -0.749123      0.228923      0.366273
8590 C      0.356813      1.221157      0.592489
8591 C      1.588782      1.000573      -0.274274
8592 O      2.226603      -0.254941      0.045546
8593 O      1.867639      -1.208950      -0.758884
8594 O      -2.888998      -0.203964      -0.611804
8595 H      -1.967069      1.592998      -0.708991
8596 C      -0.625813      -1.165153      0.928019
8597 H      0.001192      2.230566      0.374814

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8598      H      0.665992      1.211051      1.640907
8599      H      1.340216      0.972306      -1.333044
8600      H      2.348091      1.756234      -0.075769
8601      H      -2.717138      -1.099473      -0.304838
8602      H      -0.474526      -1.911017      0.144251
8603      H      -1.516950      -1.442277      1.497998
8604      H      0.226614      -1.241311      1.599681
8605      Rotational constants (GHz):      3.5834100      1.2111900      1.0713800
8606      Vibrational harmonic frequencies (cm-1):
8607      39.9458      73.1485      128.2640
8608      167.4782      175.8704      263.8396
8609      308.0215      339.6564      396.1107
8610      471.1996      520.2774      540.9332
8611      609.5298      795.0616      861.5924
8612      923.9655      937.1037      1016.3156
8613      1031.4899      1050.5768      1093.6730
8614      1179.3530      1227.8926      1241.8213
8615      1251.0525      1320.3644      1328.3232
8616      1378.4174      1391.6522      1405.0569
8617      1421.3944      1470.4582      1481.4939
8618      1496.5170      1502.0666      1765.0900
8619      3040.3305      3053.9698      3088.4239
8620      3093.0150      3102.2243      3146.0031
8621      3158.5547      3212.6987      3861.4501
8622      Zero-point correction (Hartree): 0.139792
8623
8624      HOCHCCH3CH2CH2OO.Elmmc
8625      ~~~~~
8626      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45242156
8627      Electronic state : 2-A
8628      Cartesian coordinates (Angs):
8629      C      2.013050      -0.583300      0.048600
8630      C      0.822405      -0.037761      0.280218
8631      C      -0.330897      -0.920787      0.665404
8632      C      -1.401168      -1.046745      -0.407538
8633      O      -2.022990      0.228051      -0.691483
8634      O      -2.717012      0.653555      0.318701
8635      O      3.144830      0.064818      -0.333535
8636      H      2.192013      -1.644901      0.158839
8637      C      0.576416      1.443144      0.170143
8638      H      0.025312      -1.930256      0.878572
8639      H      -0.813437      -0.547858      1.572093
8640      H      -0.979016      -1.352464      -1.363281
8641      H      -2.195381      -1.728309      -0.105657
8642      H      2.954627      0.995628      -0.481461
8643      H      0.217636      1.728786      -0.820826
8644      H      1.471402      2.028463      0.390908
8645      H      -0.190622      1.752218      0.880397
8646      Rotational constants (GHz):      4.6129000      1.0605600      0.9487100
8647      Vibrational harmonic frequencies (cm-1):
8648      38.6505      77.3705      130.5209
8649      169.8811      176.6163      264.7294
8650      311.8036      328.6012      402.1490
8651      459.2398      517.9373      551.3201
8652      617.6214      797.0893      847.4594
8653      928.4938      943.3898      996.1643
8654      1036.3604      1052.8646      1106.3434
8655      1176.3255      1219.7146      1234.3742
8656      1269.0028      1305.5852      1318.0439
8657      1378.3035      1395.9793      1409.7986
8658      1426.5379      1469.6655      1485.0410
8659      1489.3419      1505.1048      1769.2464
8660      3047.6348      3061.1003      3088.9961
8661      3104.5789      3110.0293      3124.2378
8662      3153.5715      3211.4230      3868.8059
8663      Zero-point correction (Hartree): 0.139827
8664
8665      HOCHCCH3CH2CH2OO.Elmtt
8666      ~~~~~
8667      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45107126
8668      Electronic state : 2-A
8669      Cartesian coordinates (Angs):

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8670	C	-2.045545	-0.556310	-0.080610	
8671	C	-0.840502	-0.020493	-0.231501	
8672	C	0.320886	-0.905756	-0.581414	
8673	C	1.398805	-0.977272	0.489546	
8674	O	2.113025	0.274231	0.616461	
8675	O	2.827360	0.521781	-0.437538	
8676	O	-3.140708	0.192148	0.252576	
8677	H	-2.218904	-1.618909	-0.211558	
8678	C	-0.596830	1.451270	-0.071279	
8679	H	-0.024704	-1.925997	-0.758613	
8680	H	0.802291	-0.563348	-1.501394	
8681	H	0.977864	-1.144065	1.479792	
8682	H	2.140528	-1.740460	0.258152	
8683	H	-3.929223	-0.350927	0.223254	
8684	H	-0.062021	1.665449	0.855983	
8685	H	-1.533593	2.002421	-0.061156	
8686	H	0.029452	1.821923	-0.884911	
8687	Rotational constants (GHz):		4.9357000	1.0140300	0.9163200
8688	Vibrational harmonic frequencies (cm-1):				
8689		36.7960	71.9341		147.3537
8690		166.4145	200.7384		220.6476
8691		267.5188	297.9678		374.2763
8692		433.4844	506.7578		553.2612
8693		611.9254	806.4659		851.1981
8694		888.6263	946.0686		989.6621
8695		1041.5967	1058.7229		1110.1534
8696		1180.1000	1210.4322		1229.0814
8697		1272.1106	1305.5993		1308.5329
8698		1380.5998	1394.8994		1397.4725
8699		1430.8916	1468.7159		1487.8996
8700		1493.0969	1493.7255		1791.2177
8701		3056.7129	3057.7261		3087.8331
8702		3106.6378	3107.8842		3152.1624
8703		3161.8569	3175.6031		3920.5807
8704	Zero-point correction (Hartree):		0.139544		
8705	HOHCCH3CH2CH2OO.Elmtc				
8706	~~~~~				
8707	E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45103902				
8708	Electronic state : 2-A				
8709	Cartesian coordinates (Angs):				
8711	C	2.057130	-0.569428	-0.201725	
8712	C	0.932723	-0.082448	0.315439	
8713	C	-0.172671	-1.032065	0.687609	
8714	C	-1.412079	-0.918236	-0.180575	
8715	O	-2.063491	0.337284	0.123070	
8716	O	-3.099629	0.531724	-0.632015	
8717	O	3.138556	0.138524	-0.620488	
8718	H	2.215710	-1.631877	-0.333222	
8719	C	0.710421	1.388304	0.540609	
8720	H	0.181427	-2.060750	0.604398	
8721	H	-0.471987	-0.880858	1.728956	
8722	H	-1.171835	-0.910268	-1.243110	
8723	H	-2.133812	-1.706963	0.029789	
8724	H	2.960188	1.080858	-0.554230	
8725	H	0.152950	1.849424	-0.276981	
8726	H	1.646002	1.936518	0.665775	
8727	H	0.124727	1.546901	1.445953	
8728	Rotational constants (GHz):		4.5600900	0.9613500	0.8826200
8729	Vibrational harmonic frequencies (cm-1):				
8730		33.2861	60.1466		98.9528
8731		149.4043	179.0129		256.2755
8732		302.3820	334.3240		390.1704
8733		410.9641	501.4042		575.1685
8734		600.9007	797.4821		840.6084
8735		925.9919	961.2699		1025.1453
8736		1044.0113	1059.1274		1093.6388
8737		1180.0190	1218.9880		1237.1159
8738		1276.0249	1295.5166		1318.5902
8739		1380.5161	1398.0782		1412.0442
8740		1428.2151	1467.6952		1485.1955
8741		1498.0731	1503.1657		1769.5168

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8742          3049.7919          3050.6693          3082.3847
8743          3107.0257          3108.5436          3125.5393
8744          3142.4746          3209.4681          3871.6575
8745 Zero-point correction (Hartree): 0.139551
8746
8747 HOCHCCH3CH2CH2OO.Elmtt
8748 ~~~~~
8749 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44993064
8750 Electronic state : 2-A
8751 Cartesian coordinates (Angs):
8752   C      -2.102942      0.538206      -0.143436
8753   C      -0.937721      0.060986      0.276054
8754   C       0.166425      1.019365      0.624421
8755   C       1.406567      0.886346     -0.241243
8756   O       2.135432     -0.287980      0.187571
8757   O       3.181418     -0.493893     -0.550088
8758   O      -3.144905     -0.277302     -0.488645
8759   H      -2.283931      1.603643     -0.234672
8760   C      -0.681508     -1.410118      0.417318
8761   H      -0.189171      2.046483      0.528509
8762   H       0.472598      0.885162      1.666565
8763   H       1.166525      0.752649     -1.295559
8764   H       2.081468      1.733116     -0.121316
8765   H      -3.916446      0.249339     -0.700408
8766   H       0.027256     -1.761330     -0.335032
8767   H      -1.602277     -1.977775      0.312444
8768   H      -0.236502     -1.626603      1.390083
8769 Rotational constants (GHz):  4.9541800      0.9345000      0.8533500
8770 Vibrational harmonic frequencies (cm-1):
8771      38.2223          60.7487          118.7998
8772     167.5998         208.7623         239.9630
8773     253.9018         295.9806         369.6034
8774     380.9865         471.5233         579.6108
8775     597.9815         807.2849         841.7321
8776     891.1782         958.9019        1021.9535
8777    1049.8199        1064.5119        1098.2331
8778    1185.8944        1209.9780        1231.6886
8779    1279.2776        1296.1262        1305.4640
8780    1382.0083        1397.4037        1398.7941
8781    1432.0567        1465.6511        1490.4287
8782    1496.2937        1500.0287        1794.8727
8783    3047.2310        3058.8339        3081.9629
8784    3106.0061        3109.1757        3141.2796
8785    3163.4507        3177.9344        3921.3390
8786 Zero-point correction (Hartree): 0.139402
8787
8788 HOCHCCH3CH2CH2OO.Elpmc
8789 ~~~~~
8790 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.84408640
8791 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.77348661
8792 T1 diagnostic: 0.020724
8793 E(MP2/Aug-CC-pVTZ) (Hartree): -420.72102249
8794 E(MP3/Aug-CC-pVTZ) (Hartree): -420.76040125
8795 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72446597
8796 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76254263
8797 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18070042
8798 E(UHF/Aug-CC-pVTZ) (Hartree): -419.17544253
8799 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45265451
8800 Electronic state : 2-A
8801 Cartesian coordinates (Angs):
8802   C      -1.517607     -0.283437     -0.753321
8803   C      -0.688102      0.550324     -0.133217
8804   C       0.538745      1.038517     -0.843823
8805   C       1.838957      0.611526     -0.173038
8806   O       1.985009     -0.818500     -0.218460
8807   O       1.354129     -1.396059      0.761167
8808   O      -2.645530     -0.839962     -0.241593
8809   H      -1.353689     -0.601333     -1.774347
8810   C      -0.894450      1.005527      1.283658
8811   H       0.547096      0.688579     -1.876849
8812   H       0.549588      2.133239     -0.871075
8813   H       2.704278      0.996970     -0.709256

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8814      H      1.882456      0.910749      0.873250
8815      H      -2.716026     -0.636878     0.695306
8816      H      -0.360153      0.364472      1.988530
8817      H      -1.947769      1.023448      1.568417
8818      H      -0.519904      2.022190      1.415556
8819      Rotational constants (GHz):      3.0806800      1.3277200      1.2131600
8820      Vibrational harmonic frequencies (cm-1):
8821          63.9862          104.7020          108.6729
8822          122.1413          201.4260          273.4201
8823          300.7804          361.7789          395.4514
8824          458.0915          513.3197          555.9277
8825          598.5636          800.0066          863.5417
8826          918.9867          962.5085          1003.3209
8827          1035.1931          1053.7956          1078.6200
8828          1184.2846          1224.9307          1237.2872
8829          1246.1949          1314.7995          1323.2196
8830          1372.5476          1393.5532          1406.8474
8831          1425.4227          1469.2816          1484.0931
8832          1495.6961          1505.2614          1772.5644
8833          3040.6819          3046.7273          3093.4939
8834          3107.1019          3108.7996          3113.8965
8835          3154.7250          3216.3431          3873.0163
8836      Zero-point correction (Hartree): 0.139845
8837
8838      HOCHCCH3CH2CH2OO.Elpm
8839      ~~~~~
8840      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45177275
8841      Electronic state : 2-A
8842      Cartesian coordinates (Angs):
8843      C      -1.510210      -0.336826      -0.690902
8844      C      -0.683259      0.546226      -0.145920
8845      C      0.539959      0.977063      -0.898706
8846      C      1.847651      0.597746      -0.214740
8847      O      2.000095      -0.831905      -0.179810
8848      O      1.380285      -1.354796      0.837605
8849      O      -2.640887      -0.764850      -0.055396
8850      H      -1.323918      -0.761340      -1.671016
8851      C      -0.911633      1.122466      1.218494
8852      H      0.541037      0.556366      -1.905497
8853      H      0.548957      2.066978      -1.003651
8854      H      2.705532      0.954743      -0.781869
8855      H      1.899584      0.958318      0.811076
8856      H      -3.092511      -1.415167      -0.594411
8857      H      -0.205936      0.698501      1.936264
8858      H      -1.917224      0.908862      1.570994
8859      H      -0.766517      2.205095      1.209553
8860      Rotational constants (GHz):      3.1009500      1.3187700      1.1980700
8861      Vibrational harmonic frequencies (cm-1):
8862          57.1189          93.4475          104.6185
8863          131.9094          219.1160          232.0021
8864          276.1121          311.2246          387.5974
8865          438.8327          494.0006          557.1893
8866          600.1569          807.2122          858.7543
8867          894.0112          961.8466          999.8902
8868          1036.6439          1062.5751          1080.2574
8869          1193.8357          1210.0610          1235.1229
8870          1248.8211          1303.8493          1319.1174
8871          1375.2739          1390.0143          1398.2793
8872          1430.4524          1469.6591          1486.2454
8873          1489.9780          1504.9210          1796.2725
8874          3041.9251          3050.8094          3095.6879
8875          3102.2293          3104.9275          3157.8622
8876          3162.0273          3180.0152          3922.6773
8877      Zero-point correction (Hartree): 0.139594
8878
8879      HOCHCCH3CH2CH2OO.Elppc
8880      ~~~~~
8881      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45195093
8882      Electronic state : 2-A
8883      Cartesian coordinates (Angs):
8884      C      1.459781      -0.776614      0.420568
8885      C      0.809440      0.376741      0.306445

```

8886	C	-0.482178	0.573410	1.045944	
8887	C	-1.666117	0.819506	0.124995	
8888	O	-1.850534	-0.277332	-0.795413	
8889	O	-2.187652	-1.364440	-0.172854	
8890	O	2.617064	-1.127776	-0.198308	
8891	H	1.098108	-1.575173	1.054509	
8892	C	1.280687	1.502085	-0.571500	
8893	H	-0.703645	-0.293698	1.667310	
8894	H	-0.414759	1.443134	1.707674	
8895	H	-2.593160	0.935477	0.684486	
8896	H	-1.513927	1.681988	-0.522449	
8897	H	2.881434	-0.442781	-0.818407	
8898	H	0.815043	1.470810	-1.560068	
8899	H	2.362349	1.500720	-0.714819	
8900	H	1.027859	2.465136	-0.124337	
8901	Rotational constants (GHz):		3.1403500	1.2648500	1.0636500
8902	Vibrational harmonic frequencies (cm-1):				
8903		36.8765	52.5879		118.8400
8904		127.2007	205.7481		263.7766
8905		302.9698	348.2542		391.2698
8906		454.1732	509.8571		554.3828
8907		615.8995	799.6879		843.0226
8908		929.9481	956.6517		993.0827
8909		1035.7560	1052.2483		1089.8522
8910		1182.5724	1223.8758		1230.1082
8911		1265.2094	1299.6920		1317.9795
8912		1377.4525	1396.8678		1410.5049
8913		1426.5641	1472.3962		1486.1949
8914		1496.9209	1505.0832		1778.0527
8915		3041.6380	3043.2119		3093.3491
8916		3098.9139	3114.6308		3121.5831
8917		3151.6504	3215.2843		3874.0553
8918	Zero-point correction (Hartree): 0.139665				
8919					
8920	HOCHCCH3CH2CH2OO.Elppt				
8921	~~~~~				
8922	E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.84385432				
8923	E(CCSD/Aug-CC-pVTZ) (Hartree): -420.77372382				
8924	T1 diagnostic: 0.020573				
8925	E(MP2/Aug-CC-pVTZ) (Hartree): -420.72095663				
8926	E(MP3/Aug-CC-pVTZ) (Hartree): -420.76066693				
8927	E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72411407				
8928	E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76253098				
8929	E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18205719				
8930	E(UHF/Aug-CC-pVTZ) (Hartree): -419.17690718				
8931	E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45188619				
8932	Electronic state : 2-A				
8933	Cartesian coordinates (Angs):				
8934	C	1.428909	-0.761649	0.387917	
8935	C	0.808286	0.406145	0.287379	
8936	C	-0.489208	0.617197	1.011743	
8937	C	-1.672006	0.827860	0.080720	
8938	O	-1.862434	-0.311367	-0.786966	
8939	O	-2.193385	-1.369017	-0.113317	
8940	O	2.607110	-1.019542	-0.254484	
8941	H	1.022622	-1.570406	0.984909	
8942	C	1.341535	1.528230	-0.552156	
8943	H	-0.712932	-0.230656	1.658873	
8944	H	-0.426996	1.506181	1.647335	
8945	H	-2.598217	0.971458	0.635324	
8946	H	-1.517559	1.658184	-0.605961	
8947	H	2.895243	-1.912333	-0.060989	
8948	H	0.735260	1.673752	-1.449666	
8949	H	2.361263	1.329288	-0.871014	
8950	H	1.325889	2.467235	0.005707	
8951	Rotational constants (GHz):		3.1486200	1.2674200	1.0540300
8952	Vibrational harmonic frequencies (cm-1):				
8953		26.7941	45.7261		108.2875
8954		130.5170	215.3615		233.3374
8955		275.5859	299.0623		385.1109
8956		433.3619	493.0776		557.0090
8957		615.4538	807.4477		840.0362

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8958          902.1129          957.7869          984.3953
8959          1035.1859         1063.0966         1089.2179
8960          1192.4548         1208.3106         1233.7179
8961          1266.7916         1301.9615         1305.5584
8962          1381.0377         1389.3788         1401.8280
8963          1430.7164         1471.4674         1487.7331
8964          1490.5883         1502.7339         1800.3064
8965          3046.1368         3048.2779         3093.5697
8966          3097.0945         3117.7039         3155.1559
8967          3161.9043         3180.8921         3921.9245
8968 Zero-point correction (Hartree): 0.139390
8969
8970 HOCHCCH3CH2CH2OO.Elptc
8971 ~~~~~
8972 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45093535
8973 Electronic state : 2-A
8974 Cartesian coordinates (Angs):
8975 C      -1.721411      -0.587870      -0.547802
8976 C      -0.916644      0.407847      -0.192202
8977 C       0.248419      0.773116      -1.068863
8978 C       1.585035      0.661313      -0.362510
8979 O       1.784646      -0.724568      -0.010541
8980 O       2.857524      -0.884493      0.700195
8981 O      -2.797669      -1.055815      0.136247
8982 H      -1.576378      -1.138501      -1.467638
8983 C      -1.090617      1.192064      1.078120
8984 H       0.263101      0.147565      -1.962174
8985 H       0.157778      1.811407      -1.403676
8986 H       2.415615      0.956359      -1.002489
8987 H       1.620835      1.237491      0.561719
8988 H      -2.868588      -0.611774      0.985637
8989 H      -0.462934      0.806120      1.885350
8990 H      -2.122091      1.195651      1.433353
8991 H      -0.812046      2.235865      0.922256
8992 Rotational constants (GHz): 3.4451300 1.0522800 0.9883000
8993 Vibrational harmonic frequencies (cm-1):
8994 41.6818 55.6782 95.2414
8995 122.1272 225.6290 255.4193
8996 298.1443 341.1793 386.6297
8997 405.9443 500.7129 568.1586
8998 599.1119 800.1281 838.2699
8999 929.8089 959.6360 1024.2254
9000 1049.3828 1067.1277 1077.5407
9001 1181.2537 1223.4907 1231.4619
9002 1276.1074 1297.0730 1318.4225
9003 1380.2345 1394.1162 1412.8135
9004 1428.6500 1470.7367 1488.4428
9005 1503.7162 1508.9518 1777.2567
9006 3043.4882 3044.8136 3085.8243
9007 3100.1926 3108.8349 3116.2341
9008 3140.7489 3215.3730 3874.7341
9009 Zero-point correction (Hartree): 0.139571
9010
9011 HOCHCCH3CH2CH2OO.Elptt
9012 ~~~~~
9013 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45062207
9014 Electronic state : 2-A
9015 Cartesian coordinates (Angs):
9016 C       1.687998      -0.618795      0.492881
9017 C       0.915542      0.416456      0.192925
9018 C      -0.259700      0.749108      1.067999
9019 C      -1.591353      0.659142      0.349459
9020 O      -1.802077      -0.723348      -0.011109
9021 O      -2.887151      -0.874508      -0.704725
9022 O       2.769767      -0.965716      -0.266504
9023 H       1.492458      -1.242616      1.357736
9024 C       1.163201      1.278087      -1.009050
9025 H      -0.285528      0.095656      1.941473
9026 H      -0.170140      1.775429      1.437329
9027 H      -2.423692      0.956840      0.985921
9028 H      -1.613993      1.241844      -0.570464
9029 H       3.198522      -1.736052      0.107991

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9030      H      2.139415      1.075352      -1.441349
9031      H      1.111298      2.335820      -0.741319
9032      H      0.413215      1.102318      -1.783897
9033      Rotational constants (GHz):      3.4577100      1.0502500      0.9739700
9034      Vibrational harmonic frequencies (cm-1):
9035      27.8590      56.3095      95.1152
9036      130.4504      229.9982      233.0775
9037      279.8611      281.8680      379.0604
9038      390.0224      473.3075      569.5506
9039      599.1604      808.7278      835.2397
9040      901.7905      959.8911      1022.4905
9041      1052.1236      1073.0370      1076.6099
9042      1189.3981      1207.2794      1234.9150
9043      1275.3578      1297.3689      1306.2990
9044      1383.6717      1387.5146      1402.9185
9045      1432.2372      1469.4858      1490.7696
9046      1493.0623      1509.5911      1800.9719
9047      3046.6909      3049.0555      3088.0839
9048      3097.1853      3103.7458      3144.0555
9049      3161.8549      3181.6663      3920.9978
9050      Zero-point correction (Hartree): 0.139309
9051
9052      HOCHCCH3CH2CH2OO.Eltmc
9053      ~~~~~
9054      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45164869
9055      Electronic state : 2-A
9056      Cartesian coordinates (Angs):
9057      C      1.811935      -0.907621      0.071422
9058      C      1.027333      0.151265      0.247118
9059      C      -0.414545      -0.040563      0.622740
9060      C      -1.339242      0.420047      -0.492300
9061      O      -2.719465      0.331750      -0.081247
9062      O      -3.113306      -0.903396      -0.014655
9063      O      3.119974      -0.898855      -0.294994
9064      H      1.454965      -1.917711      0.221781
9065      C      1.516665      1.562881      0.063181
9066      H      -0.625008      -1.089135      0.831386
9067      H      -0.651596      0.533489      1.523087
9068      H      -1.198815      1.472892      -0.733562
9069      H      -1.219188      -0.188641      -1.387452
9070      H      3.407718      0.001017      -0.472667
9071      H      1.385050      1.918785      -0.961790
9072      H      2.571892      1.675366      0.319359
9073      H      0.964490      2.241889      0.714062
9074      Rotational constants (GHz):      4.7964600      0.8767900      0.7807500
9075      Vibrational harmonic frequencies (cm-1):
9076      53.7285      71.7147      89.4977
9077      116.3588      155.1504      271.1468
9078      307.8924      327.9762      383.8881
9079      406.1160      510.9140      539.2368
9080      656.5248      795.4961      837.0464
9081      933.8506      968.3074      1016.5065
9082      1043.4275      1069.7756      1081.4272
9083      1183.6477      1220.7490      1236.2731
9084      1280.1390      1307.8771      1322.0944
9085      1335.7953      1400.0742      1409.7012
9086      1425.2233      1482.0790      1491.9171
9087      1499.1111      1505.3858      1772.0821
9088      3043.5621      3050.7344      3091.7159
9089      3098.1917      3117.5938      3121.3765
9090      3154.5905      3218.4321      3871.8645
9091      Zero-point correction (Hartree): 0.139597
9092
9093      HOCHCCH3CH2CH2OO.Eltmt
9094      ~~~~~
9095      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45146190
9096      Electronic state : 2-A
9097      Cartesian coordinates (Angs):
9098      C      1.808449      -0.870946      0.073997
9099      C      1.022126      0.185896      0.234148
9100      C      -0.415721      -0.007658      0.623098
9101      C      -1.359154      0.443369      -0.480086

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9102      O      -2.733501      0.297045      -0.063681
9103      O      -3.085753      -0.951642      -0.027514
9104      O      3.119356      -0.754994      -0.294526
9105      H      1.443150      -1.880050      0.228246
9106      C      1.518328      1.587994      0.035525
9107      H      -0.622997      -1.056074      0.837927
9108      H      -0.642754      0.569183      1.524220
9109      H      -1.258428      1.504409      -0.700972
9110      H      -1.223508      -0.143918      -1.387232
9111      H      3.537838      -1.616751      -0.290378
9112      H      1.112418      2.031524      -0.876723
9113      H      2.602370      1.614041      -0.037457
9114      H      1.206935      2.222439      0.868047
9115      Rotational constants (GHz):      4.7876600      0.8777500      0.7801800
9116      Vibrational harmonic frequencies (cm-1):
9117      56.3337      61.5398      111.1569
9118      118.4974      170.4625      240.0409
9119      267.4307      321.2406      359.2031
9120      385.4776      485.3416      538.0905
9121      660.2330      793.0924      844.5286
9122      900.1542      966.8000      1014.9355
9123      1050.6590      1070.5620      1086.7521
9124      1194.8091      1209.8170      1236.0224
9125      1283.4324      1293.5699      1325.9942
9126      1339.2963      1393.4718      1406.7887
9127      1430.5021      1480.0410      1492.3605
9128      1497.0516      1499.6333      1795.6914
9129      3049.6415      3051.3162      3094.9246
9130      3099.0336      3116.9742      3159.8308
9131      3162.0614      3183.4444      3918.9380
9132      Zero-point correction (Hartree): 0.139463
9133
9134      HOCHCCH3CH2CH2OO.Eltpc
9135      ~~~~~
9136      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45201182
9137      Electronic state : 2-A
9138      Cartesian coordinates (Angs):
9139      C      -2.007490      -0.766543      -0.158771
9140      C      -1.003670      0.103506      -0.211088
9141      C      0.386922      -0.368660      -0.524399
9142      C      1.307083      -0.192810      0.672840
9143      O      2.663592      -0.544892      0.329885
9144      O      3.209099      0.359872      -0.424121
9145      O      -3.304263      -0.488022      0.135709
9146      H      -1.870260      -1.819530      -0.365650
9147      C      -1.199234      1.573372      0.052831
9148      H      0.380775      -1.418458      -0.818898
9149      H      0.807641      0.209533      -1.351093
9150      H      1.321144      0.836694      1.029090
9151      H      1.041753      -0.866617      1.485571
9152      H      -3.399346      0.442897      0.356862
9153      H      -1.153800      1.815574      1.117656
9154      H      -2.155303      1.937117      -0.329843
9155      H      -0.421692      2.153930      -0.443958
9156      Rotational constants (GHz):      5.5881300      0.8426200      0.7822800
9157      Vibrational harmonic frequencies (cm-1):
9158      53.0781      68.9128      92.6832
9159      134.5309      153.8551      269.6361
9160      308.6222      336.0594      387.3273
9161      408.3134      514.1855      543.1282
9162      658.1054      792.9716      836.2138
9163      926.7746      973.8020      1018.9343
9164      1043.2789      1062.5763      1082.5295
9165      1183.7005      1225.6114      1233.7287
9166      1283.3615      1305.6221      1327.7582
9167      1335.9956      1398.4848      1407.9966
9168      1424.1372      1481.3396      1492.3829
9169      1498.2498      1507.0122      1770.7074
9170      3041.9336      3058.3081      3092.2916
9171      3095.3268      3114.2838      3122.0515
9172      3156.0048      3216.5067      3868.2763
9173      Zero-point correction (Hartree): 0.139667

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9174
9175 HOCHCCH3CH2CH2OO.Eltp
9176 ~~~~~
9177 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45145415
9178 Electronic state : 2-A
9179 Cartesian coordinates (Angs):
9180 C -2.001604 -0.742327 -0.143488
9181 C -1.003878 0.131352 -0.193096
9182 C 0.388943 -0.341258 -0.495733
9183 C 1.325429 -0.112698 0.679639
9184 O 2.660431 -0.553504 0.354349
9185 O 3.240376 0.263637 -0.470784
9186 O -3.284177 -0.367272 0.143806
9187 H -1.843266 -1.799209 -0.327038
9188 C -1.215763 1.598121 0.043935
9189 H 0.390938 -1.403170 -0.745496
9190 H 0.796207 0.204117 -1.351080
9191 H 1.390356 0.938782 0.954426
9192 H 1.039528 -0.710211 1.543648
9193 H -3.874869 -1.114517 0.041352
9194 H -0.835668 1.906024 1.020700
9195 H -2.271803 1.852258 0.004772
9196 H -0.683224 2.183896 -0.707787
9197 Rotational constants (GHz): 5.6476000 0.8348200 0.7774800
9198 Vibrational harmonic frequencies (cm-1):
9199 49.7688 62.1260 111.8830
9200 127.3880 172.9634 210.4648
9201 261.2065 320.6001 362.4027
9202 382.3184 485.9407 542.2492
9203 657.6454 793.1815 842.6844
9204 892.9237 971.7160 1015.6927
9205 1050.5671 1064.3973 1088.9214
9206 1195.4017 1206.0764 1235.3924
9207 1278.4451 1296.7273 1326.6436
9208 1338.9397 1392.0899 1404.1120
9209 1429.8617 1479.4113 1492.5962
9210 1497.1967 1499.5171 1794.2645
9211 3052.0717 3056.5095 3095.4248
9212 3101.9954 3108.8201 3158.4228
9213 3161.4501 3179.2350 3920.3404
9214 Zero-point correction (Hartree): 0.139351
9215
9216 HOCHCCH3CH2CH2OO.Elttc
9217 ~~~~~
9218 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45091885
9219 Electronic state : 2-A
9220 Cartesian coordinates (Angs):
9221 C 2.019457 -0.817672 0.008327
9222 C 1.098313 0.106194 0.263784
9223 C -0.265828 -0.308594 0.739631
9224 C -1.331637 0.046086 -0.278635
9225 O -2.612365 -0.306310 0.287546
9226 O -3.586183 -0.017001 -0.518699
9227 O 3.280374 -0.604705 -0.449534
9228 H 1.832634 -1.872400 0.160319
9229 C 1.352064 1.578443 0.081059
9230 H -0.294439 -1.382104 0.927499
9231 H -0.506575 0.195948 1.679682
9232 H -1.359513 1.112952 -0.500090
9233 H -1.213321 -0.513727 -1.205893
9234 H 3.413792 0.330153 -0.629580
9235 H 1.084613 1.925417 -0.920047
9236 H 2.395599 1.846085 0.257166
9237 H 0.758393 2.155065 0.791451
9238 Rotational constants (GHz): 5.6123100 0.7832700 0.7367300
9239 Vibrational harmonic frequencies (cm-1):
9240 53.8263 72.5390 95.9165
9241 114.0774 128.2612 270.0024
9242 279.2909 331.3963 381.0101
9243 385.4593 495.6250 548.1192
9244 637.7717 787.1260 832.2222
9245 931.2207 1006.1629 1023.5025

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9246      1047.5933      1065.7010      1104.9684
9247      1179.5446      1217.2770      1228.0802
9248      1292.8911      1306.1027      1310.3396
9249      1333.4085      1402.8581      1413.8348
9250      1426.4010      1485.5788      1492.6064
9251      1504.5213      1508.5126      1772.3846
9252      3044.6967      3051.5936      3084.0365
9253      3099.7247      3110.5957      3118.4691
9254      3143.5100      3214.7052      3871.4970
9255      Zero-point correction (Hartree): 0.139435
9256
9257      HOCHCCH3CH2CH2OO.El1ttt
9258      ~~~~~
9259      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45055503
9260      Electronic state : 2-A
9261      Cartesian coordinates (Angs):
9262      C      2.019747      -0.786239      0.012765
9263      C      1.092870      0.133198      0.249446
9264      C      -0.268522      -0.285052      0.729399
9265      C      -1.347484      0.078620      -0.271565
9266      O      -2.613552      -0.338726      0.285451
9267      O      -3.600278      -0.055760      -0.507019
9268      O      3.268503      -0.461379      -0.437772
9269      H      1.826796      -1.842387      0.164177
9270      C      1.353458      1.598099      0.055223
9271      H      -0.298640      -1.360915      0.906120
9272      H      -0.498650      0.209545      1.677373
9273      H      -1.411543      1.151424      -0.448613
9274      H      -1.217059      -0.439965      -1.220983
9275      H      3.818674      -1.244931      -0.472194
9276      H      0.843713      1.981548      -0.831597
9277      H      2.415948      1.794482      -0.062124
9278      H      0.982964      2.166359      0.910953
9279      Rotational constants (GHz):      5.7031700      0.7796800      0.7330400
9280      Vibrational harmonic frequencies (cm-1):
9281      49.4497      85.7927      94.1556
9282      109.3073      155.9037      223.1140
9283      264.6973      296.5680      353.0401
9284      371.2835      465.2999      545.6444
9285      640.9286      785.9895      840.5879
9286      895.2056      1002.6418      1021.9917
9287      1055.0963      1069.6735      1106.7878
9288      1189.2775      1208.1309      1226.7501
9289      1292.2113      1296.0405      1310.2441
9290      1338.0122      1392.7459      1413.1792
9291      1430.7267      1482.9877      1493.2188
9292      1498.6237      1508.4037      1795.6003
9293      3050.3658      3052.0386      3087.7339
9294      3100.1541      3106.2284      3147.3929
9295      3162.0558      3180.1953      3919.4495
9296      Zero-point correction (Hartree): 0.139230
9297
9298
9299      TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Ec
9300      ~~~~~
9301      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82495066
9302      E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74993036
9303      T1 diagnostic: 0.027178
9304      E(MP2/Aug-CC-pVTZ) (Hartree): -420.69194733
9305      E(MP3/Aug-CC-pVTZ) (Hartree): -420.73018644
9306      E(PMP2/Aug-CC-pVTZ) (Hartree): -420.70966304
9307      E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74344876
9308      E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15893222
9309      E(UHF/Aug-CC-pVTZ) (Hartree): -419.13843132
9310      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.43069294
9311      Electronic state : 2-A
9312      Cartesian coordinates (Angs):
9313      C      0.897061      -0.546190      0.623516
9314      C      0.499806      0.751999      0.364265
9315      C      -0.899828      1.100331      0.734933
9316      C      -1.862983      0.349260      -0.214481
9317      O      -1.608941      -1.029261      -0.103469

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9318 O -0.379546 -1.295814 -0.660220
9319 O 2.063821 -1.066021 0.210856
9320 H 0.465226 -1.110783 1.437486
9321 C 1.222207 1.567402 -0.659583
9322 H -1.133763 0.784748 1.752116
9323 H -1.076472 2.173656 0.656888
9324 H -2.901957 0.490788 0.082090
9325 H -1.719342 0.671026 -1.248151
9326 H 2.398259 -0.574510 -0.546052
9327 H 1.015811 1.199817 -1.672535
9328 H 2.304179 1.548632 -0.511108
9329 H 0.907815 2.608579 -0.619976
9330 Rotational constants (GHz): 2.9232700 1.9578100 1.4160100
9331 Vibrational harmonic frequencies (cm-1):
9332 i584.5270 104.0146 131.1446
9333 152.9753 280.3153 301.1201
9334 328.3390 384.9481 405.1223
9335 438.5013 509.0466 585.3565
9336 622.4213 804.3175 876.8799
9337 933.8620 966.4459 987.6532
9338 1013.3413 1029.7845 1074.4238
9339 1089.5739 1180.5453 1223.0220
9340 1246.1206 1264.0096 1324.3687
9341 1343.1694 1375.3321 1386.2243
9342 1413.1340 1480.3285 1482.9774
9343 1490.9019 1502.0566 1565.9389
9344 3013.5153 3063.7344 3073.1651
9345 3083.0540 3122.8568 3133.5583
9346 3139.1511 3225.4811 3857.2312
9347 Zero-point correction (Hartree): 0.138990
9348
9349 TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Et
9350 ~~~~~
9351 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82644110
9352 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.75168260
9353 T1 diagnostic: 0.027377
9354 E(MP2/Aug-CC-pVTZ) (Hartree): -420.69320422
9355 E(MP3/Aug-CC-pVTZ) (Hartree): -420.73169845
9356 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.71075959
9357 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74484390
9358 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.16124987
9359 E(UHF/Aug-CC-pVTZ) (Hartree): -419.14094997
9360 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.43224778
9361 Electronic state : 2-A
9362 Cartesian coordinates (Angs):
9363 C 0.901440 -0.521479 0.586849
9364 C 0.502829 0.769096 0.333071
9365 C -0.894366 1.109763 0.725147
9366 C -1.864531 0.326386 -0.190794
9367 O -1.591884 -1.049777 -0.073455
9368 O -0.384427 -1.307941 -0.683039
9369 O 2.095071 -0.960328 0.136906
9370 H 0.439773 -1.087856 1.386068
9371 C 1.212414 1.628625 -0.655606
9372 H -1.109120 0.822969 1.754911
9373 H -1.083272 2.178781 0.618222
9374 H -2.898699 0.457600 0.126698
9375 H -1.748306 0.635648 -1.231358
9376 H 2.156168 -1.910354 0.265310
9377 H 1.301757 2.650040 -0.281367
9378 H 0.641760 1.676875 -1.589447
9379 H 2.203139 1.246316 -0.884335
9380 Rotational constants (GHz): 2.8787500 1.9716900 1.3999900
9381 Vibrational harmonic frequencies (cm-1):
9382 i553.2027 109.9272 129.4570
9383 161.2925 272.9190 293.9918
9384 335.0045 356.8991 383.6058
9385 430.7677 499.5686 584.3038
9386 625.0749 816.1024 874.9959
9387 937.0347 964.9763 987.8429
9388 1010.4461 1035.3106 1075.9675
9389 1087.1538 1189.3977 1224.8218

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9390      1245.0144      1264.3001      1303.5546
9391      1334.5962      1374.3540      1390.3968
9392      1422.9022      1477.8849      1482.0055
9393      1488.2023      1492.0330      1602.7358
9394      3031.4077      3066.6412      3072.5900
9395      3092.3654      3121.7575      3134.3623
9396      3168.0763      3189.7552      3887.1174
9397 Zero-point correction (Hartree): 0.139034
9398
9399
9400 TS.HOHCCH3CH2CH2O.1-6Hshift.a.Ec
9401 ~~~~~
9402 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.80543099
9403 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.73000039
9404 T1 diagnostic: 0.024966
9405 E(MP2/Aug-CC-pVTZ) (Hartree): -420.67733307
9406 E(MP3/Aug-CC-pVTZ) (Hartree): -420.71333383
9407 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.69231131
9408 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.72403263
9409 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.12957042
9410 E(UHF/Aug-CC-pVTZ) (Hartree): -419.11164555
9411 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41459562
9412 Electronic state : 2-A
9413 Cartesian coordinates (Angs):
9414 O      1.611663      -1.284114      -0.619711
9415 H      0.570609      -1.436504      0.047100
9416 C     -0.397947      -1.100677      0.836472
9417 O      2.231586      -0.228477      0.005948
9418 C     -0.728993      0.240864      0.373594
9419 C      1.585033      0.992460      -0.352959
9420 C      0.358900      1.279457      0.506288
9421 H      0.156254      -1.138816      1.772511
9422 H     -1.154259      -1.878237      0.771877
9423 C     -1.881294      0.561876      -0.234616
9424 O     -2.930091      -0.252592      -0.482316
9425 H     -2.076507      1.567403      -0.583044
9426 H      2.343442      1.759914      -0.195592
9427 H      1.326531      0.944954      -1.412172
9428 H     -0.024832      2.261609      0.223290
9429 H      0.680104      1.342327      1.549750
9430 H     -2.740806      -1.145064      -0.177763
9431 Rotational constants (GHz):      3.7713900      1.2756300      1.0917400
9432 Vibrational harmonic frequencies (cm-1):
9433 i2187.2165      79.1229      145.5697
9434      202.8478      290.9588      295.2709
9435      344.0117      403.4398      455.9409
9436      495.2855      550.5102      563.2053
9437      629.2395      656.4428      815.4285
9438      873.4114      917.9509      956.2470
9439      990.7497      1016.8466      1060.0645
9440      1081.7357      1118.5491      1190.0307
9441      1204.8801      1238.1535      1253.3422
9442      1299.2440      1329.1686      1375.6154
9443      1396.7598      1416.0353      1465.7503
9444      1478.7994      1485.3532      1530.7273
9445      1702.6711      3050.4029      3069.6122
9446      3098.1448      3102.9731      3128.3971
9447      3176.8308      3215.6662      3865.5866
9448 Zero-point correction (Hartree): 0.134451
9449
9450 TS.HOHCCH3CH2CH2O.1-6Hshift.a.Et
9451 ~~~~~
9452 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41378992
9453 Electronic state : 2-A
9454 Cartesian coordinates (Angs):
9455 O      1.601501      -1.290271      -0.618535
9456 H      0.561291      -1.438259      0.056889
9457 C     -0.401768      -1.097574      0.847814
9458 O      2.232270      -0.235626      0.001025
9459 C     -0.713173      0.247279      0.381248
9460 C      1.594707      0.986734      -0.362118
9461 C      0.371862      1.287446      0.498634

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9462      H      0.154954      -1.145404      1.781839
9463      H      -1.189898      -1.835589      0.756039
9464      C      -1.868947      0.544929      -0.223165
9465      O      -2.847699      -0.382535      -0.401426
9466      H      -2.078130      1.543523      -0.589924
9467      H      2.358378      1.750500      -0.211240
9468      H      1.332110      0.935967      -1.420313
9469      H      -0.010168      2.268012      0.206377
9470      H      0.697337      1.359552      1.540003
9471      H      -3.610527      0.016269      -0.822647
9472      Rotational constants (GHz):      3.7784100      1.2856200      1.0982000
9473      Vibrational harmonic frequencies (cm-1):
9474      i2126.1464      82.8438      145.7752
9475      213.6238      269.8116      277.2568
9476      325.9406      373.3494      448.8572
9477      472.1455      554.2206      568.7976
9478      633.4221      661.9724      823.5970
9479      875.3510      878.8346      957.0137
9480      1001.7419      1015.9198      1062.1319
9481      1082.5804      1119.0508      1198.9166
9482      1199.9316      1231.2216      1252.2669
9483      1295.3559      1318.6255      1377.5621
9484      1397.1068      1404.6352      1462.3339
9485      1478.6047      1479.7281      1516.7170
9486      1730.1079      3050.1858      3067.5503
9487      3099.5063      3107.3536      3126.1656
9488      3182.5087      3211.7110      3914.6619
9489      Zero-point correction (Hartree): 0.134291
9490
9491      TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Ec
9492      ~~~~~
9493      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41342897
9494      Electronic state : 2-A
9495      Cartesian coordinates (Angs):
9496      O      -1.809153      1.189157      -0.280637
9497      H      -0.693200      1.491482      0.191782
9498      C      0.459690      1.311138      0.776573
9499      O      -1.506597      0.067604      -1.009623
9500      C      0.653638      -0.107794      0.532762
9501      C      -1.543084      -1.075315      -0.157669
9502      C      -0.494299      -0.994585      0.960701
9503      H      0.164990      1.569807      1.791662
9504      H      1.170044      2.019741      0.358664
9505      C      1.682250      -0.631587      -0.156204
9506      O      2.736439      0.031551      -0.672135
9507      H      1.754807      -1.694854      -0.345186
9508      H      -2.553466      -1.197939      0.236613
9509      H      -1.317258      -1.896094      -0.838222
9510      H      -0.152773      -2.001917      1.198934
9511      H      -0.942200      -0.582073      1.864560
9512      H      2.654362      0.974213      -0.496627
9513      Rotational constants (GHz):      3.3187200      1.4055600      1.2662400
9514      Vibrational harmonic frequencies (cm-1):
9515      i2094.4757      79.0026      123.8287
9516      232.6307      277.1059      301.8495
9517      371.7860      378.3727      434.8235
9518      486.2273      537.4493      568.2219
9519      625.1325      708.2326      807.3081
9520      858.3569      921.8416      954.5784
9521      1018.9063      1030.5444      1058.5716
9522      1082.5619      1126.5080      1200.3832
9523      1219.9226      1253.2084      1266.0461
9524      1287.5495      1327.3345      1364.0460
9525      1396.2710      1414.5928      1482.8872
9526      1488.3685      1498.0181      1501.1903
9527      1689.9085      3068.2305      3082.1468
9528      3098.4667      3116.4651      3135.8086
9529      3174.3543      3212.3579      3857.4644
9530      Zero-point correction (Hartree): 0.134683
9531
9532      TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Et
9533      ~~~~~

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9534 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41202505
9535 Electronic state : 2-A
9536 Cartesian coordinates (Angs):
9537 O -1.801016 1.194880 -0.292037
9538 H -0.680972 1.494659 0.182105
9539 C 0.458122 1.309432 0.788425
9540 O -1.505795 0.067479 -1.018020
9541 C 0.640213 -0.110418 0.546060
9542 C -1.555137 -1.071067 -0.163841
9543 C -0.505830 -1.004294 0.957098
9544 H 0.137967 1.569895 1.795354
9545 H 1.204489 1.976818 0.373802
9546 C 1.677405 -0.607886 -0.141367
9547 O 2.680110 0.183750 -0.600182
9548 H 1.766000 -1.668997 -0.347278
9549 H -2.566519 -1.181391 0.231818
9550 H -1.340686 -1.896938 -0.842239
9551 H -0.165710 -2.015214 1.183006
9552 H -0.955428 -0.603189 1.865159
9553 H 3.325829 -0.339119 -1.078065
9554 Rotational constants (GHz): 3.3264600 1.4097200 1.2706800
9555 Vibrational harmonic frequencies (cm-1):
9556 i2051.6284 80.8964 118.0649
9557 234.7208 253.7706 296.7965
9558 327.8990 367.3283 412.4711
9559 463.3578 542.0591 565.4153
9560 629.6163 708.5276 808.9682
9561 856.5643 886.7265 954.9900
9562 1018.2313 1030.5736 1064.8990
9563 1082.5759 1127.6163 1207.4368
9564 1210.8433 1252.4923 1264.9906
9565 1289.6721 1309.7406 1357.9237
9566 1397.5991 1405.8849 1478.3326
9567 1482.6085 1488.6295 1499.8821
9568 1716.0912 3066.0063 3080.8514
9569 3108.1941 3113.8368 3133.5914
9570 3180.4327 3210.1388 3913.5482
9571 Zero-point correction (Hartree): 0.134414
9572
9573
9574 #####
9575 Z-HOCH=C(CH3)CH2CH2OO ring closure and H-shift
9576 #####
9577
9578 HOHCCH3CH2CH2OO.Zcpmm
9579 ~~~~~
9580 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44926728
9581 Electronic state : 2-A
9582 Cartesian coordinates (Angs):
9583 C 1.130828 1.189643 0.118372
9584 C 1.238603 -0.132009 -0.010035
9585 C 0.223458 -1.204350 0.298823
9586 C -1.174937 -0.855596 0.776147
9587 O -2.076071 -0.621963 -0.337399
9588 O -1.939195 0.550472 -0.866455
9589 O 0.048799 1.933320 0.470619
9590 H 2.005167 1.806843 -0.055894
9591 C 2.555327 -0.707592 -0.455973
9592 H 0.121413 -1.869420 -0.565394
9593 H 0.663012 -1.830250 1.083227
9594 H -1.627782 -1.712607 1.269338
9595 H -1.213156 0.009725 1.433576
9596 H -0.745437 1.559668 0.057560
9597 H 3.299289 0.071191 -0.610861
9598 H 2.443891 -1.258622 -1.393007
9599 H 2.945669 -1.411728 0.283331
9600 Rotational constants (GHz): 2.8902200 1.5369100 1.1689500
9601 Vibrational harmonic frequencies (cm-1):
9602 24.0365 77.6570 189.7251
9603 198.5005 212.4232 301.1457
9604 319.7088 342.3071 426.8330
9605 433.3245 555.5785 612.1342

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9606      683.9066      774.3618      863.0769
9607      915.0358      972.8046      1009.5127
9608     1050.9749     1071.7262     1096.5676
9609     1181.8355     1220.7331     1247.8945
9610     1277.4254     1332.8511     1356.0380
9611     1407.6980     1409.2349     1419.2418
9612     1438.9876     1461.5529     1484.0105
9613     1501.8632     1507.0806     1769.4280
9614     3030.3042     3041.7617     3055.8862
9615     3088.3897     3111.8810     3143.4802
9616     3168.9225     3179.4980     3648.0915
9617 Zero-point correction (Hartree): 0.140370
9618
9619 HOCHCCH3CH2CH2OO.Zcppc
9620 ~~~~~
9621 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44991842
9622 Electronic state : 2-A
9623 Cartesian coordinates (Angs):
9624 C      1.302368      1.134243      -0.052999
9625 C      1.292066      -0.197500     -0.038492
9626 C      0.113401     -1.112402      0.187562
9627 C     -1.101218     -0.564118      0.907252
9628 O     -1.906118      0.273034      0.035929
9629 O     -2.522093     -0.422441     -0.870935
9630 O      0.278841      2.017500      0.086638
9631 H      2.242014      1.657752     -0.178460
9632 C      2.581383     -0.932962     -0.282837
9633 H     -0.224491     -1.555842     -0.754835
9634 H      0.469624     -1.953295      0.789785
9635 H     -1.753771     -1.364950      1.247106
9636 H     -0.836395      0.090558      1.735721
9637 H     -0.571467      1.619975     -0.129949
9638 H      3.407289     -0.247262     -0.461502
9639 H      2.495186     -1.588545     -1.153039
9640 H      2.838972     -1.566692      0.569206
9641 Rotational constants (GHz):   3.0876200      1.3938000      1.0892800
9642 Vibrational harmonic frequencies (cm-1):
9643      41.4157      88.8959      158.4002
9644     203.7030      214.9268      267.4457
9645     306.5270      349.4743      426.3144
9646     468.9643      540.3332      555.0457
9647     616.7284      783.5881      848.6957
9648     920.2684      977.4469     1010.4465
9649    1023.8451     1070.5587     1118.5778
9650    1177.7980     1205.3420     1226.1172
9651    1285.3179     1308.7509     1328.8084
9652    1396.5434     1402.0385     1419.5250
9653    1434.5639     1466.7983     1484.7455
9654    1489.9621     1503.0773     1770.8431
9655    3041.0376     3043.7765     3071.5466
9656    3088.6966     3103.7687     3142.8778
9657    3164.1479     3197.6601     3816.3222
9658 Zero-point correction (Hartree): 0.140248
9659
9660 HOCHCCH3CH2CH2OO.Zcptt
9661 ~~~~~
9662 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44798473
9663 Electronic state : 2-A
9664 Cartesian coordinates (Angs):
9665 C      1.111782      1.202708     -0.048985
9666 C      1.321607     -0.106468      0.000181
9667 C      0.372817     -1.143483      0.544186
9668 C     -1.082610     -0.764033      0.699462
9669 O     -1.584852     -0.416972     -0.610449
9670 O     -2.785048      0.066786     -0.547755
9671 O     -0.001108      1.821837      0.451410
9672 H      1.860828      1.861847     -0.473951
9673 C      2.623586     -0.662260     -0.501470
9674 H      0.429102     -2.020392     -0.107435
9675 H      0.730553     -1.483099      1.521683
9676 H     -1.670436     -1.612639      1.049149
9677 H     -1.242637      0.091413      1.346309

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9678      H      -0.106376      2.684059      0.045726
9679      H      3.140249      -1.213026      0.288487
9680      H      3.289287      0.123328      -0.854380
9681      H      2.454407      -1.363486      -1.321472
9682      Rotational constants (GHz):      3.1846200      1.3743500      1.1036000
9683      Vibrational harmonic frequencies (cm-1):
9684          41.7350          54.6761          136.9906
9685          196.3076          224.8723          256.5599
9686          272.2639          309.1968          342.1811
9687          389.1014          449.4868          541.9392
9688          634.2976          783.3691          838.9369
9689          888.2290          1005.2984          1008.2993
9690          1044.5282          1077.3965          1102.6649
9691          1177.8265          1204.1175          1242.1809
9692          1276.9776          1294.3337          1304.8379
9693          1384.4248          1413.3817          1421.5673
9694          1433.4271          1466.7757          1483.4140
9695          1500.1768          1504.6908          1800.8913
9696          3040.9819          3045.7174          3070.2552
9697          3094.2460          3095.3060          3140.4667
9698          3175.4861          3184.9905          3907.3554
9699      Zero-point correction (Hartree): 0.139565
9700
9701      HOCHCCH3CH2CH2OO.Zctpc
9702      ~~~~~
9703      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44515262
9704      Electronic state : 2-A
9705      Cartesian coordinates (Angs):
9706      C      -1.954737      0.702111      -0.066637
9707      C      -1.292319      -0.449834      -0.007600
9708      C      0.197765      -0.675928      0.038772
9709      C      1.099300      0.522071      0.262716
9710      O      2.448422      0.069257      0.503280
9711      O      3.004518      -0.353378      -0.590800
9712      O      -1.493168      1.984059      -0.122603
9713      H      -3.036633      0.701284      -0.068602
9714      C      -2.079754      -1.732002      0.012289
9715      H      0.399791      -1.381335      0.850752
9716      H      0.521164      -1.176700      -0.878264
9717      H      1.155607      1.183685      -0.603865
9718      H      0.836007      1.076985      1.162625
9719      H      -0.546872      2.014117      -0.268205
9720      H      -3.150674      -1.546910      -0.040197
9721      H      -1.874075      -2.301120      0.921577
9722      H      -1.804015      -2.368020      -0.832066
9723      Rotational constants (GHz):      3.2170000      1.1150700      0.8728000
9724      Vibrational harmonic frequencies (cm-1):
9725          25.4172          78.3647          123.7774
9726          170.7876          196.9246          227.9818
9727          287.8662          320.1712          343.9952
9728          406.9443          474.0316          574.1455
9729          604.6082          791.2435          883.9768
9730          921.8576          975.5759          1005.4773
9731          1051.2166          1083.7976          1123.9663
9732          1173.5548          1183.5992          1246.7477
9733          1278.9744          1303.1522          1346.0534
9734          1355.9993          1411.8816          1419.2780
9735          1434.4271          1483.0102          1487.6386
9736          1504.0531          1515.7753          1779.0413
9737          3042.4192          3047.0036          3065.3448
9738          3076.6750          3095.3128          3140.2386
9739          3146.0393          3213.1117          3925.5280
9740      Zero-point correction (Hartree): 0.139759
9741
9742      HOCHCCH3CH2CH2OO.Zctpt
9743      ~~~~~
9744      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44961874
9745      Electronic state : 2-A
9746      Cartesian coordinates (Angs):
9747      C      -1.910461      0.687968      -0.132568
9748      C      -1.279218      -0.468402      0.020212
9749      C      0.193008      -0.658194      0.265105

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9750      C      1.080153      0.569106      0.189292
9751      O      2.452055      0.165698      0.416055
9752      O      2.935128     -0.475134     -0.603425
9753      O     -1.293149      1.911294     -0.076811
9754      H     -2.980286      0.712591     -0.304352
9755      C     -2.063894     -1.748177     -0.033569
9756      H      0.327699     -1.125570      1.246155
9757      H      0.572150     -1.379256     -0.464639
9758      H      1.037631      1.055505     -0.781581
9759      H      0.876641      1.290249      0.974713
9760      H     -1.926284      2.602984     -0.272360
9761      H     -3.124880     -1.566021     -0.195353
9762      H     -1.952764     -2.308170      0.897707
9763      H     -1.699699     -2.390990     -0.837673
9764      Rotational constants (GHz):      3.1892200      1.1588400      0.8959600
9765      Vibrational harmonic frequencies (cm-1):
9766          34.7291          89.3545          133.3168
9767          169.8388          185.6689          216.9190
9768          265.2060          311.7155          345.4390
9769          397.6089          456.9792          567.6594
9770          604.5898          790.8203          878.8482
9771          888.6487          966.6599          1004.5028
9772          1046.3952          1088.0718          1117.8057
9773          1174.1608          1201.1280          1238.9297
9774          1268.2535          1294.4717          1332.8919
9775          1353.3483          1407.4306          1422.2608
9776          1431.8591          1481.9638          1483.7375
9777          1493.8845          1504.6745          1803.5656
9778          3037.9988          3048.1738          3074.2592
9779          3098.3665          3123.7778          3140.1703
9780          3183.9106          3189.7624          3920.7129
9781      Zero-point correction (Hartree): 0.139584
9782
9783      HOCHCCH3CH2CH2OO.Zgmmc
9784      ~~~~~
9785      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45072057
9786      Electronic state : 2-A
9787      Cartesian coordinates (Angs):
9788      C      1.989804      0.208706      -0.313793
9789      C      0.826097      0.596713      0.196926
9790      C     -0.065618     -0.359934      0.947609
9791      C     -0.945036     -1.198469      0.032037
9792      O     -1.823393     -0.354934     -0.746128
9793      O     -2.718326      0.210818      0.003761
9794      O      2.543784     -1.034946     -0.234980
9795      H      2.629282      0.883352     -0.866545
9796      C      0.339780      2.005975      0.026131
9797      H      0.509180     -1.048789      1.575217
9798      H     -0.716760      0.191344      1.626975
9799      H     -0.361834     -1.730557     -0.718451
9800      H     -1.574360     -1.891379      0.589167
9801      H      2.003592     -1.606928      0.316729
9802      H     -0.624440      2.029662     -0.484220
9803      H      1.047187      2.600169     -0.550200
9804      H      0.201475      2.487689      0.996649
9805      Rotational constants (GHz):      3.3559600      1.2984200      1.0556100
9806      Vibrational harmonic frequencies (cm-1):
9807          40.9393          66.7204          142.3623
9808          169.4739          193.3883          289.2887
9809          302.5363          332.5190          387.9733
9810          421.2621          534.2735          570.9138
9811          613.4048          790.2132          848.8792
9812          917.2383          948.1353          1009.7677
9813          1031.0112          1071.8344          1097.2237
9814          1177.1280          1189.8680          1239.8074
9815          1266.6471          1299.3519          1313.3219
9816          1364.8695          1399.9540          1410.5359
9817          1423.9707          1481.6530          1488.0521
9818          1493.7835          1504.0293          1772.4866
9819          3041.5945          3051.1800          3087.2260
9820          3106.0248          3108.3076          3140.4678
9821          3149.7913          3219.9452          3871.8849

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9822 Zero-point correction (Hartree): 0.139837
9823
9824 HOCHCCH3CH2CH2OO.Zgmmt
9825 ~~~~~
9826 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45252662
9827 Electronic state : 2-A
9828 Cartesian coordinates (Angs):
9829 C 1.937512 -0.188903 -0.323205
9830 C 0.805674 -0.633427 0.203909
9831 C -0.070602 0.296764 1.002205
9832 C -0.912154 1.199539 0.117663
9833 O -1.770587 0.420154 -0.748972
9834 O -2.692514 -0.194761 -0.074327
9835 O 2.332130 1.115667 -0.158502
9836 H 2.592745 -0.818658 -0.913257
9837 C 0.345735 -2.044789 0.001752
9838 H -0.736259 -0.273491 1.650451
9839 H 0.540127 0.946490 1.631171
9840 H -1.556161 1.858637 0.698149
9841 H -0.290957 1.773311 -0.566664
9842 H 3.207424 1.243071 -0.526465
9843 H 0.236027 -2.554879 0.961179
9844 H 1.048398 -2.611123 -0.608111
9845 H -0.630563 -2.066941 -0.485989
9846 Rotational constants (GHz): 3.2226000 1.3598600 1.0889800
9847 Vibrational harmonic frequencies (cm-1):
9848 42.8964 65.6193 142.7389
9849 167.1418 189.3145 227.3757
9850 288.6729 320.2290 354.3743
9851 391.2909 531.7092 574.5252
9852 617.5566 798.6739 848.1971
9853 878.3959 950.0970 1009.2751
9854 1028.4883 1072.7596 1100.3847
9855 1182.1118 1197.7530 1226.2701
9856 1262.8379 1299.1358 1318.7714
9857 1362.3503 1390.7542 1407.4201
9858 1423.0941 1474.4708 1481.9141
9859 1491.8754 1503.0181 1794.6668
9860 3050.6164 3075.4455 3095.1329
9861 3105.4278 3124.1288 3136.8179
9862 3163.0238 3188.8317 3919.8657
9863 Zero-point correction (Hartree): 0.139596
9864
9865 HOCHCCH3CH2CH2OO.Zgmpc
9866 ~~~~~
9867 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44933493
9868 Electronic state : 2-A
9869 Cartesian coordinates (Angs):
9870 C 1.782933 0.110969 -0.461481
9871 C 0.787914 0.564110 0.293452
9872 C -0.004858 -0.353506 1.188551
9873 C -1.119576 -1.100004 0.464262
9874 O -2.097280 -0.166343 -0.034011
9875 O -1.863617 0.176104 -1.265665
9876 O 2.230116 -1.173930 -0.541764
9877 H 2.351128 0.759979 -1.113582
9878 C 0.402348 2.013945 0.272419
9879 H 0.633315 -1.104711 1.666413
9880 H -0.447622 0.220846 2.003959
9881 H -0.752162 -1.663208 -0.392318
9882 H -1.670244 -1.749300 1.143820
9883 H 1.742706 -1.737215 0.064959
9884 H 1.019339 2.575114 -0.427427
9885 H 0.518723 2.460585 1.262732
9886 H -0.641492 2.138175 -0.020258
9887 Rotational constants (GHz): 2.7294700 1.4523500 1.2564800
9888 Vibrational harmonic frequencies (cm-1):
9889 48.7034 88.8848 105.7465
9890 169.7326 194.4482 263.3324
9891 294.1944 342.2144 378.2690
9892 420.1903 528.8116 569.2579
9893 604.0069 779.9811 872.6524

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9894      918.2761          938.0512          1019.9914
9895      1036.1814         1069.0318         1087.0051
9896      1177.5739         1191.8773         1236.3051
9897      1258.3935         1300.3856         1329.8438
9898      1370.3998         1391.7892         1410.7006
9899      1423.2240         1481.1253         1483.1346
9900      1491.9566         1502.5607         1774.5235
9901      3036.0261         3048.8346         3086.6194
9902      3098.1440         3104.4574         3141.0885
9903      3151.2493         3221.7205         3877.9113
9904      Zero-point correction (Hartree): 0.139695
9905
9906      HOCHCCH3CH2CH2OO.Zgmpt
9907      ~~~~~
9908      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45143242
9909      Electronic state : 2-A
9910      Cartesian coordinates (Angs):
9911      C      1.737121      0.063987      -0.456171
9912      C      0.779185      0.601911      0.284741
9913      C     -0.011417     -0.262962      1.230502
9914      C     -1.095726     -1.067273      0.528296
9915      O     -2.080353     -0.182475     -0.047689
9916      O     -1.816170      0.105465     -1.286838
9917      O      2.025882     -1.274731     -0.377320
9918      H      2.322426      0.642226     -1.160931
9919      C      0.431283      2.055253      0.184803
9920      H      0.645789     -0.982963      1.721704
9921      H     -0.471362      0.351282      2.006168
9922      H     -0.687958     -1.672298     -0.278096
9923      H     -1.653186     -1.683368      1.232423
9924      H      2.762741     -1.485878     -0.951833
9925      H      1.056551      2.565317     -0.546653
9926      H      0.559200      2.551269      1.149607
9927      H     -0.611754      2.182851     -0.110643
9928      Rotational constants (GHz):      2.6594900      1.5166600      1.2947300
9929      Vibrational harmonic frequencies (cm-1):
9930      45.6868          87.5472          103.4694
9931      176.4799         193.2789         234.0679
9932      281.1618         330.6672         348.3348
9933      397.9300         526.6332         570.6983
9934      607.3737         787.0443         870.6459
9935      876.5100         939.9320         1016.1217
9936      1035.2074        1070.4997        1088.9494
9937      1183.0382        1198.2857        1234.1057
9938      1242.8935        1310.5007        1325.2313
9939      1366.3777        1382.6238        1408.4118
9940      1421.3718        1472.8623        1481.4155
9941      1485.9827        1501.6823        1796.0196
9942      3048.6422        3067.6456        3095.2545
9943      3103.2459        3114.5449        3137.1026
9944      3164.9746        3192.3371        3920.0508
9945      Zero-point correction (Hartree): 0.139521
9946
9947      HOCHCCH3CH2CH2OO.Zgmtc
9948      ~~~~~
9949      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44965828
9950      Electronic state : 2-A
9951      Cartesian coordinates (Angs):
9952      C      1.939070     -0.129593     -0.510460
9953      C      1.011908      0.552033      0.154141
9954      C      0.089828     -0.124896      1.137626
9955      C     -1.102311     -0.796531      0.478876
9956      O     -1.901160      0.241346     -0.129589
9957      O     -2.928763     -0.251629     -0.747865
9958      O      2.204870     -1.462661     -0.411107
9959      H      2.596994      0.343679     -1.226528
9960      C      0.832012      2.025207     -0.065783
9961      H      0.613282     -0.886342      1.724394
9962      H     -0.277367      0.604850      1.861275
9963      H     -0.805748     -1.479880     -0.317169
9964      H     -1.739491     -1.315071      1.194778
9965      H      1.645233     -1.868477      0.256231

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9966      H      -0.181116      2.248067      -0.403871
9967      H      1.532750      2.401156      -0.809499
9968      H      0.992846      2.578250      0.862484
9969      Rotational constants (GHz):      3.0103600      1.2180800      1.0238900
9970      Vibrational harmonic frequencies (cm-1):
9971      41.4082      75.5142      119.9922
9972      173.6373      195.7565      273.3382
9973      284.5693      314.9211      381.6568
9974      392.4674      489.2844      577.5848
9975      622.5919      786.1280      841.5853
9976      921.7769      977.9475      1025.9881
9977      1049.6434      1070.3287      1087.9050
9978      1176.7408      1196.4185      1244.8787
9979      1276.7479      1294.6012      1306.7742
9980      1367.8364      1402.7677      1410.5180
9981      1422.6055      1481.9338      1491.9293
9982      1499.3863      1505.2994      1775.1273
9983      3043.9052      3050.1255      3078.3368
9984      3098.5812      3105.7877      3137.3926
9985      3141.1266      3219.1818      3876.0556
9986      Zero-point correction (Hartree): 0.139670
9987
9988      HOCHCCH3CH2CH2OO.Zgmtt
9989      ~~~~~
9990      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45153725
9991      Electronic state : 2-A
9992      Cartesian coordinates (Angs):
9993      C      1.880460      -0.188728      -0.506354
9994      C      1.011983      0.572220      0.144584
9995      C      0.096187      -0.044062      1.170887
9996      C      -1.088956      -0.750130      0.542855
9997      O      -1.874325      0.247915      -0.150741
9998      O      -2.889016      -0.281038      -0.759924
9999      O      1.966358      -1.535761      -0.260800
10000     H      2.549319      0.206647      -1.261521
10001     C      0.889736      2.038765      -0.135028
10002     H      0.635776      -0.789604      1.756667
10003     H      -0.265876      0.721474      1.859021
10004     H      -0.775125      -1.488032      -0.193238
10005     H      -1.741217      -1.213280      1.282420
10006     H      2.681224      -1.918254      -0.771152
10007     H      -0.121915      2.284581      -0.462218
10008     H      1.588769      2.357583      -0.907021
10009     H      1.088445      2.621573      0.767096
10010     Rotational constants (GHz):      2.9146800      1.2701200      1.0549900
10011     Vibrational harmonic frequencies (cm-1):
10012     42.7504      72.7486      117.7732
10013     178.3161      198.3964      245.1979
10014     285.7025      300.6185      347.4777
10015     375.8057      479.9849      582.0684
10016     623.8398      794.2295      840.9293
10017     877.0195      983.2028      1025.2759
10018     1042.4252      1075.1355      1088.8214
10019     1181.7763      1199.4183      1228.8308
10020     1269.4839      1298.6573      1317.1769
10021     1362.1365      1396.8202      1406.5667
10022     1421.5974      1473.6656      1482.2938
10023     1502.4534      1505.0698      1794.8735
10024     3050.0418      3071.5608      3089.2414
10025     3105.2245      3118.0648      3137.4365
10026     3152.1171      3190.2015      3919.1491
10027     Zero-point correction (Hartree): 0.139541
10028
10029     HOCHCCH3CH2CH2OO.Zgpmc
10030     ~~~~~
10031     E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45240759
10032     Electronic state : 2-A
10033     Cartesian coordinates (Angs):
10034     C      1.224405      1.071636      0.115225
10035     C      1.093779      -0.235051      -0.098039
10036     C      0.100153      -0.780139      -1.085588
10037     C      -1.252678      -1.100586      -0.463721

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10038 O -1.846708 0.122595 0.018775
10039 O -1.626316 0.305916 1.289588
10040 O 0.501693 2.068096 -0.462038
10041 H 1.972419 1.462813 0.792974
10042 C 1.914167 -1.228647 0.668231
10043 H -0.054263 -0.084383 -1.913673
10044 H 0.486521 -1.704024 -1.522661
10045 H -1.953299 -1.490637 -1.200553
10046 H -1.174329 -1.775711 0.385619
10047 H -0.359671 1.738532 -0.737933
10048 H 1.276658 -1.891783 1.259108
10049 H 2.597727 -0.732283 1.354866
10050 H 2.499926 -1.858654 -0.004990
10051 Rotational constants (GHz): 2.4124700 1.7738900 1.3808600
10052 Vibrational harmonic frequencies (cm-1):
10053 53.2250 92.8312 110.8594
10054 190.7603 202.6129 259.5484
10055 307.3685 344.1491 378.7662
10056 437.9692 526.9002 582.3746
10057 602.7792 774.7668 862.8993
10058 918.0243 979.9982 993.6932
10059 1030.2699 1066.0743 1084.6708
10060 1184.8261 1199.6995 1224.5053
10061 1269.9523 1306.9516 1323.5696
10062 1366.7961 1384.1554 1411.7458
10063 1422.4428 1479.2083 1487.6470
10064 1488.9137 1500.8396 1764.8020
10065 3040.9682 3056.5544 3088.9997
10066 3091.9236 3100.8731 3138.8295
10067 3159.6501 3206.2195 3848.4104
10068 Zero-point correction (Hartree): 0.139763
10069
10070 HOCHCCH3CH2CH2OO.Zgppc
10071 ~~~~~
10072 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.84631979
10073 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.77536686
10074 T1 diagnostic: 0.021002
10075 E(MP2/Aug-CC-pVTZ) (Hartree): -420.72348730
10076 E(MP3/Aug-CC-pVTZ) (Hartree): -420.76218978
10077 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.72673939
10078 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.76408756
10079 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.18016550
10080 E(UHF/Aug-CC-pVTZ) (Hartree): -419.17484935
10081 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45480404
10082 Electronic state : 2-A
10083 Cartesian coordinates (Angs):
10084 C -1.212494 1.178878 -0.172259
10085 C -1.161420 -0.120390 0.111263
10086 C -0.063202 -0.717029 0.948967
10087 C 1.038780 -1.369346 0.134278
10088 O 1.696511 -0.421967 -0.746504
10089 O 2.167644 0.596960 -0.102567
10090 O -0.325313 2.138965 0.186655
10091 H -2.036973 1.595904 -0.737046
10092 C -2.216824 -1.058983 -0.394807
10093 H 0.382627 0.021461 1.615150
10094 H -0.480267 -1.497923 1.590496
10095 H 1.813810 -1.800446 0.767521
10096 H 0.656562 -2.124151 -0.549973
10097 H 0.523487 1.748654 0.428011
10098 H -2.961550 -0.533786 -0.990435
10099 H -2.729056 -1.555064 0.433194
10100 H -1.788407 -1.845085 -1.022259
10101 Rotational constants (GHz): 2.6040800 1.7509900 1.2063500
10102 Vibrational harmonic frequencies (cm-1):
10103 44.7648 126.1924 134.7356
10104 191.5450 199.3966 275.1822
10105 313.8253 352.8731 395.9432
10106 453.1138 531.0890 580.7217
10107 633.5081 769.4751 848.0543
10108 928.5450 971.3108 982.7232
10109 1032.1058 1072.3501 1091.7482

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10110      1189.0619          1205.0560          1249.2238
10111      1274.8693          1304.4794          1327.1191
10112      1372.8944          1403.2116          1416.6370
10113      1424.7850          1480.5896          1492.7890
10114      1495.1440          1502.5296          1770.9465
10115      3040.2241          3062.2873          3085.6176
10116      3092.1114          3115.3914          3138.1233
10117      3155.0114          3201.6968          3806.0569
10118      Zero-point correction (Hartree): 0.140187
10119
10120      HOCHCCH3CH2CH2OO.Zgppt
10121      ~~~~~
10122      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45053934
10123      Electronic state : 2-A
10124      Cartesian coordinates (Angs):
10125      C      -1.451259          0.979163          -0.222332
10126      C      -1.140884          -0.268690          0.103488
10127      C      0.033012          -0.571021          0.992191
10128      C      1.204235          -1.175474          0.235921
10129      O      1.720483          -0.246319          -0.742162
10130      O      2.350518          0.735054          -0.172919
10131      O      -0.750905          2.051340          0.251475
10132      H      -2.292076          1.204611          -0.869038
10133      C      -1.948873          -1.422287          -0.410435
10134      H      0.381536          0.331125          1.491996
10135      H      -0.260136          -1.289196          1.763415
10136      H      2.025859          -1.431021          0.902989
10137      H      0.917013          -2.045772          -0.351916
10138      H      -1.030789          2.852096          -0.193360
10139      H      -2.767359          -1.083959          -1.044064
10140      H      -2.374184          -1.998170          0.415019
10141      H      -1.338005          -2.110464          -0.999191
10142      Rotational constants (GHz):      2.5793500      1.6307200      1.1579300
10143      Vibrational harmonic frequencies (cm-1):
10144      23.6969          58.4108          132.3345
10145      164.5839          199.0826          216.6921
10146      280.8366          320.5261          381.6193
10147      386.6381          528.8669          572.3737
10148      614.8579          776.2974          854.9305
10149      893.9685          973.2870          992.2028
10150      1030.1971          1072.2597          1095.1143
10151      1184.1722          1200.4864          1231.9331
10152      1262.4902          1303.4023          1328.5719
10153      1356.8879          1397.4897          1415.4413
10154      1423.4672          1472.9296          1483.7819
10155      1495.5237          1502.2582          1800.5278
10156      3044.4417          3056.4649          3090.8389
10157      3096.1945          3134.4264          3134.7851
10158      3154.8935          3177.6820          3922.3740
10159      Zero-point correction (Hartree): 0.139516
10160
10161      HOCHCCH3CH2CH2OO.Zgpptc
10162      ~~~~~
10163      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45306200
10164      Electronic state : 2-A
10165      Cartesian coordinates (Angs):
10166      C      -1.371459          1.110287          -0.212460
10167      C      -1.279054          -0.192751          0.039897
10168      C      -0.238619          -0.760398          0.970525
10169      C      1.076458          -1.083310          0.289359
10170      O      1.692400          0.187561          -0.031864
10171      O      2.794303          0.047624          -0.699848
10172      O      -0.565969          2.095075          0.262908
10173      H      -2.159874          1.507199          -0.839848
10174      C      -2.218373          -1.170693          -0.601847
10175      H      -0.038244          -0.078086          1.801032
10176      H      -0.616913          -1.684079          1.412400
10177      H      1.770432          -1.617850          0.936960
10178      H      0.946632          -1.624807          -0.646736
10179      H      0.302756          1.738926          0.479120
10180      H      -2.920348          -0.670727          -1.267018
10181      H      -2.789432          -1.717126          0.152526

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10182      H      -1.674596      -1.914337      -1.190851
10183 Rotational constants (GHz):      2.8029500      1.4171900      1.0897600
10184 Vibrational harmonic frequencies (cm-1):
10185      57.3231      80.2590      130.1165
10186      196.3217      214.8427      249.4889
10187      312.0548      331.1202      379.1148
10188      419.9506      492.9681      589.0586
10189      621.0146      776.7252      853.3318
10190      924.1319      978.4966      1023.9317
10191      1044.5439      1072.3649      1089.5633
10192      1187.7336      1201.8755      1242.6615
10193      1288.0289      1295.5147      1324.7652
10194      1375.5354      1395.8599      1414.3787
10195      1424.0857      1480.8590      1485.3804
10196      1499.6902      1502.5269      1768.9913
10197      3039.1369      3057.5259      3085.6433
10198      3086.1935      3104.6398      3138.6926
10199      3146.6525      3200.4163      3835.2996
10200 Zero-point correction (Hartree): 0.139922
10201
10202 HOCHCCH3CH2CH2OO.Zgtml
10203 ~~~~~
10204 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45141848
10205 Electronic state : 2-A
10206 Cartesian coordinates (Angs):
10207      C      1.910795      0.759196      0.121764
10208      C      1.289882      -0.377677      -0.163657
10209      C      -0.151579      -0.373830      -0.595839
10210      C      -1.058966      -0.353502      0.623931
10211      O      -2.443031      -0.497986      0.240163
10212      O      -2.891044      0.578278      -0.330829
10213      O      1.269773      1.963812      0.025290
10214      H      2.943778      0.787010      0.449125
10215      C      1.978439      -1.700807      -0.021869
10216      H      -0.376871      0.502971      -1.201488
10217      H      -0.368963      -1.266471      -1.184824
10218      H      -0.873423      -1.199722      1.283912
10219      H      -0.959773      0.582450      1.170849
10220      H      1.885295      2.681120      0.181772
10221      H      2.995821      -1.587669      0.349828
10222      H      2.019433      -2.220512      -0.981357
10223      H      1.437702      -2.352289      0.669216
10224 Rotational constants (GHz):      3.1249400      1.1802200      0.9183300
10225 Vibrational harmonic frequencies (cm-1):
10226      43.1009      58.2287      115.8739
10227      165.0305      197.0364      238.2868
10228      252.7400      310.3572      332.7529
10229      401.3085      536.1713      573.7785
10230      594.5100      790.6777      875.4494
10231      885.5576      963.3209      1008.2226
10232      1055.7709      1071.9139      1084.4082
10233      1192.6253      1201.1349      1234.1893
10234      1271.0156      1303.6814      1323.4556
10235      1342.5573      1394.4848      1404.8444
10236      1422.0094      1481.0544      1484.2054
10237      1496.6169      1504.6700      1794.8701
10238      3045.1051      3073.9297      3094.3677
10239      3096.8570      3130.5898      3137.3229
10240      3160.9014      3185.7677      3918.9888
10241 Zero-point correction (Hartree): 0.139537
10242
10243 HOCHCCH3CH2CH2OO.Zgtpc
10244 ~~~~~
10245 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45153269
10246 Electronic state : 2-A
10247 Cartesian coordinates (Angs):
10248      C      -2.172461      -0.321246      0.095284
10249      C      -1.165908      0.518131      -0.127722
10250      C      0.187291      0.041686      -0.584998
10251      C      1.068171      -0.279022      0.612972
10252      O      2.385520      -0.687902      0.189328
10253      O      3.064743      0.317159      -0.272783

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10254	O	-2.164945	-1.672241	-0.066668		
10255	H	-3.137976	0.022345	0.441649		
10256	C	-1.322705	1.991198	0.109069		
10257	H	0.126622	-0.838889	-1.230495		
10258	H	0.680113	0.819819	-1.169329		
10259	H	1.185360	0.584699	1.265590		
10260	H	0.686718	-1.124351	1.183673		
10261	H	-1.320539	-1.962562	-0.423113		
10262	H	-2.308195	2.227326	0.506967		
10263	H	-1.184559	2.550868	-0.818376		
10264	H	-0.576415	2.360131	0.816786		
10265	Rotational constants (GHz):			3.3818200	1.0889300	0.8774500
10266	Vibrational harmonic frequencies (cm-1):					
10267		47.0904	59.3591			123.6889
10268		170.7596	199.3611			262.7582
10269		289.7434	348.5679			378.5753
10270		401.8149	542.5799			582.9100
10271		584.9880	790.7431			859.8135
10272		922.9408	969.4043			1012.0313
10273		1055.9308	1070.7385			1080.7951
10274		1181.8975	1203.1236			1241.7774
10275		1275.1277	1291.2127			1326.6449
10276		1338.6892	1396.8576			1407.5070
10277		1424.5132	1482.0798			1488.2826
10278		1500.1410	1517.0705			1774.5180
10279		3046.0285	3051.1932			3094.0154
10280		3095.2825	3107.2019			3139.8687
10281		3155.7517	3215.6197			3868.0294
10282	Zero-point correction (Hartree):			0.139827		
10283						
10284	HOHCCH3CH2CH2OO.Zgtpt					
10285	~~~~~					
10286	E(UM062X/Aug-CC-pVTZ) (Hartree):			-421.45212613		
10287	Electronic state :			2-A		
10288	Cartesian coordinates (Angs):					
10289	C	2.127603	-0.341528	-0.095140		
10290	C	1.165326	0.542943	0.129471		
10291	C	-0.187364	0.093080	0.611583		
10292	C	-1.043209	-0.328801	-0.571457		
10293	O	-2.372897	-0.693155	-0.141944		
10294	O	-3.062456	0.351967	0.198994		
10295	O	1.924794	-1.681023	0.107142		
10296	H	3.108102	-0.051935	-0.454980		
10297	C	1.367680	2.004129	-0.131708		
10298	H	-0.093737	-0.750153	1.295365		
10299	H	-0.694026	0.907621	1.130262		
10300	H	-1.146821	0.470655	-1.304120		
10301	H	-0.647740	-1.226149	-1.042759		
10302	H	2.747212	-2.160115	-0.002551		
10303	H	2.358161	2.207788	-0.536103		
10304	H	1.245541	2.581101	0.787141		
10305	H	0.627563	2.379937	-0.842295		
10306	Rotational constants (GHz):			3.3237100	1.1223700	0.8913600
10307	Vibrational harmonic frequencies (cm-1):					
10308		44.5717	62.7876			124.9787
10309		165.7322	198.6336			247.3023
10310		251.3303	323.5266			341.8888
10311		388.0639	534.2879			585.8553
10312		590.3510	792.7493			869.2410
10313		883.3122	966.9106			1011.3992
10314		1053.3917	1076.6941			1081.4453
10315		1191.2637	1199.1809			1233.0549
10316		1281.3985	1292.1512			1332.3943
10317		1337.5528	1393.4216			1403.6697
10318		1422.3264	1480.7076			1484.0234
10319		1495.7953	1503.7741			1794.3768
10320		3046.1018	3078.2855			3095.8321
10321		3096.8492	3128.8474			3136.0435
10322		3162.9429	3187.1175			3917.9089
10323	Zero-point correction (Hartree):			0.139628		
10324						
10325	HOHCCH3CH2CH2OO.Zgttc					

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10326 ~~~~~
10327 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45042784
10328 Electronic state : 2-A
10329 Cartesian coordinates (Angs):
10330 C 2.104641 -0.568463 -0.240010
10331 C 1.312290 0.440597 0.107703
10332 C -0.027993 0.218210 0.760028
10333 C -1.112626 0.082160 -0.291915
10334 O -2.377396 -0.051830 0.392218
10335 O -3.360089 -0.181256 -0.444657
10336 O 1.870417 -1.896168 -0.060880
10337 H 3.059988 -0.404822 -0.720364
10338 C 1.705336 1.861328 -0.170639
10339 H -0.036159 -0.666473 1.402354
10340 H -0.266928 1.063845 1.407142
10341 H -1.175497 0.961918 -0.931327
10342 H -0.976950 -0.802550 -0.913781
10343 H 1.034099 -2.032532 0.393316
10344 H 2.655471 1.914321 -0.699395
10345 H 1.798883 2.428605 0.757942
10346 H 0.953749 2.368736 -0.780328
10347 Rotational constants (GHz): 3.3294000 1.0160900 0.8374500
10348 Vibrational harmonic frequencies (cm-1):
10349 38.7932 77.6442 94.8878
10350 139.8178 200.9508 250.4780
10351 290.2145 327.8353 372.3155
10352 417.0661 482.9092 583.9397
10353 592.0907 785.2912 855.9910
10354 925.0215 1001.1203 1021.6723
10355 1060.4102 1069.2113 1106.8713
10356 1179.7885 1189.0477 1240.3022
10357 1286.7704 1294.3287 1310.4366
10358 1338.5068 1401.1275 1410.1341
10359 1425.0838 1483.4063 1498.2418
10360 1503.4465 1519.3107 1774.2744
10361 3045.0797 3053.4774 3085.9181
10362 3093.3019 3098.8228 3140.5612
10363 3143.5995 3217.9271 3868.9362
10364 Zero-point correction (Hartree): 0.139643
10365
10366 HOCHCCH3CH2CH2OO.Zgttt
10367 ~~~~~
10368 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45104760
10369 Electronic state : 2-A
10370 Cartesian coordinates (Angs):
10371 C -2.053189 0.599099 -0.225343
10372 C -1.317933 -0.453371 0.106343
10373 C 0.021659 -0.269816 0.769411
10374 C 1.093315 -0.063957 -0.283016
10375 O 2.369121 0.010541 0.392306
10376 O 3.344002 0.172234 -0.447333
10377 O -1.626086 1.874716 0.028101
10378 H -3.014937 0.501082 -0.715376
10379 C -1.764448 -1.849604 -0.202493
10380 H 0.006837 0.594417 1.432625
10381 H 0.267704 -1.151374 1.363568
10382 H 1.148329 -0.892628 -0.988741
10383 H 0.949566 0.869895 -0.824176
10384 H -2.309986 2.504765 -0.202678
10385 H -2.716664 -1.859774 -0.730790
10386 H -1.874359 -2.432432 0.714363
10387 H -1.029221 -2.367983 -0.822790
10388 Rotational constants (GHz): 3.3026200 1.0414100 0.8528300
10389 Vibrational harmonic frequencies (cm-1):
10390 35.2380 76.3247 96.6421
10391 134.4576 191.2049 232.7439
10392 239.3380 307.2442 337.3690
10393 392.6337 476.7409 587.3282
10394 593.6222 784.7065 865.6428
10395 884.6411 1000.0943 1019.4168
10396 1061.7149 1066.9938 1109.0101
10397 1185.1855 1197.6959 1224.3470

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10398      1291.9015      1296.4355      1313.5955
10399      1338.5135      1394.3958      1409.3311
10400      1422.4374      1481.1256      1490.5724
10401      1501.6101      1505.9176      1795.8774
10402      3045.8563      3073.8538      3087.7664
10403      3095.3978      3123.9218      3137.3848
10404      3150.5048      3187.7628      3918.4496
10405 Zero-point correction (Hartree): 0.139339
10406
10407 HOCHCCH3CH2CH2OO.Zlpmt
10408 ~~~~~
10409 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45151641
10410 Electronic state : 2-A
10411 Cartesian coordinates (Angs):
10412   C      1.709130      -0.226743      -0.323255
10413   C      0.795301      0.611124      0.149026
10414   C     -0.135776      0.198069      1.251049
10415   C     -1.593007      0.117408      0.813127
10416   O     -1.758911     -0.884811     -0.205799
10417   O     -1.500924     -0.409033     -1.388435
10418   O      1.864615     -1.493909      0.166624
10419   H      2.384572      0.062005     -1.120454
10420   C      0.651378      1.990819     -0.417397
10421   H      0.163263     -0.765875      1.658631
10422   H     -0.093554      0.929779      2.064129
10423   H     -2.229950     -0.209878      1.632958
10424   H     -1.960679      1.057390      0.405589
10425   H      2.506297     -1.971295     -0.360311
10426   H     -0.318260      2.112806     -0.904269
10427   H      1.422064      2.196291     -1.158778
10428   H      0.725858      2.746742      0.368080
10429 Rotational constants (GHz):      2.4927700      1.5844300      1.3619900
10430 Vibrational harmonic frequencies (cm-1):
10431      38.5354      95.0414      105.8187
10432     171.9951      201.3511      235.2032
10433     277.7503      319.9738      379.0078
10434     387.2898      530.7926      560.7205
10435     611.0331      778.5857      863.2415
10436     888.8703      973.1139      999.1345
10437    1033.8970     1072.5724     1078.9874
10438    1185.7482     1204.4895     1233.3178
10439    1243.8367     1315.2524     1326.5390
10440    1359.1635     1393.7535     1416.5175
10441    1419.5859     1471.0735     1483.8980
10442    1491.5533     1505.6461     1794.0954
10443    3046.5267     3048.6438     3096.0378
10444    3101.3892     3132.5287     3136.3074
10445    3157.4578     3183.7466     3922.8972
10446 Zero-point correction (Hartree): 0.139590
10447
10448 HOCHCCH3CH2CH2OO.Zlppt
10449 ~~~~~
10450 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45063142
10451 Electronic state : 2-A
10452 Cartesian coordinates (Angs):
10453   C      1.819552     -0.330908     -0.295792
10454   C      0.907450      0.556593      0.077349
10455   C     -0.151373      0.204237      1.084539
10456   C     -1.554601      0.556428      0.624112
10457   O     -1.857585     -0.056339     -0.648478
10458   O     -1.921103     -1.348537     -0.548453
10459   O      1.866143     -1.596525      0.219269
10460   H      2.588540     -0.082635     -1.018835
10461   C      0.908945      1.941423     -0.497872
10462   H     -0.110448     -0.857348      1.317768
10463   H      0.020190      0.753581      2.016356
10464   H     -2.305341      0.217826      1.336218
10465   H     -1.677583      1.621621      0.436252
10466   H      2.486993     -2.129793     -0.278425
10467   H      1.785546      2.109178     -1.121442
10468   H      0.908141      2.695031      0.293948
10469   H      0.024480      2.117110     -1.114549

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10470 Rotational constants (GHz):    2.5875400    1.5287200    1.1667400
10471 Vibrational harmonic frequencies (cm-1):
10472     25.7644         49.2800         143.5286
10473     167.0971        194.1854        236.4249
10474     278.4320        313.8739        362.1245
10475     405.1788        512.5127        567.3335
10476     624.1476        775.2516        848.2362
10477     891.7903        976.0122        984.2137
10478     1030.8415       1070.1423       1099.5314
10479     1187.0526       1205.5319       1235.7481
10480     1259.3822       1295.7444       1330.1128
10481     1357.1006       1401.9563       1418.2209
10482     1421.4405       1472.1631       1484.9152
10483     1492.4410       1509.2736       1800.8498
10484     3041.9735       3043.3968       3091.0038
10485     3098.1414       3136.7252       3141.4738
10486     3157.9596       3179.4653       3920.8526
10487 Zero-point correction (Hartree): 0.139512
10488
10489 HOCHCCH3CH2CH2OO.Zlptt
10490 ~~~~~
10491 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45028605
10492 Electronic state : 2-A
10493 Cartesian coordinates (Angs):
10494   C      -1.999039      0.048185      -0.452034
10495   C      -0.949007     -0.534742      0.109762
10496   C      -0.098358      0.197613      1.112093
10497   C       1.387094      0.049875      0.860514
10498   O       1.669237      0.580826     -0.453851
10499   O       2.902767      0.373239     -0.795236
10500   O      -2.371765      1.330853     -0.154412
10501   H      -2.623033     -0.474901     -1.167680
10502   C      -0.587990     -1.950106     -0.229491
10503   H      -0.365097      1.252916      1.129000
10504   H      -0.285842     -0.197648      2.115933
10505   H       1.981323      0.618614      1.574282
10506   H       1.718042     -0.987696      0.863734
10507   H      -3.072826      1.612212     -0.743375
10508   H      -1.339358     -2.404120     -0.873313
10509   H      -0.502860     -2.560579      0.673214
10510   H       0.371533     -2.003091     -0.748869
10511 Rotational constants (GHz):    3.1424900    1.1632600    1.0333300
10512 Vibrational harmonic frequencies (cm-1):
10513     31.1387         57.4874         108.7861
10514     193.6568        213.3292        241.8764
10515     280.4807        312.9197        337.6982
10516     395.8865        470.8439        561.6418
10517     628.8962        777.3126        841.8577
10518     886.3631        973.2580       1014.9300
10519     1045.7805       1075.9053       1095.4822
10520     1182.3439       1204.6011       1236.3738
10521     1270.4945       1298.6339       1322.9877
10522     1356.8018       1401.3671       1418.2395
10523     1424.0884       1470.8202       1485.0320
10524     1497.3576       1514.2876       1801.0893
10525     3043.5390       3045.9127       3091.0014
10526     3095.0292       3129.7364       3138.1720
10527     3148.3095       3183.1646       3920.9824
10528 Zero-point correction (Hartree): 0.139483
10529
10530 HOCHCCH3CH2CH2OO.Zpmtc
10531 ~~~~~
10532 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.44892315
10533 Electronic state : 2-A
10534 Cartesian coordinates (Angs):
10535   C       1.225893      1.208723      0.077346
10536   C       1.410632     -0.105668     -0.028430
10537   C       0.343809     -1.167296     -0.161927
10538   C      -1.005756     -0.923354      0.481733
10539   O      -1.808500     -0.110126     -0.414995
10540   O      -3.030709      0.014428      0.005569
10541   O       0.073591      1.925072      0.060217

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10542      H      2.079423      1.862132      0.207285
10543      C      2.814589      -0.644409      -0.047855
10544      H      0.183558      -1.430688      -1.213029
10545      H      0.736846      -2.074807      0.302965
10546      H      -1.558074      -1.849666      0.622762
10547      H      -0.932562      -0.385217      1.426376
10548      H      -0.657800      1.417526      -0.308304
10549      H      3.551357      0.153489      0.021877
10550      H      3.006202      -1.197355      -0.971065
10551      H      2.980993      -1.338376      0.779600
10552      Rotational constants (GHz):      3.6361300      1.2623400      0.9796100
10553      Vibrational harmonic frequencies (cm-1):
10554      19.6519      76.2984      145.2685
10555      207.5452      220.5482      267.3857
10556      294.9970      345.4938      349.8160
10557      448.9702      518.0648      563.8675
10558      624.1732      787.7658      832.0384
10559      925.1017      1004.3463      1016.8289
10560      1036.8728      1075.0445      1108.9520
10561      1184.7616      1207.4077      1234.1039
10562      1280.7706      1305.7384      1323.5230
10563      1391.9311      1412.2769      1419.7006
10564      1431.2856      1463.8643      1485.3120
10565      1500.8632      1503.7261      1772.1061
10566      3039.4061      3041.9396      3077.8754
10567      3087.7320      3096.2801      3142.7642
10568      3155.4912      3200.5034      3814.3305
10569      Zero-point correction (Hartree): 0.139977
10570
10571      HOCHCCH3CH2CH2OO.Zptpc
10572      ~~~~~
10573      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.45311898
10574      Electronic state : 2-A
10575      Cartesian coordinates (Angs):
10576      C      -1.337776      1.167113      0.144008
10577      C      -1.356078      -0.137348      -0.121298
10578      C      -0.086233      -0.827402      -0.549217
10579      C      0.933326      -0.932568      0.592911
10580      O      2.279812      -0.698882      0.113257
10581      O      2.414009      0.523274      -0.297511
10582      O      -0.265061      1.992419      0.069056
10583      H      -2.225219      1.700550      0.458868
10584      C      -2.610523      -0.947993      0.004703
10585      H      -0.305186      -1.817407      -0.945692
10586      H      0.390244      -0.264818      -1.356330
10587      H      0.747120      -0.187308      1.364677
10588      H      0.975110      -1.922479      1.039906
10589      H      0.546981      1.524914      -0.173442
10590      H      -2.881161      -1.403777      -0.950454
10591      H      -3.446566      -0.332927      0.334061
10592      H      -2.487689      -1.762045      0.723351
10593      Rotational constants (GHz):      3.2290800      1.3886100      1.0409300
10594      Vibrational harmonic frequencies (cm-1):
10595      70.9878      75.4034      181.5667
10596      196.5113      214.0703      295.3972
10597      296.6820      349.5854      401.9228
10598      527.4069      567.3644      592.9057
10599      606.8148      804.7100      871.8093
10600      930.0972      964.8976      1014.9382
10601      1033.8493      1073.4721      1075.2889
10602      1200.6918      1213.1969      1246.7772
10603      1288.4881      1302.6108      1325.8487
10604      1368.4561      1398.8044      1406.8098
10605      1423.7255      1482.5153      1494.0460
10606      1503.4373      1508.8030      1762.0564
10607      3042.6950      3059.0856      3090.0887
10608      3100.2097      3121.8062      3137.0446
10609      3166.2918      3210.1517      3747.9121
10610      Zero-point correction (Hartree): 0.140671
10611
10612
10613      TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Zh

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10614 ~~~~~
10615 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82290136
10616 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74780200
10617 T1 diagnostic: 0.027632
10618 E(MP2/Aug-CC-pVTZ) (Hartree): -420.68959699
10619 E(MP3/Aug-CC-pVTZ) (Hartree): -420.72757334
10620 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.70732238
10621 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74089315
10622 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15569713
10623 E(UHF/Aug-CC-pVTZ) (Hartree): -419.13522923
10624 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.42867123
10625 Electronic state : 2-A
10626 Cartesian coordinates (Angs):
10627 C -0.225486 1.261185 -0.046634
10628 C -1.014997 0.183361 0.288575
10629 C -0.363531 -0.892676 1.084760
10630 C 0.671914 -1.572693 0.150479
10631 O 1.553838 -0.605444 -0.371589
10632 O 0.868505 0.186239 -1.267089
10633 O 0.726247 1.683063 0.817033
10634 H -0.561307 1.977356 -0.789752
10635 C -2.230068 -0.138468 -0.510283
10636 H 0.163980 -0.494518 1.949035
10637 H -1.084801 -1.640822 1.415571
10638 H 1.293669 -2.278879 0.700038
10639 H 0.165493 -2.081734 -0.672729
10640 H 1.456220 2.067705 0.320778
10641 H -2.071248 -1.044599 -1.103181
10642 H -2.493173 0.669297 -1.190938
10643 H -3.084554 -0.328926 0.142964
10644 Rotational constants (GHz): 2.5274700 2.1855300 1.6981700
10645 Vibrational harmonic frequencies (cm-1):
10646 1607.7865 138.5662 158.4735
10647 173.2502 238.6210 275.5832
10648 323.6091 378.7176 434.5920
10649 442.6917 493.6161 596.9295
10650 629.7035 804.2215 874.7583
10651 916.7996 979.4077 996.0024
10652 1008.2363 1035.3478 1071.6900
10653 1083.2220 1187.9358 1218.4413
10654 1238.7452 1263.3048 1313.8985
10655 1321.9079 1364.1076 1396.5419
10656 1416.4615 1474.0568 1476.2740
10657 1485.8078 1494.4816 1580.6759
10658 3035.2683 3061.8629 3082.5547
10659 3086.4816 3128.0387 3140.5013
10660 3146.2336 3165.6929 3852.5523
10661 Zero-point correction (Hartree): 0.138936
10662
10663 TS.HOCHCCH3CH2CH2OO.cycHOCHCCH3CH2CH2OO.Zp
10664 ~~~~~
10665 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.82459295
10666 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.74901814
10667 T1 diagnostic: 0.026545
10668 E(MP2/Aug-CC-pVTZ) (Hartree): -420.69314458
10669 E(MP3/Aug-CC-pVTZ) (Hartree): -420.73006351
10670 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.71010883
10671 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.74269577
10672 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.15379424
10673 E(UHF/Aug-CC-pVTZ) (Hartree): -419.13410207
10674 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.42980062
10675 Electronic state : 2-A
10676 Cartesian coordinates (Angs):
10677 C 0.264881 1.272855 -0.006594
10678 C 1.007221 0.142348 -0.318909
10679 C 0.312532 -0.947264 -1.060958
10680 C -0.752520 -1.543270 -0.111180
10681 O -1.543094 -0.494526 0.416411
10682 O -0.761392 0.238666 1.298738
10683 O -0.752451 1.742482 -0.753384
10684 H 0.698749 2.032966 0.632045
10685 C 2.234549 -0.182764 0.460105

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10686      H      -0.185913      -0.568288      -1.954860
10687      H      1.007489      -1.731098      -1.362977
10688      H      -1.439278      -2.204613      -0.639172
10689      H      -0.278491      -2.076997      0.713862
10690      H      -1.414245      1.040369      -0.847075
10691      H      2.049751      -1.019782      1.140764
10692      H      2.570915      0.664760      1.054642
10693      H      3.046541      -0.481714      -0.206128
10694      Rotational constants (GHz):      2.5474400      2.2040800      1.7088700
10695      Vibrational harmonic frequencies (cm-1):
10696      i589.2412      148.4698      166.7360
10697      186.3656      244.1548      319.1700
10698      376.0619      425.6069      442.8246
10699      467.7017      500.0235      595.2845
10700      636.0796      795.4367      881.5022
10701      903.5941      973.4984      995.5179
10702      1005.8630      1031.3427      1069.6499
10703      1073.5617      1184.2861      1214.3732
10704      1262.1894      1269.6616      1312.8932
10705      1340.3680      1369.4256      1395.9655
10706      1416.7420      1475.8834      1481.4894
10707      1487.0234      1499.0715      1554.8259
10708      3035.0817      3069.2795      3071.9588
10709      3088.6041      3120.4220      3135.5229
10710      3141.8760      3197.3187      3731.1289
10711      Zero-point correction (Hartree): 0.139182
10712
10713
10714      TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Zc
10715      ~~~~~
10716      E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41388538
10717      Electronic state : 2-A
10718      Cartesian coordinates (Angs):
10719      O      -1.953200      0.709729      -0.843874
10720      H      -1.081665      1.382104      -0.240421
10721      C      -0.088042      1.598713      0.548536
10722      O      -2.176009      -0.349107      0.009137
10723      C      0.726041      0.401034      0.371658
10724      C      -1.110227      -1.286587      -0.097239
10725      C      0.083660      -0.903718      0.775320
10726      H      -0.639485      1.655303      1.485836
10727      H      0.370484      2.537415      0.253653
10728      C      1.930202      0.489202      -0.211689
10729      O      2.779922      -0.520931      -0.504577
10730      H      2.344672      1.445286      -0.502068
10731      H      -1.537182      -2.229748      0.245099
10732      H      -0.827718      -1.372330      -1.147986
10733      H      0.790085      -1.738092      0.760909
10734      H      -0.266085      -0.821483      1.807747
10735      H      2.391381      -1.367842      -0.267779
10736      Rotational constants (GHz):      3.5653900      1.3311700      1.1269500
10737      Vibrational harmonic frequencies (cm-1):
10738      i2089.6467      73.3864      144.2458
10739      252.2848      254.3888      295.2603
10740      348.6658      402.9211      446.4342
10741      498.5905      580.1781      589.5122
10742      631.7255      644.0132      781.6250
10743      877.4454      914.9174      957.1782
10744      1014.4730      1019.6854      1050.7670
10745      1089.1779      1119.6484      1187.5560
10746      1205.4486      1238.3923      1283.2037
10747      1302.1902      1329.7816      1360.7501
10748      1395.0488      1421.0353      1461.2732
10749      1480.4697      1489.5087      1522.7000
10750      1708.9601      3049.8736      3067.4395
10751      3089.7423      3096.8584      3127.0348
10752      3191.0539      3217.8402      3869.7027
10753      Zero-point correction (Hartree): 0.134600
10754
10755      TS.HOCHCCH3CH2CH2OO.1-6Hshift.a.Zt
10756      ~~~~~
10757      E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -420.80534605

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10758 E(CCSD/Aug-CC-pVTZ) (Hartree): -420.73022356
10759 T1 diagnostic: 0.025215
10760 E(MP2/Aug-CC-pVTZ) (Hartree): -420.67701734
10761 E(MP3/Aug-CC-pVTZ) (Hartree): -420.71328940
10762 E(PMP2/Aug-CC-pVTZ) (Hartree): -420.69250327
10763 E(PMP3/Aug-CC-pVTZ) (Hartree): -420.72444558
10764 E(PUHF/Aug-CC-pVTZ) (Hartree): -419.13115853
10765 E(UHF/Aug-CC-pVTZ) (Hartree): -419.11271414
10766 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41444056
10767 Electronic state : 2-A
10768 Cartesian coordinates (Angs):
10769 O -1.958174 0.689970 -0.852131
10770 H -1.100700 1.371563 -0.255314
10771 C -0.107906 1.612556 0.537761
10772 O -2.173687 -0.365790 0.004806
10773 C 0.708535 0.416080 0.378459
10774 C -1.093869 -1.293638 -0.088837
10775 C 0.092307 -0.898487 0.784797
10776 H -0.666306 1.675348 1.470149
10777 H 0.342921 2.551728 0.231718
10778 C 1.910845 0.483199 -0.203602
10779 O 2.663257 -0.627244 -0.435099
10780 H 2.336862 1.429326 -0.517010
10781 H -1.514879 -2.238742 0.254936
10782 H -0.805100 -1.382272 -1.137196
10783 H 0.835255 -1.693932 0.735464
10784 H -0.255891 -0.826943 1.818525
10785 H 3.517194 -0.379830 -0.793344
10786 Rotational constants (GHz): 3.557000 1.3494100 1.1376500
10787 Vibrational harmonic frequencies (cm-1):
10788 i2125.9030 73.8258 144.8234
10789 242.5021 249.7489 277.2143
10790 327.3942 345.9792 434.1601
10791 488.7135 585.1494 591.6852
10792 631.5893 647.1744 787.8479
10793 874.9232 885.4648 959.9891
10794 1010.0703 1018.8154 1048.2654
10795 1086.5471 1119.0282 1196.7306
10796 1207.3084 1240.5505 1248.2845
10797 1297.1116 1342.5440 1356.1230
10798 1389.9385 1421.1517 1460.2205
10799 1479.4794 1483.1757 1522.4986
10800 1730.6236 3059.4946 3072.5546
10801 3098.4729 3125.9796 3131.2908
10802 3185.5875 3190.1089 3913.8734
10803 Zero-point correction (Hartree): 0.134375
10804
10805 TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Zc
10806 ~~~~~
10807 E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41379943
10808 Electronic state : 2-A
10809 Cartesian coordinates (Angs):
10810 O -2.172289 0.392037 -0.380920
10811 H -1.317307 1.295368 -0.178889
10812 C -0.206735 1.814036 0.262017
10813 O -1.391242 -0.629704 -0.865925
10814 C 0.611405 0.617457 0.350430
10815 C -0.866227 -1.382095 0.221721
10816 C 0.006509 -0.517110 1.144415
10817 H -0.575528 2.200157 1.210717
10818 H 0.132768 2.587840 -0.419221
10819 C 1.731349 0.477639 -0.376591
10820 O 2.518254 -0.619024 -0.430998
10821 H 2.115330 1.275673 -0.997117
10822 H -1.684337 -1.853060 0.769799
10823 H -0.276027 -2.153903 -0.274322
10824 H 0.755735 -1.145670 1.632699
10825 H -0.605105 -0.096046 1.941020
10826 H 2.158878 -1.316387 0.126103
10827 Rotational constants (GHz): 3.132990 1.5781800 1.3050800
10828 Vibrational harmonic frequencies (cm-1):
10829 i2020.1929 84.2323 122.3046

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10830	255.4016	284.1316	331.6035		
10831	358.5807	390.2188	436.0733		
10832	500.3482	540.9057	592.0663		
10833	625.1512	680.8618	806.0707		
10834	858.9725	915.1989	955.7221		
10835	1018.3961	1026.9489	1073.6031		
10836	1080.3392	1124.4093	1184.5750		
10837	1219.6511	1273.1274	1280.3392		
10838	1294.0000	1322.8966	1362.4060		
10839	1385.3673	1413.3022	1475.8292		
10840	1489.2252	1497.7021	1511.2492		
10841	1696.0246	3056.3752	3066.6361		
10842	3098.0780	3108.6079	3127.2132		
10843	3190.4441	3221.2841	3857.8356		
10844	Zero-point correction (Hartree): 0.134853				
10845					
10846	TS.HOCHCCH3CH2CH2OO.1-6Hshift.b.Zt				
10847	~~~~~				
10848	E(UM062X/Aug-CC-pVTZ) (Hartree): -421.41432079				
10849	Electronic state : 2-A				
10850	Cartesian coordinates (Angs):				
10851	O	-2.168964	0.339083	-0.413326	
10852	H	-1.346566	1.264500	-0.213022	
10853	C	-0.251609	1.827108	0.230581	
10854	O	-1.354748	-0.671518	-0.861320	
10855	C	0.581625	0.646906	0.357829	
10856	C	-0.820534	-1.388581	0.250952	
10857	C	0.004495	-0.482768	1.174198	
10858	H	-0.642849	2.226174	1.164337	
10859	H	0.078148	2.591364	-0.466420	
10860	C	1.697711	0.483597	-0.364566	
10861	O	2.402750	-0.677734	-0.310386	
10862	H	2.081282	1.259780	-1.015882	
10863	H	-1.633378	-1.880493	0.788119	
10864	H	-0.184189	-2.137160	-0.219485	
10865	H	0.785654	-1.075760	1.647731	
10866	H	-0.630097	-0.067457	1.955818	
10867	H	3.189563	-0.617176	-0.854909	
10868	Rotational constants (GHz):		3.1095600	1.6159400	1.3292500
10869	Vibrational harmonic frequencies (cm-1):				
10870	i2067.2203	80.7269	124.9799		
10871	250.6726	266.1617	300.6704		
10872	356.4600	362.9145	392.0901		
10873	485.5641	539.6044	596.8966		
10874	623.0864	686.1959	811.2804		
10875	863.2249	869.4587	959.7051		
10876	1018.4655	1026.5592	1065.5672		
10877	1082.7047	1121.8113	1197.6638		
10878	1225.5901	1247.1964	1275.1394		
10879	1282.8936	1324.1650	1362.3878		
10880	1380.6641	1412.3404	1475.0907		
10881	1485.7310	1494.0201	1503.3449		
10882	1716.2163	3068.8958	3089.5693		
10883	3101.5952	3126.8974	3144.1488		
10884	3189.2682	3192.6181	3910.7707		
10885	Zero-point correction (Hartree): 0.134619				
10886					
10887					
10888					
10889					
10890					