

# Supporting Information to “Investigation of the oxidation of methyl vinyl ketone (MVK) by OH radicals in the atmosphere simulation chamber SAPHIR”

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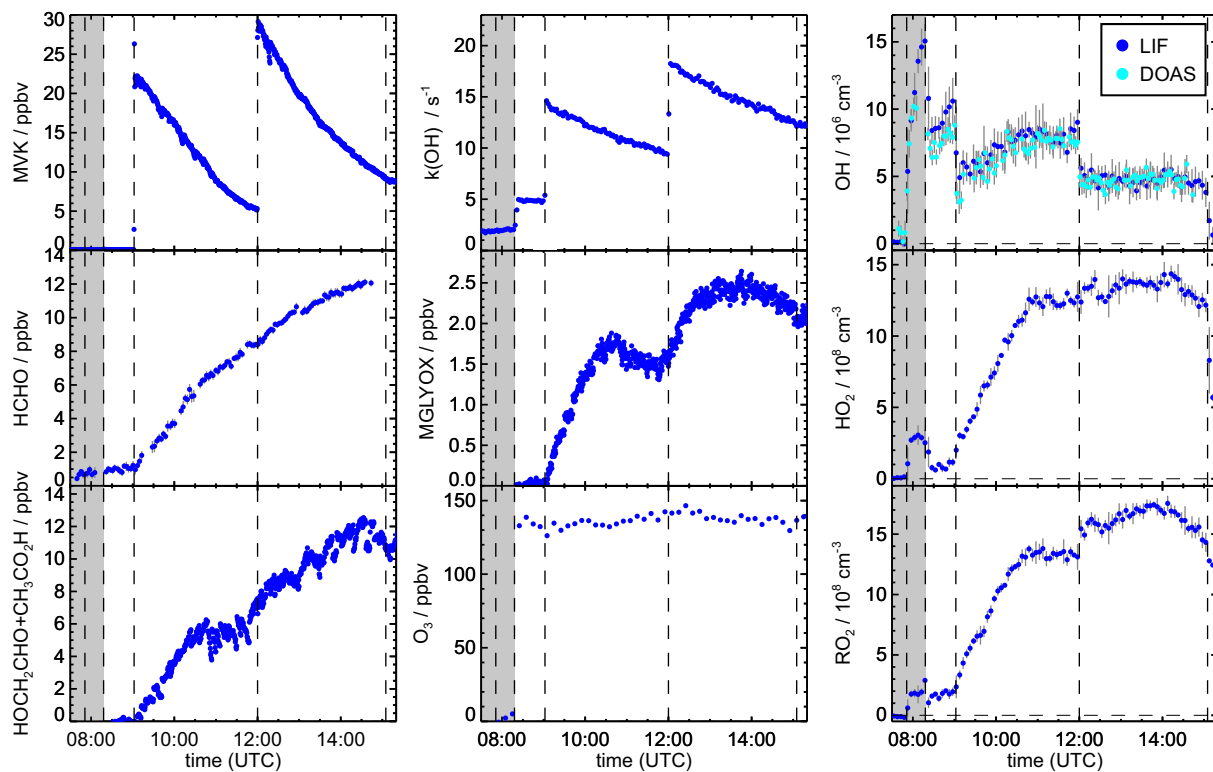
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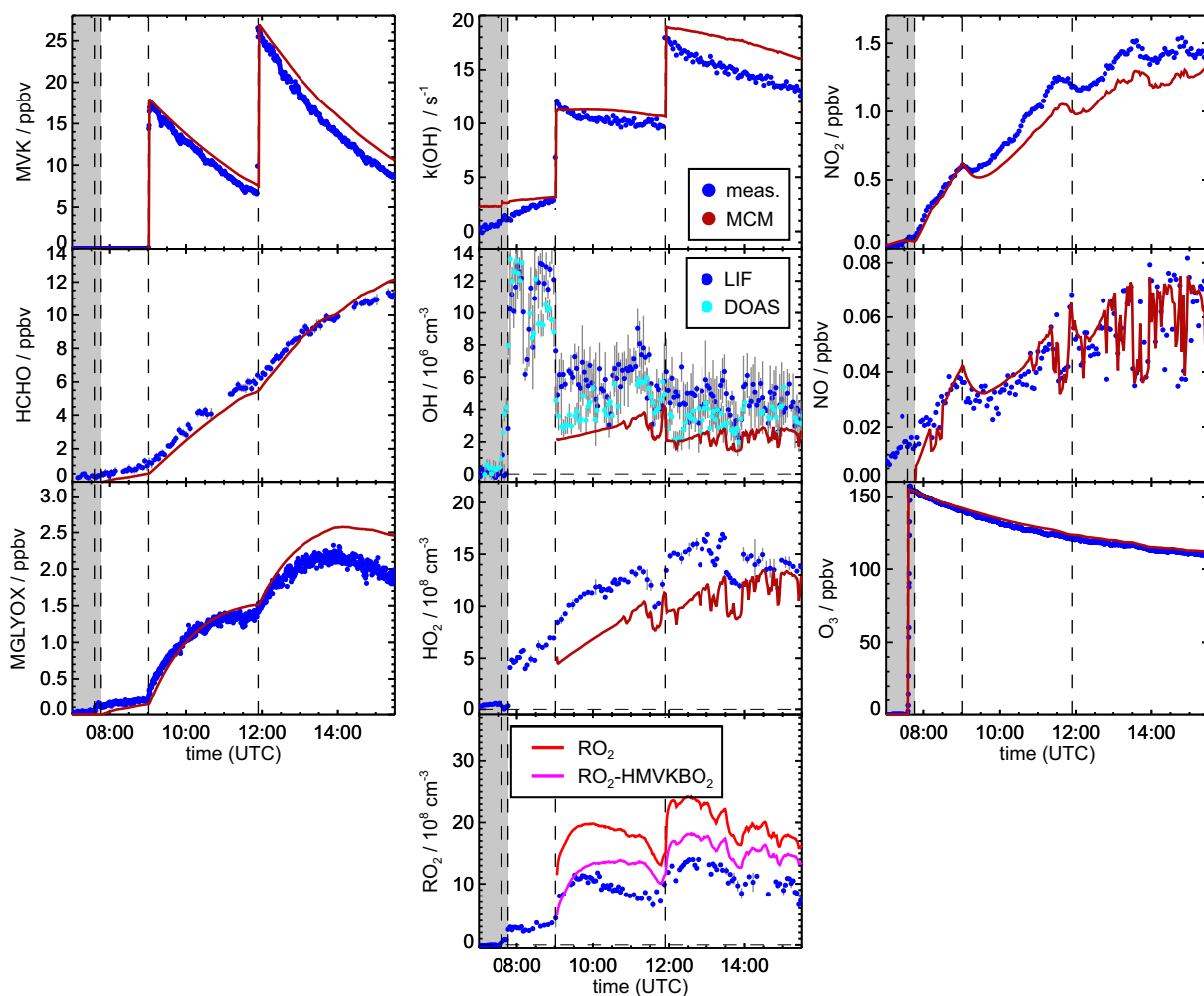
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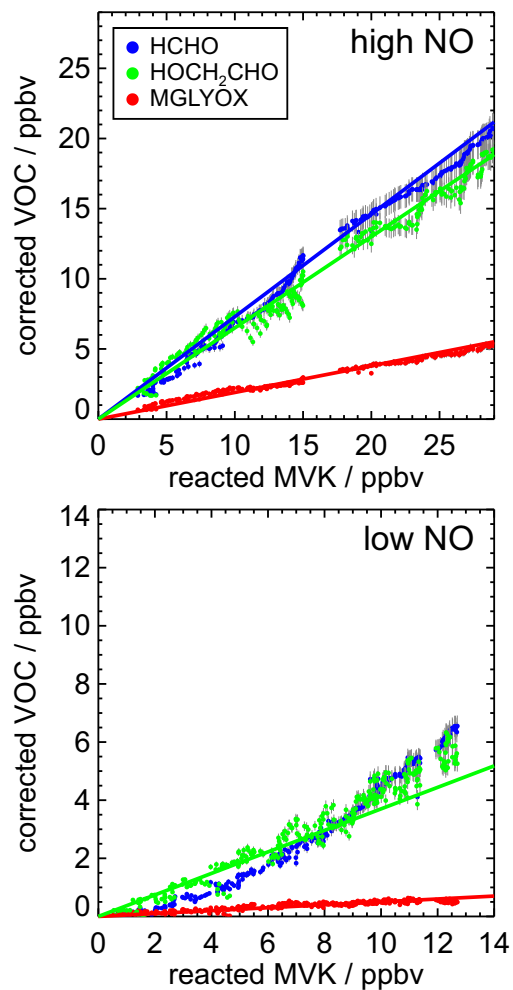
## 1 Additional Figures



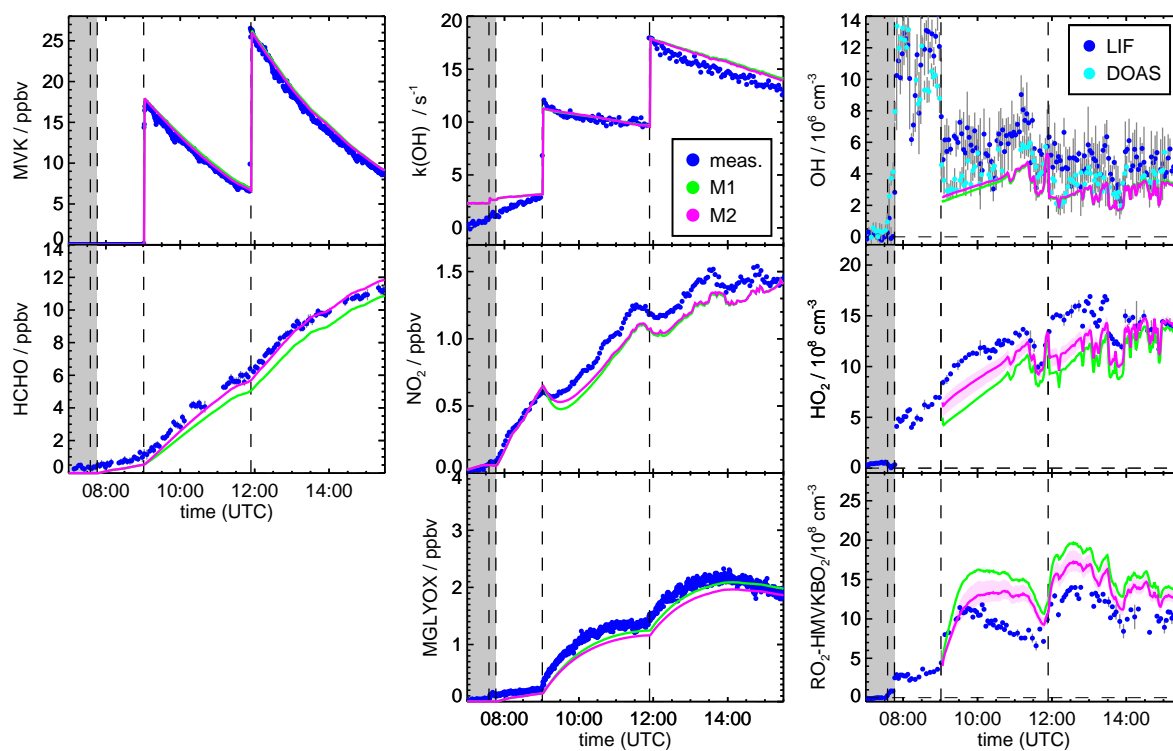
**Figure 1.** Time series of radicals, inorganic and organic species during the MVK photooxidation for the high NO experiment (17 May 2017). Dark shaded areas indicate the time before opening the chamber roof and vertical dashed line times when trace gases were injected into the chamber. Model calculations were not performed due to the lack of reliable  $\text{NO}_x$  measurements in this experiment. Approximately 8 ppbv  $\text{NO}_2$  was injected at the beginning of the experiment.



**Figure 2.** Time series of radicals, inorganic and organic species during the MVK photooxidation for the low NO experiment (23 June 2016) together with results from model calculations applying MCM. Dark shaded areas indicate the time before opening the chamber roof and vertical dashed line times when trace gases were injected into the chamber. Glycolaldehyde could not be derived from PTR-TOF-MS measurements for this experiment because no calibration was available.



**Figure 3.** Corrected product concentrations versus the MVK that reacted away. Corrections are applied to account for production not connected to the oxidation of MVK (small chamber source) and additional loss processes (reaction with OH, photolysis). The slope gives the product yield of the organic compound in the MVK reaction with OH



**Figure 4.** Time series of radicals, inorganic and organic species during the MVK photooxidation at low NO (experiment on 16 June 2016). Dark shaded areas indicate the time before opening the chamber roof and vertical dashed line times when trace gases were injected into the chamber. Model sensitivity runs include additional reaction pathways listed in Table 2 in the main paper.

## 2 Theoretical analysis of unimolecular reactions of the primary peroxy radicals

### 2.1 Theoretical methodology

The geometries of the reactants and transition states are optimized at the M06-2X/cc-pVTZ level of theory (Dunning, 1989; Zhao and Truhlar, 2008), exhaustively searching the entire conformer space afforded by the internal rotors. The lowest-lying structures, i.e those contributing 0.1 % to the population at 300 K, are then re-optimized at the M06-2X/aug-cc-pVTZ level of theory, and their harmonic vibrational wavenumbers are calculated and scaled by 0.971 (Alecú et al., 2010; Bao et al., 2017). Finally, the relative energies of the barrier heights are refined by CCSD(T)/aug-cc-pVxZ (x=D,T) single point energy calculations (Purvis and Bartlett, 1982) on the most stable conformer for each critical point, and extrapolated to the complete basis set using the aug-Schwartz4(DT) method described by (Martin, 1996). These CCSD(T)/CBS(DT)//M06-2X/aug-cc-pVTZ energies and rovibrational characteristics (see Table 1) are selected for theoretical kinetic calculations.

For the chemically most critical transition state, i.e. the 1,5-H-shift of the hydroxy-H-atom in the HMVKBO<sub>2</sub> radical, we have performed additional calculations using the B3LYP and M05-2X DFT functionals with various basis sets, as well as CBS-QB3, G3X, and G3SX calculations (Becke, 1992; Curtiss et al., 2001; Lee et al., 1988; Montgomery et al., 1999; Zhao et al., 2006). All quantum chemical calculations are performed using the Gaussian-09 program suite (Frisch et al., 2010).

The high-pressure rate coefficients for each of the elementary processes is calculated using multi-conformer canonical transition state theory, MC-CTST (Vereecken and Peeters, 2003; Zheng and Truhlar, 2013), as implemented in our in-house software. The rate is predicted based on a rigid rotor harmonic oscillator paradigm using M06 2X/aug-cc-pVTZ rovibrational characteristics and CCSD(T) barrier heights, where the population includes all conformers that contribute more than 0.1 %. The temperature range considered is 200 to 400 K. Tunnelling is included by asymmetric Eckart tunnelling (Johnston and Hecklen, 1962) with unscaled imaginary frequency, where the conformer-specific reactant and product for the lowest TS are discovered by IRC calculations. The tunnelling correction for the lowest TS is then used for all TS. For one reaction channel, we have also performed WKB tunnelling corrections (Garrett and Truhlar, 1979) based on the M06-2X/aug-cc-pVTZ minimum energy path.

### 2.2 Theoretical results

Table 1 lists barrier heights for the various reaction pathways studied in this work. For the 1,5-H-migration in HMVKBO<sub>2</sub>, we find that our calculations using a wide range of methodologies yield significantly higher energy barriers than the earlier predictions by Peeters et al. (2009). Partly, this is due to the methodologies used, where the B3LYP functional in particular is known to underestimate H-migration barrier heights, and yield TS geometries that are not ideal for single-point energy calculations. Another reason for the systematic underprediction in the earlier work is that the conformer space of the reactant was not examined exhaustively. Several lower-lying conformers were identified since, leading to a higher effective barrier height and hence lower rate coefficients for all reaction channels. The M05-2X functional seems to overpredict barrier heights somewhat, whereas the M06-2X functional leads to good agreement with higher-level single-point energy calculations. Extrapolation to

the complete basis set limit appears to have only a limited influence, though the computational cost prohibited us from applying basis sets above aug-cc-pVTZ.

The rate coefficient predictions are listed in Table 1 and Table 2. Compared to the earlier predictions by Peeters et al. (2009), we find rate coefficients that are about two orders of magnitude slower; this is mainly related to the higher energy barriers found at the levels of theory applied in this work, as discussed above. Tunnelling has a large contribution for the  $\alpha$ -OH 1,4-H-shift and  $-\text{CH}_3$  1,6-H-shift, with rate enhancements between  $10^2$  and  $10^4$ ; as expected,  $\text{HO}_2$  elimination is not affected much by tunnelling (factor 4 at 300 K) due to its high reduced mass and concomitant low imaginary wavenumber of  $\approx 1060i \text{ cm}^{-1}$ . Tunnelling has the lowest impact on the  $-\text{OH}$  1,5-H-migrations, with enhancements of a factor 2 to 3 only, with similar values obtained when using Eckart and WKB tunnelling corrections. This is related directly to the high endoenergeticity of the reaction, which leads to a broad energy profile (imaginary wavenumber  $\approx 1200i \text{ cm}^{-1}$ ) with a limited energy range accessible for tunnelling (reverse barrier only  $\approx 2.5 \text{ kcal mol}^{-1}$ ). Despite having the lowest energy barrier of the processes discussed here, its rate coefficient thus remains rather low. The highest rate coefficient is predicted for the 1,4-H-migration of the  $\alpha$ -OH hydrogen atom in  $\text{HMVKAO}_2$ . This channel is entropically slightly more favourable than a 1,5-H-shift, with less degrees of freedom for internal rotation converted to more rigid vibrations in the cyclic transition state. This channel also has the highest tunnelling factor,  $2 \times 10^4$  at 300 K, using asymmetric Eckart tunnelling.

The two fastest reactions, both H-migrations in the  $\text{HMVKAO}_2$  radicals lead to a product radical that is stabilized by vinyloxy resonance; delocalization of the unpaired electron only becomes active after the migrating H-atom is transferred to the peroxy group. It is conceivable that an Eckart potential energy barrier shape is not appropriate for these reactions. For example, allyl resonance has been shown to produce a non-Eckart energy profiles, with an minimum energy profile that cannot be reproduced accurately by the Eckart barrier shape (Nguyen et al., 2010; Peeters et al., 2009, 2014). To probe the reliability of the Eckart tunnelling, a zero-curvature tunnelling (ZCT) correction using the WKB methodology was implemented, based explicitly on the shape of the minimum energy path. In both cases, a significantly lower tunnelling correction was found, about an order of magnitude below the Eckart correction at 300 K (see Table 1). The ZCT values are expected to be a lower bound to the tunnelling correction, as corner-cutting will increase tunnelling. The effective rate coefficient is expected to be bracketed by the two tunnelling predictions. As our final rate coefficient prediction, we then employ the geometric average of the two tunnelling corrections, but with a large uncertainty of a factor 5. As none of the reactions studied theoretically in this work are contributing significantly to the oxidation of MVK, we choose not to perform additional calculations to reduce the uncertainty interval further.

**Table 1.** H-migration and HO<sub>2</sub> elimination in hydroxy–MVK–peroxy radicals. Barrier height  $E_b$  and the rate coefficient  $k$  at a temperature of 300 K are listed. aVxZ is used as abbreviation for aug-cc-pVxZ ( $x = D, T$ ); CBS(DT) refers to extrapolation to the complete basis set using the aug-Schwartz4(DT) method.

Reactant	Reaction class	Level of theory	$E_b$ kcal mol <sup>-1</sup>	$k(300)$ K s <sup>-1</sup>
<b>HMVKAO<sub>2</sub></b> CH <sub>3</sub> –C(=O)–CH(OH)–CH <sub>2</sub> OO•	–OH 1,5-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	22.0	$2.9 \times 10^{-4}$
		CCSD(T)/CB S(DT)//M06-2X/aVTZ	21.6	$5.0 \times 10^{-4}$
	$\alpha$ –OH 1,4-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	24.7	$1.3 \times 10^{-2}$
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	24.7	$1.5 \times 10^{-2}$
	–CH <sub>3</sub> 1,6-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	23.1	$7.7 \times 10^{-4}$ <sup>a</sup>
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	23.1	$1.5 \times 10^{-3}$
			$1.4 \times 10^{-3}$	
			$2.5 \times 10^{-4}$ <sup>a</sup>	
<b>HMVKBO<sub>2</sub></b> CH <sub>3</sub> –C(=O)–CH(OO•)–CH <sub>2</sub> OH	–OH 1,5-H-shift	B3LYP/6-31+G(d,p)	17.7 <sup>b</sup>	
		CBS-QB3	21.3 <sup>b</sup>	
		M05-2X/6-31+G(d,p)	24.3	
		M05-2X/aVDZ	24.0	
		M06-2X/cc-pVTZ	22.3	
		M06-2X/aug-cc-pVTZ	22.2	
		CBS-QB3//M05-2X/6-311G(d,p)	23.0	
		CBS-Q//QCISD/6-311G(d,p)	20.6 <sup>b</sup>	
		CBS-APNO	20.0 <sup>b</sup>	$7 \times 10^{-3}$ <sup>b,c</sup>
		CCSD(T)/aVDZ//M05-2X/aVDZ	24.2	
		CCSD(T)/CBS(DT)//M05-2X/6-311G(d,p)	22.4	
		G3X/B3LYP/6-31G(2df,p)	24.7	
		G3SX/B3LYP/6-31G(2df,p)	23.8	
		CCSD(T)/aVTZ//M06-2X/aVTZ	22.7	$6.0 \times 10^{-5}$
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	22.5	$8.8 \times 10^{-5}$
		$\alpha$ –OH 1,4-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	25.2
	CCSD(T)/CBS(DT)//M06-2X/aVTZ		25.1	$3.2 \times 10^{-5}$
–CH <sub>3</sub> 1,6-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	27.4	$3.6 \times 10^{-5}$	
	CCSD(T)/CBS(DT)//M06-2X/aVTZ	27.4	$3.8 \times 10^{-5}$	
HO <sub>2</sub> elimination	CCSD(T)/aVTZ//M06-2X/aVTZ	29.7	$9.5 \times 10^{-10}$	
	CCSD(T)/CBS(DT)//M06-2X/aVTZ	30.0	$6.1 \times 10^{-10}$	

<sup>a</sup>Based on WKB zero-curvature tunnelling

<sup>b</sup>Peeters et al. (2009)

<sup>c</sup>reported as  $0.01 \text{ s}^{-1}$  by Peeters et al. (2009)



**Table 2.** Temperature dependence of the rate coefficients between 200 and 400 K as a Kooij expression:  $k(T) = AT^n \exp(-E_a/T)$ . The rates are based on the CCSD(T)/CBS(DT)//M06-2X/aug-cc-pVTZ quantum chemical data.

Reactant	Reaction class	$A$ $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	$n$	$E_a$ K
<b>HMVKAO<sub>2</sub></b>	-OH 1,5-H-shift	$1.25 \times 10^{11}$	-0.03	9897
CH <sub>3</sub> -C(=O)-CH(OH)-CH <sub>2</sub> OO•	α-OH 1,4-H-shift	$4.12 \times 10^{-67}$	24.46	-2295
	-CH <sub>3</sub> 1,6-H-shift	$8.97 \times 10^{-29}$	12.54	4308
	all unimolecular	$7.4 \times 10^{-109}$	39.35	-5769
<b>HMVKBO<sub>2</sub></b>	-OH 1,5-H-shift	$7.13 \times 10^{11}$	-0.24	10571
CH <sub>3</sub> -C(=O)-CH(OO•)-CH <sub>2</sub> OH	α-OH 1,4-H-shift	$3.11 \times 10^{-81}$	29.64	-1790
	-CH <sub>3</sub> 1,6-H-shift	$2.05 \times 10^{-57}$	21.74	1083
	HO <sub>2</sub> elimination	$2.15 \times 10^{-45}$	18.86	7811
	all unimolecular	$6.71 \times 10^{-112}$	41.14	-3722

<sup>a</sup> Geometric average across the Eckart and WKB tunneling corrections

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## Quantum chemical data

### a. Population analysis at the M06-2X/cc-pVTZ level of theory

Relative energies in kcal mol<sup>-1</sup>

Population contribution in %

#### HMVKA02

Conformer	Erel	%
HMVKA02.mppt	0.34	23.2
HMVKA02.mpmt	0.00	19.4
HMVKA02.hptp	0.68	13.9
HMVKA02.mmpt	1.08	8.33
HMVKA02.mtmt	0.92	8.3
HMVKA02.hmtp	1.71	3.72
HMVKA02.hmmm	1.16	3.69
HMVKA02.mmtt	1.44	3.41
HMVKA02.mumt	1.57	3.21
HMVKA02.mmpm	1.50	2.98
HMVKA02.mmtm	1.92	2.55
HMVKA02.hpmm	1.35	1.86
HMVKA02.http	2.42	1.43
HMVKA02.mttm	2.91	1.13
HMVKA02.htm	2.64	1.05
HMVKA02.mttt	2.39	1
HMVKA02.mptt	3.01	0.394
HMVKA02.tmtm	4.17	0.127
HMVKA02.htm	4.16	0.0736
HMVKA02.hpmt	3.66	0.0597
HMVKA02.hpmp	3.50	0.0553
HMVKA02.htm	4.88	0.0445
HMVKA02.htm	4.38	0.0366
HMVKA02.tppp	4.82	0.0153
HMVKA02.hmmt	4.87	0.0114
HMVKA02.pmp	5.19	0.00546
HMVKA02.pppt	5.65	0.00484
HMVKA02.ptpt	6.12	0.00369
HMVKA02.pmpp	6.11	0.00227
HMVKA02.hppt	6.23	0.0019
HMVKA02.mmtp	6.11	0.00189
HMVKA02.hppp	6.20	0.00178
HMVKA02.mtp	6.18	0.00177
HMVKA02.ttp	6.40	0.00177
HMVKA02.tmpp	6.53	0.00124
HMVKA02.ttpt	7.10	0.000732
HMVKA02.htm	7.30	0.000598
HMVKA02.mtpp	7.02	0.000573
HMVKA02.pmpm	6.85	0.000273
HMVKA02.mppp	7.52	0.000266
HMVKA02.hppm	7.51	0.000231
HMVKA02.ptpm	8.17	0.000134
HMVKA02.cmp	8.88	5.95e-05
HMVKA02.mtm	8.78	2.12e-05
HMVKA02.mpp	8.39	1.97e-05
HMVKA02.mtpp	8.99	1.39e-05

**HMVKBO2**

Conformer	Erel	%
HMVKBO2.hhmt	0.00	52.5
HMVKBO2.pppp	1.38	6.02
HMVKBO2.ptmp	0.97	5.81
HMVKBO2.ptmm	1.38	4.12
HMVKBO2.pppt	1.39	3.99
HMVKBO2.ptmt	0.85	3.98
HMVKBO2.pmmp	1.28	3.87
HMVKBO2.pttp	1.46	3.6
HMVKBO2.hmmm	1.36	2.72
HMVKBO2.htpm	1.56	2.65
HMVKBO2.pppm	2.07	2.43
HMVKBO2.ptpp	1.55	2.2
HMVKBO2.pppt	2.32	1.38
HMVKBO2.pttm	2.02	1.09
HMVKBO2.lhmt	1.57	0.931
HMVKBO2.htpt	1.97	0.671
HMVKBO2.pptp	2.88	0.658
HMVKBO2.pppp	3.01	0.328
HMVKBO2.pppm	3.21	0.177
HMVKBO2.pppm	3.68	0.126
HMVKBO2.ltmp	3.14	0.125
HMVKBO2.lhmm	3.29	0.112
HMVKBO2.tppp	4.07	0.0611
HMVKBO2.pttt	3.98	0.0578
HMVKBO2.lppp	4.12	0.0529
HMVKBO2.tppm	4.07	0.0446
HMVKBO2.lppm	4.40	0.0426
HMVKBO2.lppt	4.21	0.0331
HMVKBO2.tmtp	4.67	0.0219
HMVKBO2.hmpm	5.92	0.0211
HMVKBO2.tmtm	4.74	0.0163
HMVKBO2.tmpm	5.21	0.0127
HMVKBO2.ttpm	4.95	0.0115
HMVKBO2.cmtp	5.39	0.00984
HMVKBO2.pmtp	5.50	0.00842
HMVKBO2.tmtt	5.43	0.00784
HMVKBO2.tptp	5.65	0.007
HMVKBO2.lttm	5.06	0.00699
HMVKBO2.lttp	5.17	0.00604
HMVKBO2.hmpt	5.60	0.00585
HMVKBO2.tmpp	5.70	0.0042
HMVKBO2.cmtm	5.52	0.00418
HMVKBO2.cmtt	5.54	0.00349
HMVKBO2.lmtt	5.48	0.00321
HMVKBO2.lmpt	5.82	0.0031
HMVKBO2.lptp	6.19	0.00168
HMVKBO2.tppm	6.61	0.000895
HMVKBO2.lpmt	7.21	0.000188

**TS.HMVKA02.14HshiftCH2OH**

Conformer	Erel	%
TS.HMVKA02.14HshiftCH2OH.dtS1	0.00	94.9
TS.HMVKA02.14HshiftCH2OH.utS1	1.79	4.93
TS.HMVKA02.14HshiftCH2OH.umSc	4.38	0.119
TS.HMVKA02.14HshiftCH2OH.dmSc	6.47	0.00315
TS.HMVKA02.14HshiftCH2OH.umS1	7.81	0.000285
TS.HMVKA02.14HshiftCH2OH.dmS1	8.06	0.000178
TS.HMVKA02.14HshiftCH2OH.dtSc	8.33	0.000139

TS.HMVKA02.14HshiftCH2OH.utSc 8.65 0.000139  
TS.HMVKA02.14HshiftCH2OH.upSc 9.08 5.71e-05

**TS.HMVKA02.15HshiftOH**

Conformer Erel %

-----  
TS.HMVKA02.15HshiftOH.md 0.05 50.1  
TS.HMVKA02.15HshiftOH.mu 0.00 49.9  
TS.HMVKA02.15HshiftOH.pd 5.66 0.00606

**TS.HMVKA02.16HshiftCH3**

Conformer Erel %

-----  
TS.HMVKA02.16HshiftCH3.a.Sp 0.00 97.9  
TS.HMVKA02.16HshiftCH3.b.Sp 2.45 1.76  
TS.HMVKA02.16HshiftCH3.a.Rm 3.52 0.237  
TS.HMVKA02.16HshiftCH3.a.Rt 4.53 0.0631  
TS.HMVKA02.16HshiftCH3.b.Rm 4.27 0.0517  
TS.HMVKA02.16HshiftCH3.b.Rt 6.17 0.00335  
TS.HMVKA02.16HshiftCH3.a.Sm 7.07 0.0011  
TS.HMVKA02.16HshiftCH3.b.Sm 9.61 1.33e-05

**TS.HMVKB02.14HshiftCH2OH**

Conformer Erel %

-----  
TS.HMVKB02.14HshiftCH2OH.umRlp 0.00 99.4  
TS.HMVKB02.14HshiftCH2OH.mmSht 3.58 0.482  
TS.HMVKB02.14HshiftCH2OH.umSlp 5.24 0.0493  
TS.HMVKB02.14HshiftCH2OH.mtShp 5.27 0.0324  
TS.HMVKB02.14HshiftCH2OH.mmRmp 5.50 0.0235  
TS.HMVKB02.14HshiftCH2OH.mmRlp 5.77 0.0217  
TS.HMVKB02.14HshiftCH2OH.mmRhm 5.65 0.0205  
TS.HMVKB02.14HshiftCH2OH.mtRhm 6.20 0.00761  
TS.HMVKB02.14HshiftCH2OH.utRhm 7.11 0.00238  
TS.HMVKB02.14HshiftCH2OH.mtShm 8.00 0.000734  
TS.HMVKB02.14HshiftCH2OH.umScm 8.10 0.000502  
TS.HMVKB02.14HshiftCH2OH.utScm 8.05 0.000494  
TS.HMVKB02.14HshiftCH2OH.mmScm 9.25 0.000384  
TS.HMVKB02.14HshiftCH2OH.mpSlp 10.27 2.29e-05  
TS.HMVKB02.14HshiftCH2OH.mtRct 9.96 2.03e-05  
TS.HMVKB02.14HshiftCH2OH.mpRhm 10.65 1.32e-05  
TS.HMVKB02.14HshiftCH2OH.utRct 10.53 7.49e-06

**TS.HMVKB02.15HshiftOH**

Conformer Erel %

-----  
TS.HMVKB02.15HshiftOH.t 0.00 56.5  
TS.HMVKB02.15HshiftOH.bis.t 0.46 43.4  
TS.HMVKB02.15HshiftOH.bis.c 4.10 0.15

**TS.HMVKB02.15HshiftCH3**

Conformer Erel %

-----  
TS.HMVKB02.15HshiftCH3.bis.pm 0.00 24.5  
TS.HMVKB02.15HshiftCH3.mp 0.34 20.2  
TS.HMVKB02.15HshiftCH3.tm 0.36 12.2  
TS.HMVKB02.15HshiftCH3.bis.mp 0.78 11.3  
TS.HMVKB02.15HshiftCH3.bis.pp 0.82 10.4  
TS.HMVKB02.15HshiftCH3.bis.pt 1.02 6.47  
TS.HMVKB02.15HshiftCH3.bis.tm 0.82 6.38  
TS.HMVKB02.15HshiftCH3.pm 0.96 5.97  
TS.HMVKB02.15HshiftCH3.mt 2.34 0.717  
TS.HMVKB02.15HshiftCH3.pp 2.40 0.626

TS.HMVKBO2.15HshiftCH3.bis.mm	2.63	0.614
TS.HMVKBO2.15HshiftCH3.bis.mt	2.74	0.466
TS.HMVKBO2.15HshiftCH3.mm	3.00	0.208
TS.HMVKBO2.15HshiftCH3.tp	4.81	0.0165
TS.HMVKBO2.15HshiftCH3.tt	5.65	0.00444

**TS.HMVKBO2.HO2elim**

Conformer	Erel %	
-----		
TS.HMVKBO2.HO2elim.cZm	0.00	95.1
TS.HMVKBO2.HO2elim.mEc	2.23	3.24
TS.HMVKBO2.HO2elim.cEc	3.29	0.723
TS.HMVKBO2.HO2elim.mEt	3.81	0.362
TS.HMVKBO2.HO2elim.mZt	4.12	0.19
TS.HMVKBO2.HO2elim.cEt	4.30	0.181
TS.HMVKBO2.HO2elim.pEt	4.50	0.101
TS.HMVKBO2.HO2elim.pZl	4.88	0.0572
TS.HMVKBO2.HO2elim.pZt	5.15	0.0356
TS.HMVKBO2.HO2elim.mZh	7.44	0.000766
TS.HMVKBO2.HO2elim.mZc	7.86	0.000462

## b. Selected energetic and rovibrational data on M06-2X/aug-cc-pVTZ geometries

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HMVKA02.mpmt
-----
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.36512897
E (CCSD/Aug-CC-pVDZ) (Hartree): -456.31464640
  T1 diagnostic: 0.022666
E (MP2/Aug-CC-pVDZ) (Hartree): -456.25443317
E (MP3/Aug-CC-pVDZ) (Hartree): -456.29038221
E (PMP2/Aug-CC-pVDZ) (Hartree): -456.25740556
E (PMP3/Aug-CC-pVDZ) (Hartree): -456.29218027
E (PUHF/Aug-CC-pVDZ) (Hartree): -454.93913768
E (UHF/Aug-CC-pVDZ) (Hartree): -454.93431610
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.75629660
E (CCSD/Aug-CC-pVTZ) (Hartree): -456.68407033
  T1 diagnostic: 0.021789
E (MP2/Aug-CC-pVTZ) (Hartree): -456.64334697
E (MP3/Aug-CC-pVTZ) (Hartree): -456.66793458
E (PMP2/Aug-CC-pVTZ) (Hartree): -456.64653130
E (PMP3/Aug-CC-pVTZ) (Hartree): -456.66981848
E (PUHF/Aug-CC-pVTZ) (Hartree): -455.04635905
E (UHF/Aug-CC-pVTZ) (Hartree): -455.04118977
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.39156917
Electronic state : 2-A
Cartesian coordinates (Angs):
  O      -1.094970      -1.312715      -0.935448
  O      -1.841554      -0.447335      -0.322886
  C      -1.230065      -0.002509      0.901537
  C       0.032742       0.803278      0.636344
  C      1.152820      -0.008357      -0.018623
  C      1.645135      -1.240473      0.684559
  H      -1.980220       0.635139      1.362652
  H      -1.035318      -0.876978      1.522377
  O      -0.266653       1.932801      -0.117518
  H       0.416194       1.093642      1.625733
  H       0.301111       1.900456      -0.902046
  O       1.631720       0.401010      -1.045504
  H       2.661406      -1.455052      0.366931
  H       1.603372      -1.124521      1.767264
  H       1.001325      -2.074415      0.405041
Rotational constants (GHz):    2.5687900    1.9095300    1.5178200
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  66.0531         93.3947         108.0521
  148.4992        219.8635         234.7154
  329.5622        406.3559         432.1195
  452.3623        523.9337         596.3041
  702.1359        769.9792         897.3103
  912.7623        963.8776         1019.8574
  1058.5634       1143.6388         1184.2557
  1204.1422       1258.8232         1268.9397
  1322.9307       1350.5397         1357.4521
  1399.3340       1427.6173         1437.4639
  1441.8474       1790.7276         2910.6599
  2987.7133       3008.6247         3055.8498
  3075.9330       3087.8866         3635.1552
Zero-point correction (Hartree): 0.115633

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HMVKA02.hmmm
-----
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38937903
Electronic state : 2-A
Cartesian coordinates (Angs):
  O      -1.937322       0.479021      -0.948134
  O      -1.432342      -0.701723      -0.751454
  C      -1.029459      -0.894725      0.624528
  C       0.131024       0.021538      0.981549
  C      1.274788      -0.216706      -0.019865
  C      1.691597       0.932166      -0.886584
  H      -1.893796      -0.697577      1.256253
  H      -0.723319      -1.935917      0.672723
  O      -0.241271       1.366752      1.115166
  H       0.506687      -0.311824      1.951697
  H      -0.911090       1.572476      0.452642
  O      1.772065      -1.311961      -0.071687
  H      2.502471       0.621653      -1.537597
  H       0.835456       1.263416      -1.478979
  H      1.986861       1.777429      -0.265645
Rotational constants (GHz):    2.7989200    1.6528800    1.5300100
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  44.3212         49.6524         150.6729
  178.3463        207.0611         257.3070
  332.0887        399.5535         424.3418
  484.2938        509.5258         532.2280
  677.8098        755.8077         849.4299
  945.7859        958.9797         1005.3203
  1038.2026       1138.4951         1203.0695
  1220.2100       1233.0585         1260.3784
  1314.9898       1343.8977         1351.6106

```



1380.0436	1418.5389	1427.3745
1432.2132	1794.9309	2977.1398
2994.1644	3019.4504	3041.2628
3093.6439	3097.0517	3701.3854

Zero-point correction (Hartree): 0.115536

HMVKAO2.hmmt

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38309537

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.436332	0.067965	0.784395
O	1.390100	-0.681042	0.601019
C	0.957413	-0.697036	-0.773050
C	-0.230137	0.233500	-0.938782
C	-1.341734	-0.216472	0.021769
C	-1.610676	0.633321	1.228201
H	1.794119	-0.378143	-1.389220
H	0.657294	-1.720906	-0.985679
O	0.222075	1.547232	-0.722541
H	-0.611216	0.088007	-1.954665
H	-0.449608	2.176615	-0.994268
O	-1.927902	-1.239882	-0.219428
H	-2.332254	0.134458	1.867296
H	-0.675338	0.818451	1.757035
H	-1.997035	1.607455	0.923124

Rotational constants (GHz): 2.9984100 1.4860700 1.4078800

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

41.6720	62.2229	78.1180
152.3784	185.1956	247.0477
257.0986	313.2798	433.9886
490.2720	507.7232	533.0408
655.6971	767.4048	861.9043
953.3239	954.1866	1000.3775
1042.3627	1140.7029	1171.5548
1199.6747	1227.4004	1270.5995
1313.4194	1344.5411	1349.8786
1358.5040	1416.4038	1422.6419
1428.1287	1796.2399	2967.5207
2979.9307	3020.0025	3040.9201
3089.1008	3095.9500	3775.0823

Zero-point correction (Hartree): 0.114836

HMVKAO2.hmtp

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38822723

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.689267	-0.141984	-0.768238
O	2.235471	-0.003363	0.441306
C	0.920311	-0.584796	0.581250
C	-0.077453	0.232779	-0.215723
C	-1.468041	-0.387781	-0.106411
C	-2.636174	0.552191	-0.120812
H	0.953936	-1.614788	0.238335
H	0.707677	-0.531944	1.647059
O	-0.132845	1.571269	0.220522
H	0.204850	0.178166	-1.274819
O	0.723804	1.983445	0.075796
O	-1.579245	-1.585526	-0.038075
H	-3.558222	-0.019550	-0.148424
H	-2.600275	1.185039	0.766028
H	-2.564809	1.222109	-0.977914

Rotational constants (GHz): 4.0708900 1.2399700 1.0458300

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

33.1847	61.5060	114.4529
162.7090	185.0760	263.9730
300.5009	336.2959	405.8084
457.8591	511.5307	568.7287
599.3044	793.8402	886.3408
914.4605	967.1365	1006.7507
1095.1418	1145.4205	1179.5804
1190.9687	1213.9713	1257.7062
1293.6214	1350.9393	1357.0994
1390.8257	1420.8311	1426.0005
1434.8168	1792.0838	2942.9012
2987.1132	3026.4237	3048.5223
3095.9960	3098.1367	3754.3004

Zero-point correction (Hartree): 0.115133

HMVKAO2.hpmm

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38912749

Electronic state : 2-A

Cartesian coordinates (Angs):

O	1.070887	-0.172680	1.441916
O	1.912846	-0.371452	0.478247
C	1.287710	-0.418494	-0.832484
C	0.003316	0.385640	-0.880161
C	-1.139945	-0.359259	-0.175454
C	-2.060063	0.440764	0.699298

H	2.042801	-0.009065	-1.498897
H	1.089488	-1.464560	-1.061345
O	0.176201	1.716971	-0.473664
H	-0.290569	0.421520	-1.933015
H	0.444119	1.721515	0.451223
O	-1.286545	-1.534508	-0.393279
H	-2.880346	-0.190035	1.026687
H	-1.509923	0.810724	1.565163
H	-2.428790	1.311359	0.157231

Rotational constants (GHz): 2.8090900 1.7425700 1.5973700  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

55.3243	93.6720	112.4145
167.5204	213.5378	254.6567
321.6953	398.5843	415.4629
463.4280	512.8632	560.2389
716.6765	764.9209	853.2719
906.7812	957.6689	1002.6551
1050.5814	1123.0351	1189.1198
1209.2447	1238.6997	1268.4701
1292.6619	1351.2038	1361.6327
1374.5378	1419.7543	1434.8696
1441.1957	1792.1344	2985.4445
2986.8555	3017.5826	3049.7165
3078.8609	3095.4665	3736.1443

Zero-point correction (Hartree): 0.115594

HMVKA02.hpmp

-----  
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38552622  
Electronic state : 2-A  
Cartesian coordinates (Angs):

O	1.059916	-1.078945	1.111721
O	1.893560	-0.429269	0.360708
C	1.288262	-0.028536	-0.884049
C	-0.005551	0.739309	-0.662202
C	-1.149157	-0.213793	-0.291927
C	-1.913281	0.060526	0.965879
H	2.049716	0.590442	-1.356737
H	1.092226	-0.915910	-1.485133
O	0.111159	1.747414	0.311050
H	-0.290009	1.151837	-1.637835
H	0.824110	2.348586	0.081311
O	-1.405935	-1.107461	-1.056323
H	-2.671586	-0.704590	1.098082
H	-1.225801	0.081545	1.810464
H	-2.369896	1.049140	0.906394

Rotational constants (GHz): 2.7161900 1.7574900 1.6038000  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

66.0101	101.0653	117.4223
173.0801	184.6929	221.3036
246.5522	306.4058	415.9394
468.4214	511.0148	548.6454
714.9243	756.6897	873.2843
915.0342	961.4854	1017.7253
1046.4212	1138.2614	1164.0215
1207.1803	1221.4494	1253.2902
1304.6069	1351.4107	1356.3746
1383.4674	1419.8776	1428.5781
1443.7143	1795.9519	2940.7250
2987.8783	3004.8792	3052.7252
3062.7606	3097.4692	3765.8756

Zero-point correction (Hartree): 0.115027

HMVKA02.hpmt

-----  
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38501930  
Electronic state : 2-A  
Cartesian coordinates (Angs):

O	-1.037225	-1.240566	-0.944952
O	-1.875425	-0.462590	-0.336476
C	-1.306495	0.102169	0.862666
C	-0.000372	0.817976	0.583209
C	1.131540	-0.186907	0.311012
C	1.845849	-0.110581	-1.006992
H	-2.064260	0.799602	1.210344
H	-1.146444	-0.699378	1.582094
O	-0.230169	1.747866	-0.447059
H	0.274379	1.312042	1.522459
H	0.519914	2.340822	-0.528612
O	1.433032	-0.951761	1.189803
H	2.519214	-0.957164	-1.097153
H	1.126977	-0.090444	-1.823813
H	2.425384	0.814989	-1.055212

Rotational constants (GHz): 2.6665500 1.7800900 1.6071900  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

47.0286	106.0288	119.0716
174.4696	191.6539	214.1697
238.8637	298.4593	415.0036
478.4024	512.8252	542.1990
705.3374	753.2893	876.1455
917.5224	963.1422	1010.7247

1054.9147	1137.3928	1169.1519
1202.5621	1229.8541	1267.2414
1314.5091	1345.4941	1359.7238
1369.4588	1421.6331	1431.9671
1437.7506	1795.0989	2951.3054
2973.4202	3017.6621	3047.0486
3082.0968	3097.7616	3779.6146

Zero-point correction (Hartree): 0.115081

HMVKAO2.hptp

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38999356

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.699607	0.512275	-0.036585
O	2.210113	-0.684949	-0.144115
C	0.879355	-0.779969	0.408919
C	-0.078411	0.148458	-0.314103
C	-1.521643	-0.313024	-0.083523
C	-2.556930	0.757192	0.087451
H	0.591189	-1.817234	0.266537
H	0.938316	-0.528310	1.467751
O	0.045036	1.490240	0.084297
H	0.097733	0.040478	-1.394058
H	0.981541	1.718469	0.063581
O	-1.775231	-1.490456	-0.077619
H	-3.540531	0.301642	0.138511
H	-2.343354	1.323748	0.993759
H	-2.495319	1.468390	-0.736368

Rotational constants (GHz): 4.2678100 1.2729400 1.0187700

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

38.9724	53.4639	150.1838
163.8450	205.0663	281.8801
310.9090	395.0146	442.9044
453.2489	519.5213	555.0789
601.7913	796.5157	886.0312
951.2771	961.9388	1003.8463
1069.5111	1153.0967	1193.4934
1202.6976	1217.5372	1260.5183
1307.8089	1350.9797	1352.1497
1391.1871	1420.0396	1425.0613
1439.3784	1792.9337	2918.1379
2988.5289	3010.3327	3049.6105
3094.2506	3099.5669	3713.9030

Zero-point correction (Hartree): 0.115486

HMVKAO2.htm

-----

E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38653665

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.739667	-0.501148	0.645118
O	1.487379	-0.177987	0.544921
C	1.061438	-0.068166	-0.832814
C	-0.320307	0.549531	-0.775552
C	-1.298264	-0.431433	-0.106692
C	-2.067269	0.047283	1.088378
H	1.770834	0.575101	-1.348711
H	1.035974	-1.065885	-1.265300
O	-0.302071	1.829644	-0.194543
H	-0.673514	0.670971	-1.801138
H	0.201690	1.799237	0.625009
O	-1.408505	-1.536307	-0.571137
H	-2.758459	-0.726245	1.407234
H	-1.369517	0.277856	1.896404
H	-2.592356	0.972059	0.851711

Rotational constants (GHz): 2.9987400 1.4181000 1.2484800

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

38.7405	53.7813	110.4226
175.7166	185.8578	250.5812
319.1218	330.4689	400.8328
465.7606	507.9985	529.7145
679.3516	736.2681	895.4801
929.2844	960.3914	1028.4491
1042.7013	1122.9171	1187.6321
1214.9293	1248.2141	1260.3485
1293.2981	1340.5126	1351.8391
1370.2210	1420.6334	1430.4574
1442.6362	1796.4649	2979.0797
3007.2382	3018.8053	3042.7534
3083.7883	3097.3238	3740.2881

Zero-point correction (Hartree): 0.115176

HMVKAO2.htm

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38441394

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.721512	-0.585591	0.569285
O	1.462073	-0.280977	0.522404
C	1.067055	0.124200	-0.802731

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C      -0.346301      0.663454     -0.706114
C      -1.264377     -0.436870     -0.158634
C      -1.938856     -0.197437      1.155835
H       1.774066      0.880735     -1.143447
H       1.100314     -0.749551     -1.451644
O      -0.441093      1.804800      0.112712
H      -0.690759      0.865103     -1.725873
H       0.124918      2.501165     -0.229306
O      -1.385337     -1.444419     -0.805559
H      -2.534644     -1.065626      1.418431
H      -1.179431     -0.000743      1.913648
H      -2.556821      0.698332      1.097318
Rotational constants (GHz):  2.9134900    1.4499700    1.2755500
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  44.4456          52.6062          102.5225
 161.9025         175.1203          231.0717
 255.8608         316.6670          390.6067
 476.7800         498.6264          532.1321
 681.8647         753.0173          888.8975
 936.1481         963.8890         1023.2228
1052.1217         1133.7905         1161.1244
1209.0530         1224.5081         1260.4553
1309.7224         1346.7688         1350.9645
1378.1331         1419.0953         1423.3386
1443.2917         1798.2646         2960.0752
2986.0737         2998.6409         3048.3240
3061.8767         3099.1163         3767.1540
Zero-point correction (Hartree): 0.114770

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HMVKAO2.htmt

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38381153
Electronic state : 2-A
Cartesian coordinates (Angs):
  O      2.701373      -0.656466      0.469981
  O      1.454874     -0.300516      0.478134
  C      1.056499      0.243363     -0.797035
  C      -0.366605      0.735364     -0.650406
  C      -1.248065     -0.433165     -0.179926
  C      -1.768594     -0.398828      1.226334
  H       1.732197      1.060620     -1.039683
  H      1.115319     -0.553397     -1.535871
  O      -0.355156      1.840455      0.222587
  H      -0.714710      1.006524     -1.651548
  H      -1.191249      2.308736      0.171664
  O      -1.464178     -1.330739     -0.951850
  H      -2.280190     -1.331079      1.443518
  H      -0.940123     -0.233202      1.915036
  H      -2.455957      0.439529      1.352268
Rotational constants (GHz):  2.8243500    1.4707200    1.2985900
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  52.1938          62.7039          107.5678
 157.4896         165.9704          225.3072
 248.2663         308.4853          386.4867
 474.5078         504.3817          530.8604
 668.9022         758.2235          896.5823
 932.5623         963.8940         1021.4739
1044.7157         1131.7217         1190.7293
1204.1415         1231.0694         1261.0120
1301.7642         1342.6621         1352.9531
1370.8932         1417.2942         1428.4291
1437.7623         1796.9992         2971.8308
2981.0543         3014.9580         3043.2169
3078.9689         3096.8454         3777.5855
Zero-point correction (Hartree): 0.114829

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HMVKAO2.htm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38266297
Electronic state : 2-A
Cartesian coordinates (Angs):
  O      3.219527     -0.288710      0.231858
  O      2.152491      0.163439     -0.350869
  C      0.964239     -0.436054      0.197581
  C      -0.222826      0.314435     -0.361520
  C      -1.521877     -0.446386     -0.058657
  C      -2.761562      0.382039      0.121080
  H       0.935249     -1.484162     -0.089481
  H      1.020378     -0.357190      1.285109
  O      -0.271128      1.661713      0.045799
  H      -0.136010      0.337627     -1.452756
  H      -0.050674      1.729702      0.979118
  O      -1.519919     -1.649571     -0.005717
  H      -3.628007     -0.270885      0.150772
  H      -2.691033      0.951059      1.048904
  H      -2.845521      1.114684     -0.681145
Rotational constants (GHz):  4.3537400    1.1208100    0.9288800
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  19.0722          50.0898          84.4035
 152.2733         158.1273         212.7663
 261.8703         312.2695         391.9313

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398.3336	516.4385	551.5671
608.6673	790.1938	883.2225
939.5702	984.8704	1033.5761
1044.6022	1156.1051	1169.0321
1190.4175	1254.8563	1267.2915
1284.5482	1348.2583	1355.5589
1377.1209	1417.4589	1428.4307
1452.3995	1792.1516	2970.4463
2986.0995	2991.6522	3046.5927
3072.1493	3096.6880	3750.5292

Zero-point correction (Hartree): 0.114499

HMVKAO2.http

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38707391  
Electronic state : 2-A  
Cartesian coordinates (Angs):

O	3.194829	-0.281486	0.314191
O	2.131532	0.141518	-0.297241
C	0.934262	-0.494408	0.198889
C	-0.219022	0.268103	-0.416096
C	-1.539285	-0.420504	-0.069197
C	-2.696588	0.458513	0.297133
H	0.935982	-1.537154	-0.108351
H	0.936476	-0.409161	1.284570
O	-0.257439	1.606023	0.022483
H	-0.128234	0.219653	-1.509184
H	0.565605	2.038055	-0.224116
O	-1.605195	-1.621778	-0.123115
H	-3.580925	-0.153413	0.442468
H	-2.456403	1.015304	1.203005
H	-2.858518	1.202273	-0.483306

Rotational constants (GHz): 4.3828500 1.1309400 0.9418900  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

23.5481	56.1398	101.3017
146.1245	167.1784	265.1543
308.7196	343.2977	397.4449
420.2489	511.1563	551.9320
601.5554	788.8277	888.2451
945.3259	975.8449	1021.8631
1077.2863	1152.8319	1179.2898
1193.0603	1216.5560	1256.3249
1291.8255	1352.4573	1358.1275
1387.5093	1419.6446	1425.2936
1445.6919	1794.0651	2933.0239
2987.2803	3013.2904	3047.7659
3083.2144	3099.3731	3753.0309

Zero-point correction (Hartree): 0.114919

HMVKAO2.mmt

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38884339  
Electronic state : 2-A  
Cartesian coordinates (Angs):

O	-2.456112	-0.245068	-0.784754
O	-1.366082	-0.833298	-0.390233
C	-0.947786	-0.406692	0.918375
C	0.220457	0.559815	0.786758
C	1.305353	-0.002494	-0.132746
C	1.826302	-1.381718	0.150072
H	-1.791016	0.082406	1.398825
H	-0.660752	-1.310683	1.455014
O	-0.218583	1.797020	0.331383
H	0.671196	0.653785	1.785604
H	0.294461	2.004830	-0.463148
O	1.696346	0.674040	-1.048704
H	2.780116	-1.521966	-0.349335
H	1.925472	-1.557448	1.220930
H	1.110024	-2.105936	-0.244178

Rotational constants (GHz): 2.9169000 1.5753800 1.3408700  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

18.8404	74.9240	87.6395
158.1056	188.4142	260.3961
336.8073	402.6684	430.5932
469.7190	511.2312	578.8863
676.5003	770.3057	872.9785
949.1313	965.8152	1015.7850
1042.1477	1146.1248	1174.8874
1201.1619	1240.0734	1287.8877
1319.1635	1344.6046	1353.7789
1387.3394	1419.9918	1435.6573
1440.3832	1795.9622	2912.3961
2977.9095	3009.4804	3043.2612
3080.8192	3091.0123	3644.0730

Zero-point correction (Hartree): 0.115238

HMVKAO2.mmpm

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38911290  
Electronic state : 2-A  
Cartesian coordinates (Angs):

O	2.068339	0.577820	-0.577347
O	1.927989	-0.438918	0.221202
C	0.775860	-1.222851	-0.124517
C	-0.515412	-0.692072	0.511517
C	-0.866244	0.701149	-0.014617
C	-0.262737	1.903472	0.646867
H	0.681535	-1.236357	-1.208878
H	0.970225	-2.221929	0.257788
O	-1.524004	-1.601567	0.180929
H	-0.397280	-0.648354	1.597459
H	-2.047407	-1.186089	-0.520463
O	-1.668411	0.779647	-0.912419
H	-0.112083	2.690533	-0.086971
H	-0.983270	2.255499	1.389260
H	0.668165	1.672647	1.157391

Rotational constants (GHz): 2.6359600 1.8528400 1.2856600  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

38.1236	67.0561	94.2133
162.1301	210.6093	285.9233
314.5478	349.1289	429.4013
461.1153	549.8518	597.6666
634.2725	756.4624	931.3650
962.4828	994.0660	1019.0486
1077.8145	1115.5951	1172.4412
1198.5848	1254.7533	1269.3855
1305.9176	1341.6692	1354.7727
1398.8560	1431.1245	1436.6890
1442.3620	1786.1864	2978.4616
2981.9621	3015.9064	3055.7621
3084.0487	3097.1041	3639.4080

Zero-point correction (Hartree): 0.115659

HMVKA02.mmpm

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38954508

Electronic state : 2-A

Cartesian coordinates (Angs):

O	2.533484	0.419224	-0.416863
O	1.880747	-0.380553	0.370813
C	0.782242	-1.042780	-0.283808
C	-0.533653	-0.693923	0.415262
C	-1.045974	0.694930	0.037005
C	-0.168921	1.880684	0.302244
H	0.791553	-0.759197	-1.334095
H	0.946468	-2.113515	-0.177538
O	-1.468982	-1.668053	0.070066
H	-0.351218	-0.693791	1.497601
H	-2.231592	-1.198774	-0.300362
O	-2.137741	0.783278	-0.469301
H	-0.767245	2.786531	0.279407
H	0.355981	1.780636	1.251060
H	0.593828	1.933478	-0.478020

Rotational constants (GHz): 3.0248900 1.5914300 1.1301200  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

47.2227	81.7230	111.8291
176.3485	212.9832	291.7050
306.0841	357.5337	435.4580
475.1429	524.9477	578.5752
636.8265	747.0483	928.0651
965.4282	973.5848	1023.3643
1088.3998	1137.7454	1180.1716
1189.8514	1261.9081	1278.5302
1293.0466	1349.6656	1361.4048
1397.8028	1426.4253	1436.1664
1448.3632	1784.2316	2935.4829
2980.5208	3011.3493	3046.3715
3076.7360	3092.9530	3631.0164

Zero-point correction (Hartree): 0.115626

HMVKA02.mmtm

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38932208

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-2.588263	0.630343	-0.635974
O	-2.235831	-0.076676	0.392311
C	-0.871638	0.200058	0.764915
C	0.081702	-0.378876	-0.269571
C	1.494266	0.158953	-0.069042
C	1.700706	1.646863	-0.098639
H	-0.778171	1.280818	0.856919
H	-0.734733	-0.292725	1.725260
O	0.065178	-1.769791	-0.221795
H	-0.256946	-0.020200	-1.251541
H	0.981753	-2.056794	-0.099272
O	2.396164	-0.623351	0.097473
H	1.557471	2.040339	0.909986
H	2.718752	1.864652	-0.408459
H	0.983671	2.137712	-0.754991

Rotational constants (GHz): 3.5968600 1.3035900 1.0560700  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

51.1625	71.8067	120.6617
154.8383	196.1412	262.0396
325.3506	389.0274	411.4303
456.7741	547.2398	561.4819
629.1568	820.1374	900.2869
931.2981	967.4570	1006.7449
1089.0421	1141.3179	1188.0387
1211.0296	1236.9668	1279.2870
1311.7761	1351.4861	1362.5997
1393.7405	1427.5288	1429.1911
1441.7931	1788.4735	2932.5124
2979.0855	3011.2719	3045.6536
3077.3424	3088.6399	3646.5822

Zero-point correction (Hartree): 0.115519

HMVKA02.mppt

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E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.36447322  
E (CCSD/Aug-CC-pVDZ) (Hartree): -456.31424675  
T1 diagnostic: 0.022692  
E (MP2/Aug-CC-pVDZ) (Hartree): -456.25346708  
E (MP3/Aug-CC-pVDZ) (Hartree): -456.28996447  
E (PMP2/Aug-CC-pVDZ) (Hartree): -456.25635073  
E (PMP3/Aug-CC-pVDZ) (Hartree): -456.29171757  
E (PUHF/Aug-CC-pVDZ) (Hartree): -454.94047181  
E (UHF/Aug-CC-pVDZ) (Hartree): -454.93576234  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.75578191  
E (CCSD/Aug-CC-pVTZ) (Hartree): -456.68380725  
T1 diagnostic: 0.021786  
E (MP2/Aug-CC-pVTZ) (Hartree): -456.64247456  
E (MP3/Aug-CC-pVTZ) (Hartree): -456.66766572  
E (PMP2/Aug-CC-pVTZ) (Hartree): -456.64556846  
E (PMP3/Aug-CC-pVTZ) (Hartree): -456.66950140  
E (PUHF/Aug-CC-pVTZ) (Hartree): -455.04765520  
E (UHF/Aug-CC-pVTZ) (Hartree): -455.04259446  
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.39079856

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-2.479236	0.197130	-0.617633
O	-1.836708	0.286801	0.508534
C	-0.884596	-0.780459	0.655683
C	0.269752	-0.660900	-0.342642
C	1.170590	0.537294	-0.053252
C	0.576553	1.913568	-0.096861
H	-0.532419	-0.713799	1.683858
H	-1.394939	-1.726306	0.489516
O	0.999855	-1.846522	-0.277705
H	-0.166209	-0.523355	-1.339123
H	1.911742	-1.597793	-0.064533
O	2.332366	0.332388	0.202292
H	1.372194	2.648671	-0.172810
H	-0.128484	2.011438	-0.921142
H	0.014111	2.085756	0.822761

Rotational constants (GHz): 3.0574000 1.5833300 1.1646600

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

45.9000	73.9665	141.8265
159.7013	201.3066	287.2900
308.9659	353.8382	431.4591
457.1968	551.6724	592.1856
634.0541	745.4390	925.2148
957.2824	973.8735	1022.3296
1093.1384	1136.5243	1189.0421
1195.2579	1246.2433	1275.9191
1294.5337	1351.1883	1360.9925
1399.3596	1422.9120	1436.0124
1447.9794	1782.3110	2953.1140
2983.4728	3013.6931	3047.7724
3077.7398	3091.9292	3630.6979

Zero-point correction (Hartree): 0.115652

HMVKA02.mptt

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38762419

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-3.144348	-0.488120	-0.272461
O	-2.127133	0.057597	0.317698
C	-0.893057	-0.330687	-0.315086
C	0.224059	0.402889	0.403039
C	1.586505	-0.158762	0.001837
C	1.841048	-1.626968	0.191780
H	-0.810644	-1.413404	-0.224296
H	-0.943005	-0.035090	-1.362175
O	0.154896	1.768709	0.146112
H	0.111497	0.211371	1.479980
H	1.021647	2.034511	-0.194117
O	2.412790	0.594642	-0.446872
H	2.909591	-1.800777	0.278495
H	1.316088	-2.015525	1.063179
H	1.473875	-2.162536	-0.686293

Rotational constants (GHz): 3.9321700 1.1593600 0.9482900

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

54.9632	76.9741	96.3934
156.8415	162.1109	256.3337
335.1344	367.8861	407.2047
444.2978	467.8995	589.6304
631.8637	820.4356	897.0323
952.7943	971.5637	1033.0031
1078.9590	1145.1832	1181.4230
1223.9606	1238.3767	1256.6885
1314.3277	1350.6375	1364.0348
1395.2613	1426.9265	1435.1303
1444.4384	1791.4260	2919.3429
2979.5858	2999.3969	3045.8763
3061.5053	3090.4310	3644.4143

Zero-point correction (Hartree): 0.115222

HMVKA02.mtm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.39003314

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-2.707871	-0.523962	-0.501435
O	-1.465855	-0.151371	-0.520940
C	-1.027157	0.285862	0.780955
C	0.423568	0.707970	0.655123
C	1.260279	-0.354197	-0.061256
C	1.176509	-1.767572	0.436125
H	-1.643247	1.130710	1.080873
H	-1.160366	-0.545366	1.472864
O	0.524466	1.935852	0.007600
H	0.822941	0.777680	1.677235
H	1.146766	1.816629	-0.724720
O	1.951516	-0.018254	-0.987895
H	2.010470	-2.343407	0.046846
H	1.163929	-1.801914	1.525399
H	0.242269	-2.204831	0.077175

Rotational constants (GHz): 2.8513500 1.5466700 1.2359000

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

50.4405	80.2300	120.4407
159.9724	170.6262	262.6058
341.1771	387.3799	407.5405
435.8850	487.8237	600.4469
689.1991	764.2914	902.7885
933.9365	959.7116	1037.9678
1054.9706	1142.3648	1181.8151
1203.8190	1256.6117	1262.0736
1331.4079	1351.3732	1357.5931
1391.7556	1424.5184	1439.3132
1444.4454	1796.9812	2916.3570
2978.3086	3005.6891	3042.8044
3067.3373	3091.1395	3645.8175

Zero-point correction (Hartree): 0.115384

HMVKA02.mtm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38673248

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-3.144129	-0.502243	-0.322911
O	-2.128337	-0.030725	0.330159
C	-0.895000	-0.307117	-0.360201
C	0.216531	0.353676	0.440943
C	1.573758	-0.141430	-0.056466
C	1.993232	-1.542935	0.280632
H	-0.795885	-1.390094	-0.423165
H	-0.959427	0.128384	-1.356310
O	0.130415	1.740880	0.342431
H	0.107103	0.050416	1.489222
H	0.891818	2.032726	-0.179391
O	2.279066	0.622653	-0.665568
H	2.761257	-1.876111	-0.411092
H	2.412973	-1.526665	1.288892
H	1.154921	-2.236339	0.289517

Rotational constants (GHz): 3.8806600 1.1428900 0.9614600

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

52.2819	57.6277	74.2192
102.2574	167.4903	253.2880
321.0248	376.0466	395.0560
436.0323	489.9314	610.5484
614.8621	833.0515	894.2333
945.7864	974.6595	1030.8643
1075.6596	1136.5001	1174.7851
1213.0947	1244.7064	1259.1878
1304.2716	1355.5133	1365.4888
1391.0496	1426.7108	1433.5427
1443.8018	1791.2480	2950.3555
2982.3242	3001.1129	3050.2723
3062.8517	3093.4871	3649.4865

Zero-point correction (Hartree): 0.115046

HMVKA02.tmtm



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-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38379567
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.666954      -0.102077      0.857345
O      -2.274104      -0.017583      -0.376299
C      -0.958721      -0.578199      -0.543268
C       0.077851       0.273951      0.159714
C       1.454004      -0.395731      0.094149
C       2.641221       0.498390      0.316980
H      -0.957023      -1.592004      -0.152803
H      -0.797879      -0.597724      -1.621660
O       0.109501       1.606086      -0.299998
H      -0.194575       0.332863      1.217811
H       0.133733       1.619336      -1.261244
O       1.551260      -1.579487      -0.109703
H       3.527303      -0.110256      0.467540
H       2.778478       1.143227      -0.551776
H       2.466215       1.158581      1.165922
Rotational constants (GHz):   3.9592800   1.2274900   1.0474300
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  33.4619      59.7255      113.0360
 134.9421     188.9764     244.2672
 265.6634     303.4995     378.7914
 467.1706     512.8112     572.3056
 605.9303     800.4753     884.0376
 918.2081     975.5425    1019.0587
1055.3383    1146.8642    1180.4708
1186.9668    1241.7074    1276.1955
1296.4107    1352.8056    1362.9387
1374.0704    1418.7859    1428.9692
1441.4032    1789.5760    2982.9262
2986.7212    3009.0926    3047.2028
3082.6137    3096.1299    3746.6155
Zero-point correction (Hartree): 0.114921

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HMVKAO2.tppp

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-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38340412
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.554109      -0.057422      0.892221
O      -1.973085      -0.647658      -0.107147
C      -1.076508      0.251333      -0.785972
C       0.130674       0.564326      0.088331
C       1.190318      -0.535292      0.009956
C       2.551975      -0.188004      0.538301
H      -0.791613      -0.265963      -1.698109
H      -1.628278       1.163712      -1.006347
O       0.744095       1.780082      -0.284017
H      -0.210825       0.598416      1.130411
H       0.205097       2.515991      0.016354
O       0.908420      -1.613721      -0.441945
H       3.154607      -1.087911      0.610457
H       3.020477       0.527825      -0.137235
H       2.469217       0.303509      1.507886
Rotational constants (GHz):   3.3000500   1.3937300   1.1388600
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  44.2196      63.3972      118.3372
 145.1153     202.1860     278.1230
 287.1753     329.4333     385.0060
 447.5637     514.7723     586.8065
 612.4401     736.6090     911.8375
 953.4319     977.9932    1025.0465
1069.0636    1134.5136    1176.2887
1189.2965    1211.7459    1264.9204
1300.7930    1350.5097    1370.3267
1394.5539    1423.9446    1430.3500
1434.1345    1802.6620    2944.7735
2986.5210    3012.3735    3048.9798
3085.9154    3095.5167    3766.7338
Zero-point correction (Hartree): 0.115230

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HMVKBO2.hmmm

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-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38601666
Electronic state : 2-A
Cartesian coordinates (Angs):
C      -0.295418      -0.120935      -0.248545
H      -0.490830      -0.161200      -1.323563
C       1.196278       0.116204      -0.031796
C      -1.167808       0.954802      0.390267
O      -0.609874      -1.413645      0.305360
O       1.594738       1.242253      0.137986
C       2.103906      -1.076294      -0.070026
H       1.880463      -1.692818      -0.941269
H       1.917746      -1.696427      0.807906
H       3.137692      -0.746005      -0.082562
O      -1.042387       2.169040      -0.299866
H      -2.205925       0.634769      0.316643
H      -0.904645       1.052851      1.447916

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H      -0.132920      2.468388      -0.189225
O      -1.720393     -1.885426      -0.177886
Rotational constants (GHz):  2.2424400  2.0326600  1.1226800
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  41.8211      86.1842      143.7879
 153.2770     205.7749      241.4123
 285.0609     370.9473      441.0036
 463.5506     512.4466      562.2539
 614.9058     762.9668      923.7757
 947.3793     1009.6484     1056.5799
1077.7947     1100.7797     1167.4701
1205.8266     1244.4364     1259.2896
1321.6536     1350.1286     1360.2928
1391.1680     1420.2299     1429.7315
1468.9250     1786.7622     2959.9654
2983.2563     2990.8611     3043.0634
3044.3387     3097.4613     3721.6557
Zero-point correction (Hartree): 0.115546

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HMVKBO2.hmmt

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-----
E(CCS(D)/Aug-CC-pVDZ) (Hartree): -456.36228035
E(CCS(D)/Aug-CC-pVDZ) (Hartree): -456.31196852
  T1 diagnostic: 0.022819
E(MP2/Aug-CC-pVDZ) (Hartree): -456.25052340
E(MP3/Aug-CC-pVDZ) (Hartree): -456.28759527
E(PMP2/Aug-CC-pVDZ) (Hartree): -456.25339001
E(PMP3/Aug-CC-pVDZ) (Hartree): -456.28934166
E(PUHF/Aug-CC-pVDZ) (Hartree): -454.93781106
E(UHF/Aug-CC-pVDZ) (Hartree): -454.93312479
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -456.75274738
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -456.68071667
  T1 diagnostic: 0.021933
E(MP2/Aug-CC-pVTZ) (Hartree): -456.63873437
E(MP3/Aug-CC-pVTZ) (Hartree): -456.66445591
E(PMP2/Aug-CC-pVTZ) (Hartree): -456.64181153
E(PMP3/Aug-CC-pVTZ) (Hartree): -456.66628735
E(PUHF/Aug-CC-pVTZ) (Hartree): -455.04444045
E(UHF/Aug-CC-pVTZ) (Hartree): -455.03940173
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38774592
Electronic state : 2-A

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Cartesian coordinates (Angs):

```

C      0.168693      -0.338645      0.542811
H      0.360975      -0.216773      1.611565
C     -0.489529      0.940519      0.022094
C      1.475992     -0.664231     -0.175101
O     -0.744416     -1.445959      0.462108
C     -0.193985      1.772848     -0.519474
O     -1.961836      1.114568      0.253029
H     -2.234430      0.784923      1.255645
H     -2.507838      0.486219     -0.451389
H     -2.229110      2.155266      0.098726
O      2.473257      0.254985      0.183371
H      1.806863     -1.653116      0.139046
H      1.295747     -0.682355     -1.252650
H      2.210769      1.111088     -0.173205
O     -1.155687     -1.619189     -0.761596

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Rotational constants (GHz):  2.5812600  1.9422000  1.2647800
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
  54.8136      107.9351      145.0558
 150.4859     188.8972     254.3537
 272.1788     384.2404     430.9141
 471.0983     507.3485     578.8845
 664.9822     755.6207     920.2916
 957.3054     985.7546     1033.3337
1076.4458     1105.8887     1168.0677
1202.6481     1205.0512     1289.8933
1328.0027     1348.4916     1355.8334
1390.9839     1422.9861     1431.3208
1470.1653     1788.6138     2976.1864
2985.8059     3001.7244     3041.9637
3049.5521     3095.8439     3721.0237

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Zero-point correction (Hartree): 0.115715

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HMVKBO2.htpm

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-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38560665
Electronic state : 2-A

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Cartesian coordinates (Angs):

```

C     -0.275109     -0.109746     -0.528328
H     -0.399952     -0.490528     -1.546293
C      1.211314     -0.142509     -0.182253
C     -0.871287      1.283166     -0.413569
O     -0.942266     -1.042076      0.349854
O      1.869319      0.852689     -0.355233
C      1.780734     -1.428402     0.335177
H      1.458985     -2.265591     -0.284680
H      1.386182     -1.610637      1.336022
H      2.863504     -1.359672      0.366106
O     -0.583336      1.891866      0.818869
H     -0.507891      1.876765     -1.255370

```

H	-1.953552	1.193118	-0.493222	
H	0.341637	2.156634	0.808521	
O	-2.126569	-1.341872	-0.088145	
Rotational constants (GHz):	2.4594600	1.9322500	1.2338200	
Vibrational harmonic frequencies (cm-1):	(Scaled by 0.9710)			
47.6130	82.9656		133.6649	
166.0596	209.1338		215.3120	
303.6500	385.5156		428.6993	
454.8453	502.8540		560.3778	
684.9740	796.1875		850.5170	
928.0016	964.2144		1023.8657	
1066.3216	1113.7771		1174.4969	
1206.0177	1249.6644		1284.1323	
1311.1610	1358.2685		1361.5554	
1378.6846	1420.7760		1429.8616	
1451.6729	1790.1856		2977.8438	
2982.3002	2988.3199		3043.5675	
3046.4503	3096.4365		3747.7734	

Zero-point correction (Hartree): 0.115475

HMVKBO2.htpt

-----  
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38498868  
Electronic state : 2-A  
Cartesian coordinates (Angs):

C	-0.171767	0.165805	0.811420
H	0.068122	0.186162	1.878527
C	0.893460	-0.672283	0.098911
C	-1.583189	-0.372196	0.625790
O	-0.079354	1.542545	0.405251
O	0.601198	-1.763722	-0.318896
C	2.279332	-0.102224	0.002396
H	2.532115	0.470517	0.893913
H	2.315447	0.581064	-0.846252
H	2.987617	-0.910137	-0.155453
O	-1.972216	-0.465036	-0.714856
H	-1.630121	-1.340199	1.133847
H	-2.278560	0.307714	1.116393
H	-1.415644	-1.126532	-1.138910
O	0.064623	1.650813	-0.885645

Rotational constants (GHz): 2.6133200 2.0378500 1.4509700  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

59.9358	93.2346	120.3062
175.3317	204.4379	218.0102
317.3178	330.7297	441.4846
473.3125	520.8014	577.3602
686.6530	800.8391	868.3274
934.6709	971.1242	1021.0531
1041.4595	1125.4804	1160.3434
1201.6176	1210.9168	1302.9794
1331.7900	1357.8512	1360.1541
1391.4469	1425.9508	1434.6136
1448.6704	1792.1918	2963.1050
2987.1661	2989.7979	3035.6634
3055.3390	3091.6888	3739.4762

Zero-point correction (Hartree): 0.115580

HMVKBO2.ltm

-----  
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38275007  
Electronic state : 2-A  
Cartesian coordinates (Angs):

C	-0.269109	-0.146356	-0.529960
H	-0.389395	-0.448199	-1.572907
C	1.087726	-0.605771	-0.005250
C	-0.453455	1.357343	-0.387441
O	-1.285093	-0.821704	0.238438
O	1.176661	-1.457377	0.833906
C	2.277097	0.096883	-0.601614
H	2.347484	1.088259	-0.149427
H	2.167601	0.225106	-1.678768
H	3.176979	-0.466802	-0.375799
O	-0.092650	1.804752	0.897798
H	0.196410	1.870111	-1.095085
H	-1.489478	1.599818	-0.634808
H	-0.678965	1.407467	1.549005
O	-2.446943	-0.711715	-0.332219

Rotational constants (GHz): 2.7045200 1.7251000 1.2996300  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

57.3966	91.4060	113.8358
170.7709	193.3369	209.9038
316.1493	361.6076	374.3667
462.3873	477.4024	574.2544
679.5297	812.0626	853.6056
935.6415	953.2807	1038.9404
1056.2030	1108.0326	1157.2511
1192.8550	1247.2049	1250.0158
1312.8826	1346.8165	1362.6181
1376.0668	1426.7965	1438.3994
1464.9343	1816.0856	2977.3779
2983.4431	2999.8109	3042.4519

3042.7286                    3091.8938                    3745.9751  
Zero-point correction (Hartree): 0.115236

HMVKBO2.ltmp

-----  
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38307280  
Electronic state : 2-A  
Cartesian coordinates (Angs):  
C     -0.270934            0.219250            -0.596878  
H     -0.484882           -0.017106           -1.641676  
C     0.487232            -0.945161           0.051044  
C     0.505774            1.519853           -0.473379  
O     -1.516567           0.431270           0.074432  
O     0.009667           -1.573862           0.950891  
C     1.862492           -1.199592           -0.504526  
H     2.538419           -0.448601           -0.090323  
H     1.878962           -1.107151           -1.590587  
H     2.196610           -2.187304           -0.202041  
O     1.000711           1.711980           0.830849  
H     1.368942           1.488245           -1.136311  
H     -0.137349           2.344591           -0.790673  
H     0.263629           1.747241           1.448417  
O     -2.385275           -0.492640           -0.212968  
Rotational constants (GHz):    2.3897800        1.9802600        1.3450600  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)  
65.1638                    95.2324                    110.8721  
154.6955                   162.5004                   255.8422  
306.0399                   349.2375                   384.5720  
433.1074                   492.8386                   599.2923  
663.0260                   793.7187                   866.5581  
941.9997                   955.4868                   1031.1973  
1062.6538                   1114.3263                   1159.1461  
1205.0048                   1241.3257                   1252.4847  
1309.5465                   1344.9532                   1355.3348  
1380.7233                   1426.2816                   1438.2127  
1461.5598                   1820.2171                   2974.2037  
2977.1634                   3001.3954                   3042.1990  
3042.9910                   3091.6192                   3744.7470  
Zero-point correction (Hartree): 0.115216

HMVKBO2.ltmr

-----  
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38557278  
Electronic state : 2-A  
Cartesian coordinates (Angs):  
C     0.169954            -0.047912            0.825026  
H     -0.063288           -0.120015            1.889070  
C     -1.028048           -0.549641            0.008751  
C     0.520989            1.390634            0.454511  
O     1.287183            -0.932823            0.658548  
O     -0.934365           -1.502191           -0.710401  
C     -2.286135           0.259766            0.166721  
H     -2.159686           1.188863           -0.392305  
H     -2.467007           0.514852            1.211159  
H     -3.126159           -0.295689           -0.238869  
O     0.406625            1.644314           -0.922386  
H     -0.178108           2.058425            0.957102  
H     1.525302            1.605510            0.829999  
H     1.001568            1.038186           -1.378290  
O     1.891410            -0.747703           -0.476750  
Rotational constants (GHz):    2.6420400        1.9810700        1.4753200  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)  
70.7910                    112.8546                    144.0210  
149.7968                   208.8947                   248.4337  
329.9750                   351.7887                   434.1508  
500.7448                   533.8174                   570.1607  
694.6942                   798.8306                   868.9105  
941.2740                   970.9506                   1018.9021  
1034.0424                   1118.1087                   1154.7921  
1198.4145                   1227.0856                   1246.0614  
1341.8251                   1344.8153                   1362.3830  
1393.3283                   1426.7489                   1438.1171  
1459.3515                   1819.1844                   2970.5536  
2978.4292                   3010.2307                   3032.7122  
3044.4124                   3091.0465                   3721.2178  
Zero-point correction (Hartree): 0.115813

HMVKBO2.pmp

-----  
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38605168  
Electronic state : 2-A  
Cartesian coordinates (Angs):  
C     -0.073869           -0.446687           -0.202854  
H     -0.057929           -0.673670           -1.270866  
C     0.179497            1.052735           -0.018916  
C     -1.401288           -0.887950           0.407452  
O     0.974231           -1.208608           0.423441  
O     -0.768431           1.797722           0.037018  
C     1.597899            1.528172           0.063512  
H     2.165790            1.158338           -0.790736  
H     2.071660            1.112634           0.953949

H	1.611019	2.612649	0.099588
O	-2.477712	-0.401967	-0.348915
H	-1.446491	-1.975464	0.386771
H	-1.453029	-0.560839	1.450322
H	-2.449420	0.560556	-0.299286
O	1.990033	-1.401125	-0.364659
Rotational constants (GHz):	2.6560700	1.8096900	1.1499900
Vibrational harmonic frequencies (cm-1):	(Scaled by 0.9710)		
29.3370	92.1224		137.4153
187.4753	214.7167		245.0729
293.7142	370.1615		423.1506
471.4444	519.0918		583.6509
612.5507	739.7493		920.8275
948.6184	1026.0429		1039.0144
1085.6430	1105.1152		1177.4556
1203.9053	1244.1436		1270.4952
1305.1716	1352.0703		1358.1149
1396.0066	1421.3734		1430.6372
1472.1997	1780.4187		2960.8289
2984.3219	3004.9277		3040.6368
3044.8809	3099.0686		3712.5695

Zero-point correction (Hartree): 0.115678

HMVKBO2.ppm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38187741

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.097276	-0.067479	-0.346786
H	0.340036	-0.085975	-1.410359
C	-1.407836	-0.224091	-0.168338
C	0.823366	-1.188121	0.396316
O	0.520501	1.206636	0.165521
O	-1.930820	-1.199964	-0.639622
C	-2.146891	0.824387	0.608695
H	-2.051220	1.788618	0.108169
H	-1.697213	0.942886	1.595539
H	-3.190543	0.539000	0.693014
O	2.217114	-1.052871	0.353571
H	0.544220	-1.162190	1.450565
H	0.473543	-2.132279	-0.029051
H	2.508035	-0.903852	-0.550590
O	1.552912	1.664402	-0.479047
Rotational constants (GHz):	2.9281300	1.5704400	1.1531500
Vibrational harmonic frequencies (cm-1):	(Scaled by 0.9710)		
34.7856	85.6573		127.4500
171.2138	178.3183		214.2633
236.7573	311.2924		386.9152
449.0142	478.8825		547.0694
586.3216	842.7041		868.2483
946.1716	984.5389		1039.9110
1078.1989	1115.8314		1165.5931
1216.6648	1248.2188		1274.4499
1308.9865	1325.6860		1357.2191
1385.3495	1419.4563		1429.1750
1464.1188	1796.1878		2972.5498
2982.3487	3007.1971		3027.8095
3042.8095	3096.9468		3754.2843

Zero-point correction (Hartree): 0.114867

HMVRBO2.pmp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38305263

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.276412	-0.005210	-0.301158
H	0.487136	0.079292	-1.368019
C	-1.085935	-0.682748	-0.130555
C	1.359138	-0.800129	0.414484
O	0.283971	1.321998	0.250801
O	-1.233335	-1.766873	-0.630847
C	-2.143160	0.017827	0.668947
H	-2.438840	0.935469	0.158798
H	-1.743008	0.316392	1.638959
H	-2.996600	-0.641770	0.787719
O	2.649939	-0.312474	0.147852
H	1.210455	-0.711510	1.491437
H	1.239456	-1.848335	0.135132
H	2.907420	-0.554989	-0.744926
O	-0.338668	2.163226	-0.518982
Rotational constants (GHz):	2.5086700	1.7359400	1.1607800
Vibrational harmonic frequencies (cm-1):	(Scaled by 0.9710)		
38.8721	95.2404		113.0322
175.9211	189.9353		236.5696
264.5373	291.5241		346.3134
462.7306	520.5808		574.3105
579.5246	799.9983		850.2093
952.6980	990.9950		1043.6508
1073.1789	1106.2352		1179.6281
1219.6558	1239.0379		1254.3435
1303.5145	1352.7399		1354.7301

1378.7326	1421.2466	1430.2613
1458.0333	1795.3886	2981.4968
2985.5546	3013.2393	3036.2376
3042.2121	3097.8618	3766.7791

Zero-point correction (Hartree): 0.115003

HMVKBO2.ppmt

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38262265

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.225815	-0.115045	0.472810
H	-0.385538	-0.402480	1.515320
C	1.162333	-0.622168	0.064912
C	-1.333634	-0.678229	-0.404522
O	-0.272365	1.325929	0.515148
O	1.279001	-1.782171	-0.232602
C	2.318824	0.333939	0.114285
H	2.302871	0.903734	1.043655
H	2.230729	1.054873	-0.698712
H	3.242926	-0.226894	0.017215
O	-2.613469	-0.372861	0.097112
H	-1.259218	-0.220592	-1.389447
H	-1.165238	-1.750148	-0.506947
H	-2.832498	-0.974145	0.812300
O	-0.101202	1.842187	-0.664445

Rotational constants (GHz): 2.8615600 1.7063400 1.1894100

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

30.6995	76.8091	127.8559
183.2377	195.9827	211.9420
260.8098	306.9296	348.0882
441.6987	496.8116	577.9107
655.9839	784.0356	859.6897
950.5229	990.8198	1019.4969
1060.4766	1097.3815	1163.0105
1190.7140	1229.6263	1259.2339
1340.1784	1350.6213	1353.0369
1369.0224	1422.4405	1430.5732
1459.5652	1793.1857	2985.8957
2992.0049	3005.2398	3049.2809
3058.1770	3096.0724	3773.8960

Zero-point correction (Hartree): 0.114962

HMVKBO2.pppm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38448356

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.085530	-0.062836	-0.322456
H	0.316099	-0.121091	-1.388410
C	-1.410292	-0.301944	-0.119614
C	0.932472	-1.069671	0.445281
O	0.382354	1.284945	0.113256
O	-1.835119	-1.411321	-0.305140
C	-2.275716	0.856590	0.281833
H	-2.166751	1.671449	-0.434673
H	-1.948934	1.246349	1.246552
H	-3.308227	0.526672	0.334194
O	2.261372	-1.120786	0.001267
H	0.867699	-0.833696	1.513885
H	0.493029	-2.051247	0.280826
H	2.622707	-0.228532	-0.007772
O	1.582944	1.654320	-0.216241

Rotational constants (GHz): 3.0053900 1.5981800 1.1042900

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

24.3305	49.4088	138.2027
187.2052	200.2285	221.0619
332.0613	395.2853	396.8329
416.5813	449.8376	544.3039
592.3846	836.3206	846.1745
944.7846	1001.9338	1049.1484
1066.2250	1101.2570	1186.8150
1204.1434	1240.6986	1261.8346
1305.8180	1346.1158	1358.2028
1388.8844	1420.7169	1431.2297
1461.0865	1800.3194	2943.3956
2983.8046	3004.1170	3044.0688
3054.9615	3098.1627	3733.2039

Zero-point correction (Hartree): 0.115108

HMVKBO2.pppp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38544420

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.261460	-0.055277	-0.333960
H	0.463923	0.020518	-1.401860
C	-1.141421	-0.625106	-0.120922
C	1.306271	-0.918781	0.353522
O	0.399179	1.263434	0.232450
O	-1.373717	-1.712171	-0.580035

C	-2.134995	0.176435	0.666144
H	-2.358418	1.104679	0.138764
H	-1.708103	0.459569	1.629440
H	-3.038134	-0.409651	0.801663
O	2.612043	-0.496609	0.054215
H	1.119794	-0.921573	1.433104
H	1.192607	-1.934947	-0.016128
H	2.754896	0.377998	0.426094
O	-0.159310	2.175318	-0.506604

Rotational constants (GHz): 2.5316200 1.7502900 1.1591400  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

33.1502	101.3747	122.0450
171.3028	186.7654	250.6214
277.7278	336.2307	351.5365
454.8613	521.0974	572.1374
578.8619	794.2581	850.5543
952.6400	994.3599	1048.9013
1077.5756	1098.4816	1190.4935
1216.6849	1232.2015	1251.8481
1300.5122	1350.4082	1354.5593
1375.7838	1421.6538	1430.2523
1459.2989	1796.8678	2949.4225
2981.7498	3030.9733	3042.4802
3063.4235	3098.3650	3759.5137

Zero-point correction (Hartree): 0.115154

HMVKBO2.pptp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38559643

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.201634	-0.145643	0.502130
H	-0.323498	-0.387436	1.560199
C	1.204248	-0.562109	0.063598
C	-1.294530	-0.817259	-0.311220
O	-0.355592	1.292503	0.470732
O	1.378327	-1.694314	-0.302033
C	2.307653	0.452056	0.162748
H	2.257485	0.979166	1.115854
H	2.185135	1.199967	-0.621126
H	3.261998	-0.051807	0.047080
O	-2.572701	-0.515322	0.193207
H	-1.187685	-0.530061	-1.359475
H	-1.151974	-1.891728	-0.234975
H	-2.776891	0.405010	0.007573
O	-0.244908	1.756459	-0.739239

Rotational constants (GHz): 2.9395000 1.6979800 1.2038200  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

34.1663	84.5920	132.5795
175.2633	184.8622	256.3641
287.5115	332.9495	355.5396
447.6494	490.3882	578.4060
657.7165	776.6129	857.9300
952.3378	989.9856	1020.7370
1078.0167	1093.6517	1171.9210
1187.5010	1226.5372	1257.7610
1337.5590	1353.9156	1355.5643
1370.0442	1423.8223	1433.6211
1457.5495	1797.6352	2985.0581
2987.6623	3008.0366	3048.2969
3072.3986	3096.0977	3761.7874

Zero-point correction (Hartree): 0.115246

HMVKBO2.pptp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38319855

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.269735	-0.008816	-0.281047
H	0.471285	0.114474	-1.345707
C	-1.084888	-0.706839	-0.110473
C	1.378711	-0.798241	0.375601
O	0.263680	1.302567	0.312649
O	-1.180337	-1.846608	-0.483195
C	-2.216234	0.060624	0.505783
H	-2.453677	0.926045	-0.114142
H	-1.917699	0.449885	1.479944
H	-3.078771	-0.591305	0.597504
O	2.603050	-0.251667	-0.059467
H	1.269878	-0.727200	1.463221
H	1.260768	-1.840553	0.074696
H	3.327672	-0.681338	0.399348
O	-0.306818	2.179411	-0.456743

Rotational constants (GHz): 2.5415400 1.7689900 1.1430300  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

27.9185	97.9612	116.5699
181.9591	197.7506	210.6049
270.6874	287.7640	348.1112
443.6351	517.1663	567.2144
584.7587	795.8430	866.7977
947.6971	996.4104	1053.4444

1090.3072	1108.6697	1189.6189
1211.1619	1244.5519	1254.0372
1262.0759	1309.8692	1353.8205
1416.3269	1421.9616	1429.9800
1471.6997	1795.2592	2948.9335
2983.3987	3012.7190	3023.1671
3043.7955	3098.8050	3784.2259

Zero-point correction (Hartree): 0.114886

HMVKBO2.pptt

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38385697

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.227521	-0.099929	-0.475074
H	0.373600	-0.319987	-1.535478
C	-1.153923	-0.616431	-0.058753
C	1.351591	-0.707601	0.328407
O	0.267689	1.343270	-0.423402
O	-1.259147	-1.738211	0.361061
C	-2.327559	0.300353	-0.257124
H	-2.262690	0.804063	-1.221699
H	-2.312736	1.076242	0.508665
H	-3.243547	-0.276732	-0.179653
O	2.560381	-0.355475	-0.311676
H	1.300330	-0.319774	1.348737
H	1.195765	-1.786765	0.351998
H	3.300424	-0.645285	0.225064
O	0.063962	1.776652	0.783721

Rotational constants (GHz): 2.9057200 1.6946600 1.2100900

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

41.9529	87.0286	129.4222
170.2735	190.9055	213.9529
256.4142	308.1670	352.5393
454.6422	484.5264	577.2760
661.9600	779.9339	871.6284
951.1732	1004.5754	1035.3765
1074.6016	1097.0879	1169.9718
1204.6371	1212.8751	1252.0693
1279.2774	1344.0204	1355.0891
1413.9729	1423.7619	1433.0009
1474.7444	1798.8531	2976.8026
2986.1378	3000.8442	3028.3669
3049.8639	3095.8275	3787.5883

Zero-point correction (Hartree): 0.115037

HMVKBO2.ptmm

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38541874

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.207111	-0.081349	-0.632725
H	-0.324968	-0.325954	-1.688003
C	1.264917	-0.197614	-0.246708
C	-0.721224	1.321462	-0.343717
O	-0.971672	-1.041224	0.135531
O	2.062314	0.378729	-0.938130
C	1.630587	-0.980298	0.976943
H	1.300930	-2.014478	0.875074
H	1.104427	-0.559688	1.835290
H	2.704599	-0.932635	1.126004
O	-0.578423	1.648401	1.020163
H	-0.114460	2.022249	-0.914095
H	-1.759394	1.392500	-0.673362
H	-1.253846	1.188036	1.525392
O	-2.194757	-1.128811	-0.293696

Rotational constants (GHz): 2.6449000 1.6748400 1.3717600

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

56.0002	68.9391	115.6606
163.1310	197.0979	214.3560
282.1476	344.2629	389.1909
428.8006	502.2004	567.6253
676.5713	788.4973	862.2212
924.0932	979.7005	1031.6174
1045.2235	1099.0648	1178.5429
1210.4048	1246.2574	1258.3690
1300.9182	1351.7209	1359.0597
1366.6487	1420.4869	1429.4954
1456.3396	1802.4164	2982.4722
2988.8938	3029.1413	3045.4470
3055.5251	3097.3201	3759.3561

Zero-point correction (Hartree): 0.115141

HMVKBO2.ptmp

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E (UM062X/Aug-CC-pVTZ) (Hartree): -457.38616208

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.200181	0.262901	-0.667408
H	-0.014395	0.434566	-1.721658
C	-0.647214	-0.918442	-0.182856



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C      1.675206      -0.018547      -0.439751
O      -0.087990      1.477394      0.051790
O      -0.617148      -1.918165      -0.849367
C      -1.417283      -0.784337      1.094848
H      -2.184234      -0.016645      0.990640
H      -0.741332      -0.463281      1.888539
H      -1.869405      -1.740140      1.339519
O      1.951595      -0.247996      0.924169
H      1.929671      -0.927794      -0.980463
H      2.268578      0.808189      -0.837427
H      1.885087      0.583573      1.401265
O      -1.263870      1.947777      -0.240269
Rotational constants (GHz):  2.1504900      2.0699500      1.4157600
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
60.3906      105.0131      112.2804
158.9012      172.3129      247.9999
282.1159      342.4722      368.5942
487.2192      501.2833      553.3674
664.8032      778.1565      875.6863
924.3854      982.3656      1025.7450
1046.7165      1105.4728      1181.6672
1217.3587      1250.1195      1263.2864
1291.2312      1350.2354      1355.9515
1370.7613      1421.3988      1431.0105
1457.4311      1801.6516      2977.8896
2984.1615      3031.5200      3048.4822
3055.4916      3097.6252      3759.2044
Zero-point correction (Hartree): 0.115297

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HMVKBO2.ptmt

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38651897
Electronic state : 2-A
Cartesian coordinates (Angs):
C      -0.116533      0.131926      -0.854754
H      0.083683      0.291361      -1.913404
C      1.231199      -0.038425      -0.140910
C      -0.871311      1.321327      -0.275544
O      -0.893411      -1.088531      -0.834921
O      2.095271      0.751377      -0.409413
C      1.382883      -1.145382      0.856663
H      1.199112      -2.109077      0.380633
H      0.634143      -1.027639      1.641247
O      2.382250      -1.111053      1.278336
O      -0.889773      1.340379      1.129825
H      -0.342845      2.216959      -0.597061
H      -1.879594      1.336184      -0.699019
H      -1.418355      0.591243      1.421048
O      -1.614064      -1.228806      0.236445
Rotational constants (GHz):  2.5880700      1.8948500      1.5155800
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
65.2674      91.5164      135.3830
168.0937      206.6647      245.0121
298.5172      382.5474      418.6313
483.7740      491.7933      577.0722
696.5067      794.7127      836.7653
945.4678      985.1181      998.9883
1028.1956      1115.4329      1186.7456
1213.9712      1229.1401      1243.3893
1338.7468      1351.6332      1355.5719
1386.3746      1420.5855      1430.9494
1448.3091      1802.7665      2970.0614
2983.7571      3035.8041      3046.5786
3048.9355      3097.4236      3745.3665
Zero-point correction (Hartree): 0.115672

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HMVKBO2.ptpp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38573015
Electronic state : 2-A
Cartesian coordinates (Angs):
C      -0.019616      -0.417300      -0.534748
H      0.346524      -0.565198      -1.553350
C      0.120357      1.068906      -0.186089
C      -1.457573      -0.890457      -0.400404
O      0.811475      -1.221267      0.326352
O      -0.805901      1.799152      -0.436405
C      1.398777      1.540525      0.434325
H      2.249663      1.235741      -0.175234
H      1.524661      1.060163      1.405963
H      1.365895      2.619419      0.546353
O      -2.035848      -0.526188      0.827777
H      -2.021912      -0.494254      -1.246723
H      -1.469569      -1.977891      -0.454371
H      -2.238646      0.413685      0.792340
O      2.029239      -1.314410      -0.116910
Rotational constants (GHz):  2.4709700      1.9727300      1.2665900
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
33.3405      97.7831      112.7793
183.8623      188.2793      257.4453
307.6236      389.9054      414.5123

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452.7363	497.0320	555.4023
672.1927	792.7407	851.0493
932.4196	966.7542	1024.2907
1060.1629	1121.5695	1185.6749
1205.9792	1254.0582	1287.3592
1293.7897	1355.5532	1360.7531
1381.0659	1421.1339	1427.7896
1449.2558	1783.9538	2983.8085
2985.4759	3001.9224	3045.1487
3045.1918	3098.8830	3747.8877

Zero-point correction (Hartree): 0.115496

HMVKBO2.pttm

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38457772

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.261432	-0.095853	-0.610895
H	-0.423200	-0.351396	-1.657271
C	1.216950	-0.274615	-0.267496
C	-0.682340	1.334014	-0.349547
O	-1.044600	-1.006897	0.192629
O	2.020668	0.231708	-1.005310
C	1.573487	-1.028825	0.975277
H	1.209058	-2.054253	0.907041
H	1.067120	-0.565828	1.823311
H	2.650528	-1.013536	1.108954
O	-0.333125	1.634669	0.986693
H	-0.147372	1.968062	-1.060712
H	-1.758414	1.416377	-0.517968
H	-0.603869	2.530052	1.198114
O	-2.277174	-1.051706	-0.209700

Rotational constants (GHz): 2.6356000 1.6976700 1.3813700

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

66.3023	82.6482	120.1623
167.8721	178.9902	199.7035
216.5603	303.0397	383.6611
427.0117	503.6255	567.8711
661.9545	800.9025	874.3112
933.9567	984.1521	1039.4178
1073.4055	1109.1335	1161.0414
1212.3320	1235.5293	1253.6985
1299.1084	1311.3344	1356.7202
1398.4878	1420.7526	1429.9668
1467.8101	1801.0880	2968.1492
2983.2765	3015.5040	3033.0184
3046.8383	3096.9583	3789.4607

Zero-point correction (Hartree): 0.114907

HMVKBO2.pttp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38522117

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.040028	-0.395706	-0.634049
H	0.238531	-0.505859	-1.681171
C	0.184703	1.064891	-0.221122
C	-1.488721	-0.769671	-0.420453
O	0.761618	-1.311590	0.134039
O	-0.269061	1.912170	-0.943284
C	0.904178	1.344037	1.061341
H	1.942741	1.021704	0.980786
H	0.444119	0.762369	1.860866
H	0.854985	2.407392	1.273218
O	-1.812895	-0.459242	0.919744
H	-2.082638	-0.184414	-1.126157
H	-1.619443	-1.834603	-0.629256
H	-2.737631	-0.654309	1.083214
O	2.020156	-1.200537	-0.169974

Rotational constants (GHz): 2.2423500 2.0264800 1.4304800

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

70.0097	108.7506	114.6693
167.4057	175.7500	207.1586
254.2924	289.0592	353.3932
487.5893	496.8874	553.8032
653.6210	784.8339	884.9331
936.1688	983.0298	1021.3123
1092.8179	1117.3398	1172.3681
1209.6483	1237.8308	1251.5239
1296.3613	1303.7654	1351.9150
1408.6215	1424.0275	1429.9098
1465.0896	1800.2201	2963.9023
2984.1362	3010.2189	3034.0693
3049.0904	3097.0753	3787.1405

Zero-point correction (Hartree): 0.115034

TS.HMVKAO2.14HshiftCH2OH.dtS1

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34602051

Electronic state : 2-A

Cartesian coordinates (Angs):

O	1.884171	0.188745	-1.055055
O	1.852812	0.548972	0.277798
C	1.123920	-0.489998	0.893118
C	-0.104567	-0.650375	-0.015422
H	0.648553	-0.322220	-1.015917
H	0.900320	-0.181208	1.914315
H	1.672279	-1.432968	0.878928
O	-0.593223	-1.907358	-0.057665
H	-1.546562	-1.831176	-0.241213
C	-1.193966	0.393339	-0.015825
O	-2.327034	0.006330	-0.200933
C	-0.830192	1.834260	0.159317
H	-0.071840	2.116848	-0.570816
H	-0.386807	1.988826	1.143882
H	-1.720905	2.445021	0.050537

Rotational constants (GHz): 2.9661000 1.7353800 1.3023300  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

i12103.8767	92.9891	125.7682
182.2763	218.3234	281.4142
325.3019	373.9734	405.0106
483.8817	564.7528	618.2414
652.0706	684.0746	740.0971
933.8709	963.0414	973.5332
1044.2322	1046.0252	1060.0143
1159.8413	1202.2727	1211.6371
1279.5388	1348.7362	1369.2613
1383.3540	1418.8511	1432.7145
1456.8753	1698.4056	1748.0782
2985.4161	2986.0010	3046.7891
3048.4940	3095.5150	3564.4345

Zero-point correction (Hartree): 0.110753

TS.HMVKA02.15HshiftOH.md

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E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.32252047  
E (CCSD/Aug-CC-pVDZ) (Hartree): -456.26584391  
T1 diagnostic: 0.035376  
E (MP2/Aug-CC-pVDZ) (Hartree): -456.20231883  
E (MP3/Aug-CC-pVDZ) (Hartree): -456.23515652  
E (PMP2/Aug-CC-pVDZ) (Hartree): -456.20749097  
E (PMP3/Aug-CC-pVDZ) (Hartree): -456.23842643  
E (PUHF/Aug-CC-pVDZ) (Hartree): -454.86974318  
E (UHF/Aug-CC-pVDZ) (Hartree): -454.86206821  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.71475739  
E (CCSD/Aug-CC-pVTZ) (Hartree): -456.63566900  
T1 diagnostic: 0.033944  
E (MP2/Aug-CC-pVTZ) (Hartree): -456.59254836  
E (MP3/Aug-CC-pVTZ) (Hartree): -456.61373848  
E (PMP2/Aug-CC-pVTZ) (Hartree): -456.59792785  
E (PMP3/Aug-CC-pVTZ) (Hartree): -456.61710646  
E (PUHF/Aug-CC-pVTZ) (Hartree): -454.97777406  
E (UHF/Aug-CC-pVTZ) (Hartree): -454.96980049  
E (UM062X/Aug-CC-pVTZ) (Hartree): -457.35092637  
Electronic state : 2-A

Cartesian coordinates (Angs):

O	-2.194552	0.560661	-0.341599
O	-1.376592	-0.347004	-0.972750
C	-0.859745	-1.192702	-0.020123
C	0.156353	-0.295562	0.879044
O	-0.490127	0.804216	1.266050
H	-1.527908	0.901480	0.464448
H	-1.631658	-1.554724	0.656101
H	-0.292442	-1.977730	-0.512487
H	0.403470	-0.986455	1.698519
C	1.400321	-0.065880	0.005497
O	2.169709	-0.977478	-0.149342
C	1.549924	1.290269	-0.610553
H	2.431720	1.312457	-1.242577
H	0.652566	1.526328	-1.185575
H	1.615637	2.038732	0.179502

Rotational constants (GHz): 3.3642900 1.5528300 1.4423400  
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

i1254.5188	58.4025	86.4330
167.5849	191.7071	268.2428
386.3769	422.2017	485.1879
523.9390	555.6501	641.2558
680.5528	700.9230	774.9743
883.7553	951.0160	965.6347
986.8015	1024.1314	1082.1581
1165.3930	1204.0555	1217.2889
1241.6209	1268.4149	1315.2966
1352.4414	1416.7158	1425.6615
1438.7196	1770.9353	1796.8264
2910.7482	2980.9627	3009.3562
3041.9162	3098.5096	3101.2741

Zero-point correction (Hartree): 0.109317

TS.HMVKA02.15HshiftOH.mu

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IRC pathway available  
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.32262687

E(CCSD/Aug-CC-pVDZ) (Hartree): -456.26547103  
 T1 diagnostic: 0.040391  
 E(MP2/Aug-CC-pVDZ) (Hartree): -456.20041131  
 E(MP3/Aug-CC-pVDZ) (Hartree): -456.23338339  
 E(PMP2/Aug-CC-pVDZ) (Hartree): -456.20547813  
 E(PMP3/Aug-CC-pVDZ) (Hartree): -456.23662340  
 E(PUHF/Aug-CC-pVDZ) (Hartree): -454.86836382  
 E(UHF/Aug-CC-pVDZ) (Hartree): -454.86083426  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.71525572  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -456.63558622  
 T1 diagnostic: 0.038365  
 E(MP2/Aug-CC-pVTZ) (Hartree): -456.59115793  
 E(MP3/Aug-CC-pVTZ) (Hartree): -456.61244759  
 E(PMP2/Aug-CC-pVTZ) (Hartree): -456.59645225  
 E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61579632  
 E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97676820  
 E(UHF/Aug-CC-pVTZ) (Hartree): -454.96891190  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -457.35136408  
 Electronic state : 2-A  
 Cartesian coordinates (Angs):  
 O 2.421102 0.568993 0.284794  
 O 2.058305 -0.742989 0.096903  
 C 0.738987 -0.882780 0.466299  
 C -0.101163 -0.076133 -0.647893  
 O 0.381045 1.161292 -0.735574  
 H 1.597110 1.080473 -0.230205  
 H 0.469663 -1.934205 0.417473  
 H 0.549910 -0.426079 1.438454  
 H -0.039670 -0.667377 -1.569183  
 C -1.544636 -0.169451 -0.080214  
 O -2.155652 -1.188275 -0.231977  
 C -2.051004 1.044497 0.635661  
 H -3.015634 0.831354 1.084670  
 H -1.326843 1.364928 1.384805  
 H -2.126043 1.861949 -0.082311  
 Rotational constants (GHz): 4.0840000 1.3513100 1.1612800  
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)  
 i1175.4275 66.3794 100.6276  
 156.0419 183.5656 269.9151  
 370.4835 399.0959 512.9335  
 513.7438 554.8283 578.3265  
 693.6849 700.4782 772.6359  
 883.6102 939.9847 975.7201  
 993.5901 1048.7162 1114.4712  
 1173.5535 1180.5114 1203.4188  
 1268.1748 1280.3517 1321.2393  
 1349.7902 1414.1226 1420.1917  
 1433.8348 1775.0689 1804.2545  
 2950.6215 2986.2198 2993.7107  
 3046.9900 3094.5837 3101.0906  
 Zero-point correction (Hartree): 0.109396

TS.HMVKA02.16HshiftCH3.a.Sp

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 IRC pathway available  
 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.32282572  
 E(CCSD/Aug-CC-pVDZ) (Hartree): -456.26825438  
 T1 diagnostic: 0.024330  
 E(MP2/Aug-CC-pVDZ) (Hartree): -456.21180407  
 E(MP3/Aug-CC-pVDZ) (Hartree): -456.24375974  
 E(PMP2/Aug-CC-pVDZ) (Hartree): -456.22202486  
 E(PMP3/Aug-CC-pVDZ) (Hartree): -456.25029721  
 E(PUHF/Aug-CC-pVDZ) (Hartree): -454.88015200  
 E(UHF/Aug-CC-pVDZ) (Hartree): -454.86685827  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.71395585  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -456.63705508  
 T1 diagnostic: 0.023234  
 E(MP2/Aug-CC-pVTZ) (Hartree): -456.60076598  
 E(MP3/Aug-CC-pVTZ) (Hartree): -456.62086538  
 E(PMP2/Aug-CC-pVTZ) (Hartree): -456.61127981  
 E(PMP3/Aug-CC-pVTZ) (Hartree): -456.62756435  
 E(PUHF/Aug-CC-pVTZ) (Hartree): -454.98634600  
 E(UHF/Aug-CC-pVTZ) (Hartree): -454.97268688  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34948846  
 Electronic state : 2-A  
 Cartesian coordinates (Angs):  
 O -2.034844 0.381901 -0.558831  
 H -1.343551 1.192867 -0.092088  
 C -0.284735 1.733053 0.588736  
 O -1.788701 -0.734668 0.198473  
 C 0.757086 0.826163 0.089710  
 C -0.558452 -1.313862 -0.196905  
 C 0.658119 -0.644102 0.479413  
 H -0.666170 1.541014 1.586562  
 H -0.189588 2.769722 0.290608  
 H -0.599297 -2.352546 0.125735  
 H -0.453846 -1.263187 -1.280849  
 O 1.643684 1.179359 -0.657519  
 O 1.802278 -1.333181 0.082637  
 H 0.530287 -0.714396 1.564007  
 H 2.310719 -0.728276 -0.477777

Rotational constants (GHz): 2.8338200 1.9070400 1.2979500  
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

i1872.5623	101.2725	119.9780
244.3469	295.0858	324.0826
354.7458	414.7901	441.5113
522.3909	546.6416	600.5345
641.4140	665.5430	759.3995
892.8739	949.9451	976.4107
1009.7079	1051.5321	1069.0764
1119.1297	1136.9355	1190.5607
1235.1835	1260.3616	1295.5344
1334.0887	1402.7679	1408.2471
1434.8895	1447.7660	1736.9053
2968.1232	3000.1752	3043.4983
3066.4384	3146.8376	3638.5821

Zero-point correction (Hartree): 0.109914

TS.HMVKA02.16HshiftCH3.b.St

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34542770

Electronic state : 2-A

Cartesian coordinates (Angs):

O	-2.151359	0.140081	-0.305700
H	-1.478585	1.018788	0.042125
C	-0.435404	1.698677	0.646150
O	-1.264356	-0.821926	-0.716329
C	0.651286	0.884346	0.102687
C	-0.550072	-1.313282	0.412009
C	0.781905	-0.556221	0.599827
H	-0.710163	1.531518	1.682543
H	-0.487939	2.718290	0.285309
H	-1.195990	-1.244055	1.285903
H	-0.309772	-2.353130	0.198295
O	1.393254	1.271961	-0.773465
O	1.812983	-1.197807	-0.081447
H	1.003171	-0.531457	1.675095
H	2.168811	-0.559550	-0.717779

Rotational constants (GHz): 2.7254600 2.0162200 1.4085000

Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)

i1862.5122	85.5569	115.6288
264.9617	279.5386	335.7266
403.8751	413.7656	446.8780
501.1056	519.5281	590.6030
614.2366	693.3021	811.5645
899.6150	928.0395	984.4128
989.2139	1039.7892	1054.5468
1101.7804	1147.2013	1169.3000
1220.6310	1285.0151	1303.0087
1337.4599	1393.4307	1410.5817
1427.1204	1440.5856	1728.6471
2927.3395	3005.1192	3046.6354
3068.5662	3148.8787	3631.4786

Zero-point correction (Hartree): 0.109720

TS.HMVKB02.14HshiftCH2OH.umRlp

IRC pathway available

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31676020

E(CCSD/Aug-CC-pVDZ) (Hartree): -456.26121932

T1 diagnostic: 0.024454

E(MP2/Aug-CC-pVDZ) (Hartree): -456.20488418

E(MP3/Aug-CC-pVDZ) (Hartree): -456.23592090

E(PMP2/Aug-CC-pVDZ) (Hartree): -456.21278298

E(PMP3/Aug-CC-pVDZ) (Hartree): -456.24067724

E(PUHF/Aug-CC-pVDZ) (Hartree): -454.86786824

E(UHF/Aug-CC-pVDZ) (Hartree): -454.85692566

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.70766299

E(CCSD/Aug-CC-pVTZ) (Hartree): -456.62976787

T1 diagnostic: 0.023693

E(MP2/Aug-CC-pVTZ) (Hartree): -456.59335513

E(MP3/Aug-CC-pVTZ) (Hartree): -456.61254242

E(PMP2/Aug-CC-pVTZ) (Hartree): -456.60152856

E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61744357

E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97407001

E(UHF/Aug-CC-pVTZ) (Hartree): -454.96277393

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34102477

Electronic state : 2-A

Cartesian coordinates (Angs):

O	0.030855	1.693522	-0.905691
O	0.278002	1.581015	0.468525
C	-0.123051	0.261882	0.744546
C	-1.537333	0.238381	0.139886
H	-1.087115	0.971146	-0.829715
O	-2.123173	-0.935785	-0.159351
H	-1.423473	-1.586982	-0.350916
H	-2.225324	0.916677	0.643108
C	0.817364	-0.758675	0.102187
H	-0.105425	0.122473	1.829707
O	0.395450	-1.843896	-0.232519
C	2.247922	-0.354227	-0.051545
H	2.630568	0.036422	0.891808

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H      2.298585      0.460911     -0.774239
H      2.833698     -1.203650     -0.387907
Rotational constants (GHz):   2.5144600   2.1689300   1.3592700
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1720.0102      70.0149      151.7520
176.5398      237.4238      240.8273
302.9182      431.1423      461.7598
485.3768      547.5701      625.7265
684.7628      701.5996      774.6627
906.2657      947.0595      958.4325
1013.2427     1057.1299     1066.7569
1171.9378     1193.3112     1235.1972
1250.4523     1314.0060     1334.8429
1356.5694     1418.0833     1425.5807
1429.0119     1750.9040     1768.6382
2982.7178     2985.6879     3033.2588
3048.3434     3098.4020     3501.0526
Zero-point correction (Hartree): 0.110598

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TS.HMVKB02.15HshiftCH3.mp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -457.33644494
Electronic state : 2-A
Cartesian coordinates (Angs):
O      0.201107      1.711954     -0.627580
O     -0.275255      1.245265      0.585368
C     -0.271170     -0.183531      0.540160
C      1.124183     -0.664273      0.138014
C      2.140221      0.405979     -0.000860
H      1.321141      1.311043     -0.591765
H      2.319121      1.005619      0.887705
H      3.001357      0.160155     -0.608588
O      1.324777     -1.824982     -0.120056
H     -0.493634     -0.487286      1.564562
C     -1.341109     -0.718921     -0.399036
O     -2.621355     -0.316697      0.020832
H     -1.126636     -0.387852     -1.418661
H     -1.308401     -1.805569     -0.376099
H     -2.659893      0.644043      0.004656
Rotational constants (GHz):   2.9586100   1.7846500   1.2436200
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1999.0682      68.7395      108.2236
174.7116      255.6608      302.2956
354.4028      367.8836      457.7299
503.5329      526.9672      573.1544
598.8990      681.7914      816.9942
883.2750      921.8354      952.0351
984.4238      1045.3135     1091.4188
1096.0339     1108.0500     1167.6634
1194.7102     1231.9245     1311.2107
1351.9559     1375.3268     1379.1848
1460.9286     1571.4736     1766.0710
2974.4332     3014.0022     3036.8963
3061.6024     3147.2530     3751.9136
Zero-point correction (Hartree): 0.109497

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TS.HMVKB02.15HshiftCH3.bis.pm

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IRC pathway available
E(CCS2(T)/Aug-CC-pVDZ) (Hartree): -456.31237540
E(CCS2(Aug-CC-pVDZ) (Hartree): -456.25856605
T1 diagnostic: 0.022101
E(MP2/Aug-CC-pVDZ) (Hartree): -456.20268700
E(MP3/Aug-CC-pVDZ) (Hartree): -456.23458198
E(PMP2/Aug-CC-pVDZ) (Hartree): -456.21229527
E(PMP3/Aug-CC-pVDZ) (Hartree): -456.24064295
E(PUHF/Aug-CC-pVDZ) (Hartree): -454.87136962
E(UHF/Aug-CC-pVDZ) (Hartree): -454.85871419
E(CCS2(T)/Aug-CC-pVTZ) (Hartree): -456.70300785
E(CCS2(Aug-CC-pVTZ) (Hartree): -456.62694511
T1 diagnostic: 0.021103
E(MP2/Aug-CC-pVTZ) (Hartree): -456.59114466
E(MP3/Aug-CC-pVTZ) (Hartree): -456.61113840
E(PMP2/Aug-CC-pVTZ) (Hartree): -456.60107187
E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61737601
E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97746327
E(UHF/Aug-CC-pVTZ) (Hartree): -454.96441293
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.33727492
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.541131     -1.501412     -0.253918
O      0.164209     -1.431274     -0.160893
C     -0.262151     -0.197213     -0.724566
C      0.530727      0.955242     -0.098392
C      1.433896      0.567494      1.007693
H      1.858203     -0.593629      0.446336
H      2.248758      1.248362      1.217172
H      0.943250      0.106213      1.860867
O      0.442557      2.065876     -0.556308
H     -0.078277     -0.184962     -1.801829
C     -1.741850     -0.070472     -0.415196

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O      -1.973330   -0.032670   0.975626
H      -2.094497   0.872496   -0.828591
H      -2.284359   -0.890549   -0.892147
H      -1.753343   -0.892394   1.344901
Rotational constants (GHz):   2.4049100   2.0563600   1.4501700
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1984.4981           82.6755           109.9682
159.5793            262.1384           291.0805
347.9969            376.4799           435.4536
504.2152            526.0002           577.8632
626.3082            689.2824           772.4624
877.3116            925.2918           944.2674
1016.7547           1036.5645          1069.8357
1104.6733           1110.0099          1161.8959
1212.2982           1275.6507          1290.1107
1353.5253           1371.8910          1376.7065
1455.3543           1569.0197          1774.7764
2973.1973           2992.0208          3035.6566
3051.3003           3146.2402          3759.0546
Zero-point correction (Hartree): 0.109439

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TS.HMVKBO2.15HshiftOH.t
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IRC pathway available
E(CCS(D(T)/Aug-CC-pVDZ) (Hartree): -456.31841429
E(CCS(D/Aug-CC-pVDZ) (Hartree): -456.26241001
  T1 diagnostic: 0.035348
E(MP2/Aug-CC-pVDZ) (Hartree): -456.19762041
E(MP3/Aug-CC-pVDZ) (Hartree): -456.23292148
E(PMP2/Aug-CC-pVDZ) (Hartree): -456.20220625
E(PMP3/Aug-CC-pVDZ) (Hartree): -456.23583228
E(PUHF/Aug-CC-pVDZ) (Hartree): -454.87036633
E(UHF/Aug-CC-pVDZ) (Hartree): -454.86348135
E(CCS(D(T)/Aug-CC-pVTZ) (Hartree): -456.70991292
E(CCS(D/Aug-CC-pVTZ) (Hartree): -456.63172003
  T1 diagnostic: 0.033539
E(MP2/Aug-CC-pVTZ) (Hartree): -456.58735544
E(MP3/Aug-CC-pVTZ) (Hartree): -456.61111167
E(PMP2/Aug-CC-pVTZ) (Hartree): -456.59214593
E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61411650
E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97787761
E(UHF/Aug-CC-pVTZ) (Hartree): -454.97068590
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34568179

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Electronic state : 2-A
Cartesian coordinates (Angs):
O      0.745605   1.501524   -0.620875
O      0.525690   1.231735   0.715991
C      0.116002   -0.084617   0.828991
C      1.341605   -1.004066   0.389523
O      1.799705   -0.579280   -0.802316
H      1.370616   0.652473   -0.913900
H      2.086464   -0.951690   1.189223
H      0.870296   -1.994835   0.318864
H      -0.077107   -0.255372   1.890267
C      -1.154136   -0.432817   0.030386
O      -1.349639   -1.570229   -0.296362
C      -2.129430   0.685590   -0.199325
H      -3.047786   0.277482   -0.608948
H      -2.323876   1.205862   0.739379
H      -1.693744   1.411536   -0.883843
Rotational constants (GHz):   2.8483700   1.9725100   1.4629400
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1158.7670           54.9385           113.6510
130.0334            204.4073           270.6639
335.2259            417.8518           467.2986
518.1767            570.4574           607.4376
673.7363            775.2853           794.0243
873.4363            925.9955           964.5587
972.0458            1038.5901          1062.5708
1139.6786           1179.2062          1205.6529
1241.0571           1283.6026          1323.1509
1349.7309           1422.7638          1431.1558
1454.4978           1755.7741          1803.3453
2896.2745           2980.7331          2987.9592
3009.9441           3055.9995          3099.9579
Zero-point correction (Hartree): 0.108843

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TS.HMVKBO2.15HshiftOH.bis.c
-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.33974626
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.043193   -1.018306   0.443766
O      -0.768707   -1.157121   -0.057623
C      -0.032754   -0.077789   0.359886
C      -0.626854   1.210855   -0.445540
O      -1.945881   1.238620   -0.249758
H      -2.277737   -0.012157   0.127477
H      -0.108463   2.056806   0.026760
H      -0.323068   1.078372   -1.491014
H      -0.196682   0.128820   1.419089

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C      1.435821    -0.249294    -0.002334
O      1.802043    -1.178971    -0.663090
C      2.357317     0.838196     0.483881
H      3.378627     0.469596     0.470850
H      2.286070     1.690195    -0.195677
H      2.085969     1.182787     1.480803
Rotational constants (GHz):   3.4716400   1.5030500   1.1684700
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1013.8197           43.1844           119.0336
 147.8901           193.0349           208.9061
 340.3352           367.1566           469.6613
 481.4378           530.3842           604.0190
 646.9820           671.0444           879.1713
 892.7017           935.8769           967.3829
1009.5274           1072.7320          1123.7730
1172.3153           1206.3595          1217.9980
1226.8518           1275.4401          1344.3337
1362.9907           1426.5258          1437.6367
1469.3026           1808.2405          1831.5482
2895.1876           2961.7268          2979.0601
3005.3212           3045.3523          3092.2116
Zero-point correction (Hartree): 0.109011

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TS.HMVKBO2.15HshiftOH.bis.t
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31690208
E(CCSD/Aug-CC-pVDZ) (Hartree): -456.26077363
  T1 diagnostic: 0.037099
E(MP2/Aug-CC-pVDZ) (Hartree): -456.19580528
E(MP3/Aug-CC-pVDZ) (Hartree): -456.23028948
E(PMP2/Aug-CC-pVDZ) (Hartree): -456.20066373
E(PMP3/Aug-CC-pVDZ) (Hartree): -456.23344478
E(PUHF/Aug-CC-pVDZ) (Hartree): -454.86814107
E(UHF/Aug-CC-pVDZ) (Hartree): -454.86099526
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.70918662
E(CCSD/Aug-CC-pVTZ) (Hartree): -456.63076391
  T1 diagnostic: 0.035250
E(MP2/Aug-CC-pVTZ) (Hartree): -456.58628082
E(MP3/Aug-CC-pVTZ) (Hartree): -456.60915747
E(PMP2/Aug-CC-pVTZ) (Hartree): -456.59135563
E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61241794
E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97640047
E(UHF/Aug-CC-pVTZ) (Hartree): -454.96893868
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.34522621
Electronic state : 2-A

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Cartesian coordinates (Angs):
O      -1.872571     1.215932    -0.410969
O      -0.555085     1.153499    -0.021354
C      -0.038682    -0.056620    -0.434548
C      -0.771555    -1.187352     0.465574
O      -2.091096    -0.997269     0.356708
H      -2.237036     0.248610    -0.044487
H      -0.419101    -2.113343    -0.006419
H      -0.384772    -1.082437     1.486730
H      -0.292586    -0.270700    -1.472514
C      1.457171    -0.144926    -0.172208
O      2.046132    -1.103971    -0.593114
C      2.090804     0.953012     0.627682
H      3.142305     0.729862     0.776189
H      1.967556     1.902771     0.106115
H      1.578167     1.055016     1.585211
Rotational constants (GHz):   3.4397400   1.5178900   1.1907400
Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)
i1201.7934           45.2626           147.6267
 158.5306           183.1466           212.5315
 321.2716           411.0014           473.1626
 486.1009           546.3366           568.8128
 665.5663           681.8361           831.6410
 863.2232           917.4099           982.8861
1012.1289           1069.8365          1123.7764
1189.4767           1195.1637          1204.1936
1229.2232           1276.5268          1320.4431
1357.5302           1419.0248          1426.6049
1466.8381           1778.1354          1802.4415
2903.7104           2966.9422          2983.3432
3027.4038           3044.1597          3099.6627
Zero-point correction (Hartree): 0.108847

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TS.HMVKBO2.HO2elim.pZm
-----
IRC pathway available
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31014617
E(CCSD/Aug-CC-pVDZ) (Hartree): -456.24990038
  T1 diagnostic: 0.033259
E(MP2/Aug-CC-pVDZ) (Hartree): -456.19833979
E(MP3/Aug-CC-pVDZ) (Hartree): -456.21898987
E(PMP2/Aug-CC-pVDZ) (Hartree): -456.22754672
E(PMP3/Aug-CC-pVDZ) (Hartree): -456.24442716
E(PUHF/Aug-CC-pVDZ) (Hartree): -454.87061449
E(UHF/Aug-CC-pVDZ) (Hartree): -454.83893501
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.69941482

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E(CCSD/Aug-CC-pVTZ) (Hartree): -456.61634437  
   T1 diagnostic: 0.033018  
 E(MP2/Aug-CC-pVTZ) (Hartree): -456.58459471  
 E(MP3/Aug-CC-pVTZ) (Hartree): -456.59304969  
 E(PMP2/Aug-CC-pVTZ) (Hartree): -456.61504853  
 E(PMP3/Aug-CC-pVTZ) (Hartree): -456.61953681  
 E(PUHF/Aug-CC-pVTZ) (Hartree): -454.97780129  
 E(UHF/Aug-CC-pVTZ) (Hartree): -454.94481991  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -457.33102745  
 Electronic state : 2-A  
 Cartesian coordinates (Angs):  
   O   -1.600602    1.577093    -0.473492  
   O   -0.381432    1.683747    -0.299410  
   C    0.007739    -0.031122    0.846214  
   C   -1.230978    -0.677766    0.715075  
   H   -1.771137    0.353518    0.220605  
   O   -1.428894    -1.718010    -0.170292  
   H   -0.649465    -1.775960    -0.744313  
   H   -1.816856    -0.804403    1.621860  
   C    1.177094    -0.322897    -0.012823  
   H    0.174297    0.574827    1.725566  
   O    1.094585    -1.112130    -0.933774  
   C    2.440989    0.424506    0.294026  
   H    3.218798    0.143151    -0.408547  
   H    2.245208    1.496359    0.230771  
   H    2.760839    0.210581    1.314851  
 Rotational constants (GHz):    2.4029100    1.8353600    1.2661800  
 Vibrational harmonic frequencies (cm-1): (Scaled by 0.9710)  
   i1027.9926           69.8267           111.2287  
   131.0264            148.6305           204.2438  
   249.0331            340.6202           364.4529  
   456.6042            517.6168           550.8328  
   624.2639            691.3864           715.6867  
   844.1860            909.3656           958.2840  
   1003.7957           1022.7406           1110.1159  
   1171.2932           1196.2076           1257.0953  
   1333.0390           1348.0429           1386.3677  
   1423.0189           1429.0542           1434.3050  
   1509.3672           1549.4444           1736.7490  
   2977.9066           3039.3516           3053.5596  
   3095.1894           3128.6717           3590.9805  
 Zero-point correction (Hartree): 0.109529