



Supplement of

Investigation of the oxidation of methyl vinyl ketone (MVK) by OH radicals in the atmospheric simulation chamber SAPHIR

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S1 Additional Figures

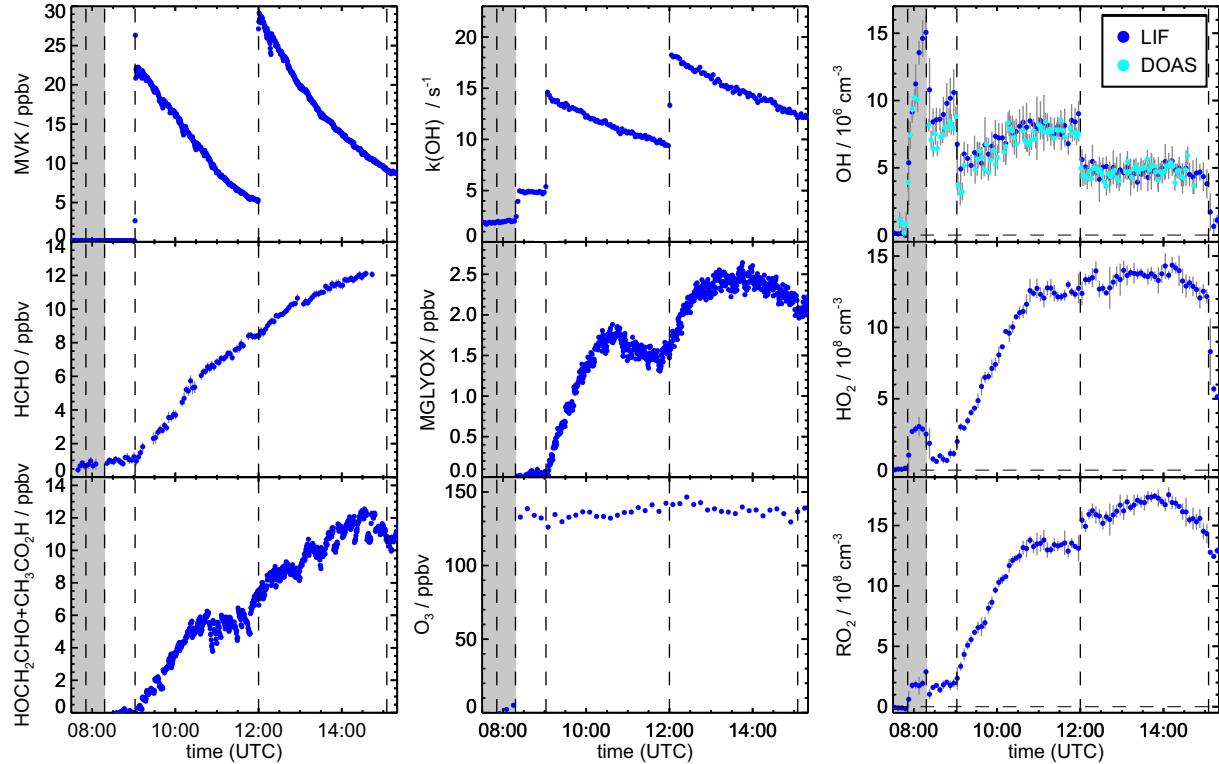


Figure S1 . Time series of radicals, inorganic and organic species during the MVK photooxidation for the high NO experiment (17 May 2017). Dark shaded areas indicate the time before opening the chamber roof and vertical dashed line times when trace gases were injected into the chamber. Model calculations were not performed due to the lack of reliable NO_x measurements in this experiment. Approximately 8 ppbv NO_2 was injected at the beginning of the experiment.

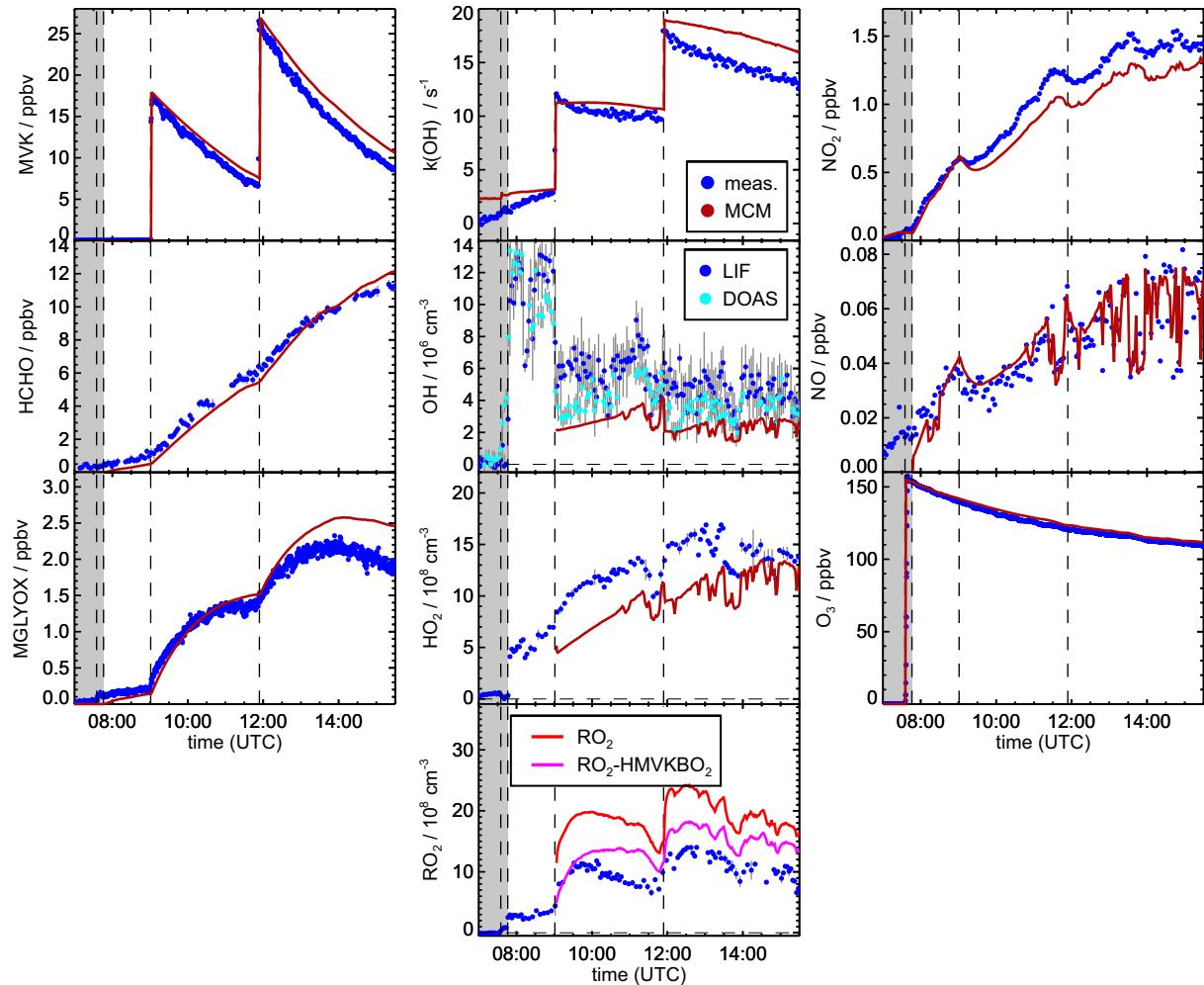


Figure S2 . Time series of radicals, inorganic and organic species during the MVK photooxidation for the low NO experiment (23 June 2016) together with results from model calculations applying MCM. Dark shaded areas indicate the time before opening the chamber roof and vertical dashed line times when 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.

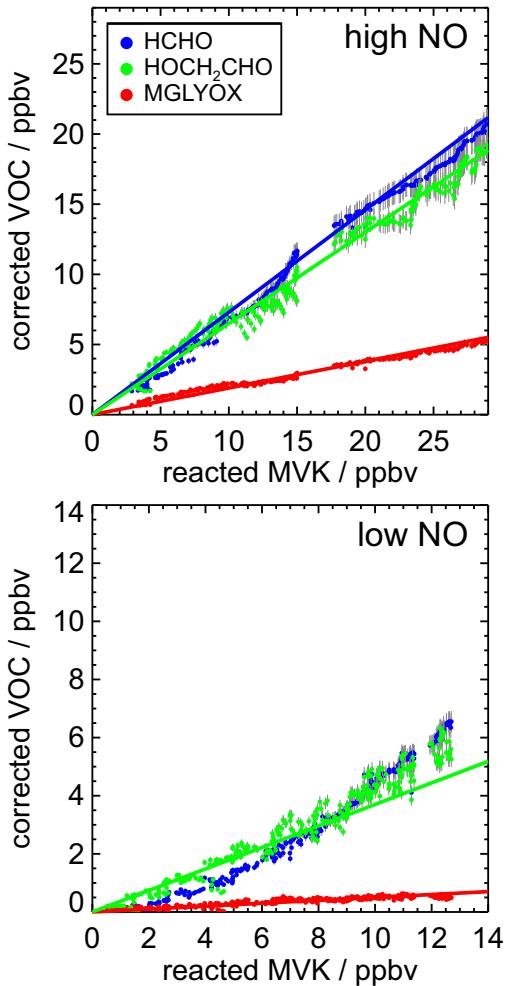


Figure S3 . Corrected product concentrations versus the MVK that reacted away. Corrections are applied to account for production not connected to the oxidation of MVK (small chamber source) and additional loss processes (reaction with OH, photolysis). The slope gives the product yield of the organic compound in the MVK reaction with OH

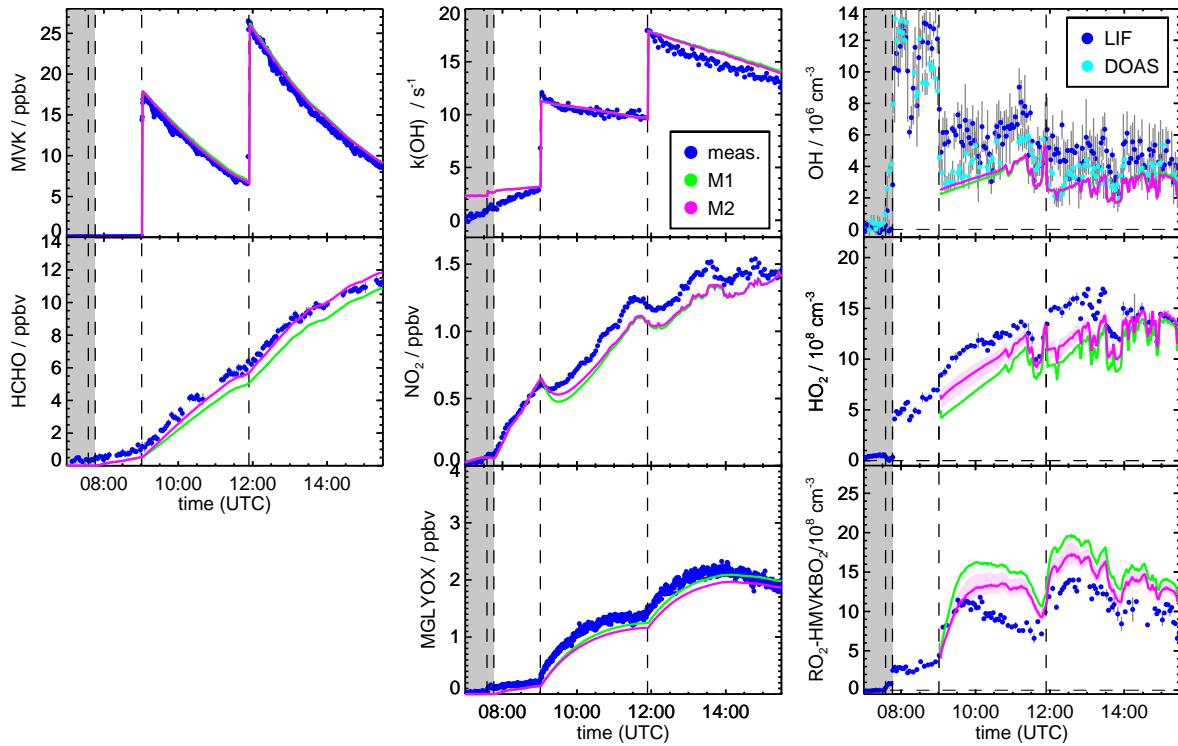


Figure S4. Time series of radicals, inorganic and organic species during the MVK photooxidation at low NO (experiment on 23 June 2016). Dark shaded areas indicate the time before opening the chamber roof and vertical dashed lines when trace gases were injected into the chamber. Model sensitivity runs include additional reaction pathways listed in Table 2 in the main paper.

S2 Theoretical analysis of unimolecular reactions of the primary peroxy radicals

S2.1 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 (Alecu 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 HMVKBO₂ 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 Heicklen, 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.

S2.2 Theoretical results

Table 1 lists barrier heights for the various reaction pathways studied in this work , with the preferred values shown in Fig. 5. For the 1,5-H-migration in HMVKBO₂, 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 α -OH 1,4-H-shift and $-\text{CH}_3$ 1,6-H-shift, with rate enhancements between 10^2 and 10^4 ; as expected, HO₂ 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 endoenergicity 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 α -OH hydrogen atom in HMVKAO₂. 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, 2×10^4 at 300 K, using asymmetric Eckart tunnelling.

The two fastest reactions, both H-migrations in the HMVKAO₂ radicals lead to a product radical that is stabilized by vinoxy 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 S1 . H-migration and HO₂ 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 ⁻¹	$k(300)$ K s ⁻¹
HMVKAO₂ CH ₃ –C(=O)–CH(OH)–CH ₂ OO [•]	–OH 1,5-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	22.0	2.9×10^{-4}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	21.6	5.0×10^{-4}
	α –OH 1,4-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	24.7	1.3×10^{-2}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	24.7	1.5×10^{-2}
				7.7×10^{-4} ^a
	–CH ₃ 1,6-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	23.1	1.5×10^{-3}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	23.1	1.4×10^{-3}
				2.5×10^{-4} ^a
HMVKBO₂ CH ₃ –C(=O)–CH(OO [•])–CH ₂ OH	–OH 1,5-H-shift	B3LYP/6-31+G(d,p)	17.7 ^b	
		CBS-QB3	21.3 ^b	
		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 ^b	
		CBS-APNO	20.0 ^b	7×10^{-3} ^{b,c}
		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	6.0×10^{-5}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	22.5	8.8×10^{-5}
	α –OH 1,4-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	25.2	2.7×10^{-5}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	25.1	3.2×10^{-5}
	–CH ₃ 1,6-H-shift	CCSD(T)/aVTZ//M06-2X/aVTZ	27.4	3.6×10^{-5}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	27.4	3.8×10^{-5}
	HO ₂ elimination	CCSD(T)/aVTZ//M06-2X/aVTZ	29.7	9.5×10^{-10}
		CCSD(T)/CBS(DT)//M06-2X/aVTZ	30.0	6.1×10^{-10}

^aBased on WKB zero-curvature tunnelling

^b Peeters et al. (2009)

^c reported as 0.01 s⁻¹ by Peeters et al. (2009)

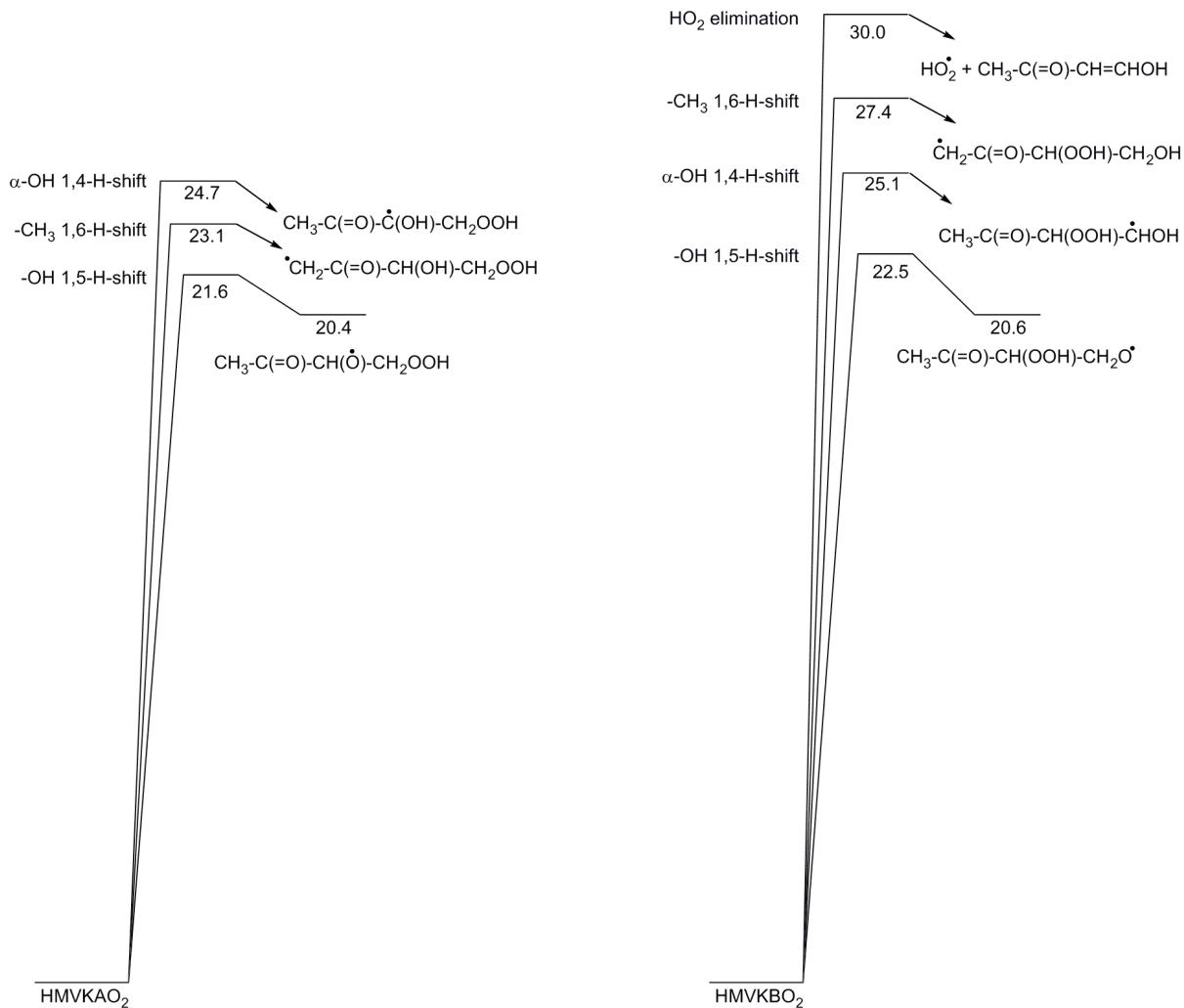


Figure S5. ZPE-corrected potential energy surface at the CCSD(T)/CBS(DT)//M06-2X/aug-cc-pVTZ level of theory, showing the energetics of the HMVKAO₂ and HMVKBO₂ reactions.

Table S2 . 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 cm ³ molecule ⁻¹ s ⁻¹	n	E _a K
HMVKAO₂ CH ₃ —C(=O)—CH(OH)—CH ₂ OO [•]	—OH 1,5-H-shift	1.25×10^{11}	-0.03	9897
	α—OH 1,4-H-shift	4.12×10^{-67}	24.46	-2295
	—CH ₃ 1,6-H-shift	8.97×10^{-29}	12.54	4308
	all unimolecular	7.4×10^{-109}	39.35	-5769
HMVKBO₂ CH ₃ —C(=O)—CH(OO [•])—CH ₂ OH	—OH 1,5-H-shift	7.13×10^{11}	-0.24	10571
	α—OH 1,4-H-shift	3.11×10^{-81}	29.64	-1790
	—CH ₃ 1,6-H-shift	2.05×10^{-57}	21.74	1083
	HO ₂ elimination	2.15×10^{-45}	18.86	7811
	all unimolecular	6.71×10^{-112}	41.14	-3722

^aGeometric 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⁻¹

Population contribution in %

HMVKAO2

Conformer	Erel	%
HMVKAO2.mppt	0.34	23.2
HMVKAO2.mpmt	0.00	19.4
HMVKAO2.hptp	0.68	13.9
HMVKAO2.mmppt	1.08	8.33
HMVKAO2.mtmt	0.92	8.3
HMVKAO2.hmtp	1.71	3.72
HMVKAO2.hmmm	1.16	3.69
HMVKAO2.mmtt	1.44	3.41
HMVKAO2.mmmmt	1.57	3.21
HMVKAO2.mmpm	1.50	2.98
HMVKAO2.mmtm	1.92	2.55
HMVKAO2.hpmm	1.35	1.86
HMVKAO2.http	2.42	1.43
HMVKAO2.mttm	2.91	1.13
HMVKAO2.htmm	2.64	1.05
HMVKAO2.mttt	2.39	1
HMVKAO2.mptt	3.01	0.394
HMVKAO2.tmtm	4.17	0.127
HMVKAO2.htmp	4.16	0.0736
HMVKAO2.hpmt	3.66	0.0597
HMVKAO2.hpmp	3.50	0.0553
HMVKAO2.htm	4.88	0.0445
HMVKAO2.hmt	4.38	0.0366
HMVKAO2.tppp	4.82	0.0153
HMVKAO2.hmmt	4.87	0.0114
HMVKAO2.pmp	5.19	0.00546
HMVKAO2.ppt	5.65	0.00484
HMVKAO2.ptpt	6.12	0.00369
HMVKAO2.pmp	6.11	0.00227
HMVKAO2.hppt	6.23	0.0019
HMVKAO2.mmt	6.11	0.00189
HMVKAO2.hpp	6.20	0.00178
HMVKAO2.mpt	6.18	0.00177
HMVKAO2.tpp	6.40	0.00177
HMVKAO2.tmp	6.53	0.00124
HMVKAO2.ttpt	7.10	0.000732
HMVKAO2.hpp	7.30	0.000598
HMVKAO2.mtt	7.02	0.000573
HMVKAO2.pmp	6.85	0.000273
HMVKAO2.mpp	7.52	0.000266
HMVKAO2.hpp	7.51	0.000231
HMVKAO2.ptp	8.17	0.000134
HMVKAO2.cmp	8.88	5.95e-05
HMVKAO2.mtm	8.78	2.12e-05
HMVKAO2.mmp	8.39	1.97e-05
HMVKAO2.mtp	8.99	1.39e-05

HMVKBO2

Conformer	Erel	%
HMVKBO2.hmmt	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.pmmm	1.28	3.87
HMVKBO2.pttp	1.46	3.6
HMVKBO2.hmmm	1.36	2.72
HMVKBO2.hptm	1.56	2.65
HMVKBO2.pppm	2.07	2.43
HMVKBO2.ptpp	1.55	2.2
HMVKBO2.pptt	2.32	1.38
HMVKBO2.pttm	2.02	1.09
HMVKBO2.ltmt	1.57	0.931
HMVKBO2.htpt	1.97	0.671
HMVKBO2.pptp	2.88	0.658
HMVKBO2.pppm	3.01	0.328
HMVKBO2.ppmr	3.21	0.177
HMVKBO2.pppm	3.68	0.126
HMVKBO2.ltpp	3.14	0.125
HMVKBO2.ltmm	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.tmtt	4.67	0.0219
HMVKBO2.hmpm	5.92	0.0211
HMVKBO2.tmtm	4.74	0.0163
HMVKBO2.tppm	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.ltmm	5.06	0.00699
HMVKBO2.ltpp	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.ltmt	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 . HMVKAO2 . 14HshiftCH2OH

Conformer	Erel	%
TS . HMVKAO2 . 14HshiftCH2OH.dts1	0.00	94.9
TS . HMVKAO2 . 14HshiftCH2OH.uts1	1.79	4.93
TS . HMVKAO2 . 14HshiftCH2OH.umSc	4.38	0.119
TS . HMVKAO2 . 14HshiftCH2OH.dmSc	6.47	0.00315
TS . HMVKAO2 . 14HshiftCH2OH.umSl	7.81	0.000285
TS . HMVKAO2 . 14HshiftCH2OH.dmSl	8.06	0.000178
TS . HMVKAO2 . 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.HMVKBO2.14HshiftCH2OH

Conformer	Erel	%
TS.HMVKBO2.14HshiftCH2OH.umRlp	0.00	99.4
TS.HMVKBO2.14HshiftCH2OH.mmSht	3.58	0.482
TS.HMVKBO2.14HshiftCH2OH.umSlp	5.24	0.0493
TS.HMVKBO2.14HshiftCH2OH.mtShp	5.27	0.0324
TS.HMVKBO2.14HshiftCH2OH.mmRmp	5.50	0.0235
TS.HMVKBO2.14HshiftCH2OH.mmRlp	5.77	0.0217
TS.HMVKBO2.14HshiftCH2OH.mmRhm	5.65	0.0205
TS.HMVKBO2.14HshiftCH2OH.mtRhm	6.20	0.00761
TS.HMVKBO2.14HshiftCH2OH.utRhm	7.11	0.00238
TS.HMVKBO2.14HshiftCH2OH.mtShm	8.00	0.000734
TS.HMVKBO2.14HshiftCH2OH.umScm	8.10	0.000502
TS.HMVKBO2.14HshiftCH2OH.utScm	8.05	0.000494
TS.HMVKBO2.14HshiftCH2OH.mmScm	9.25	0.000384
TS.HMVKBO2.14HshiftCH2OH.mpSlt	10.27	2.29e-05
TS.HMVKBO2.14HshiftCH2OH.mtRct	9.96	2.03e-05
TS.HMVKBO2.14HshiftCH2OH.mpRhm	10.65	1.32e-05
TS.HMVKBO2.14HshiftCH2OH.utRct	10.53	7.49e-06

TS.HMVKBO2.15HshiftOH

Conformer	Erel	%
TS.HMVKBO2.15HshiftOH.t	0.00	56.5
TS.HMVKBO2.15HshiftOH.bis.t	0.46	43.4
TS.HMVKBO2.15HshiftOH.bis.c	4.10	0.15

TS.HMVKBO2.15HshiftCH3

Conformer	Erel	%
TS.HMVKBO2.15HshiftCH3.bis.pm	0.00	24.5
TS.HMVKBO2.15HshiftCH3.mp	0.34	20.2
TS.HMVKBO2.15HshiftCH3.tm	0.36	12.2
TS.HMVKBO2.15HshiftCH3.bis.mp	0.78	11.3
TS.HMVKBO2.15HshiftCH3.bis.pp	0.82	10.4
TS.HMVKBO2.15HshiftCH3.bis.pt	1.02	6.47
TS.HMVKBO2.15HshiftCH3.bis.tm	0.82	6.38
TS.HMVKBO2.15HshiftCH3.pm	0.96	5.97
TS.HMVKBO2.15HshiftCH3.mt	2.34	0.717
TS.HMVKBO2.15HshiftCH3.pp	2.40	0.626

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TS.HMVKB02.15HshiftCH3.bis.mm 2.63 0.614
TS.HMVKB02.15HshiftCH3.bis.mt 2.74 0.466
TS.HMVKB02.15HshiftCH3.mm      3.00 0.208
TS.HMVKB02.15HshiftCH3.tp      4.81 0.0165
TS.HMVKB02.15HshiftCH3.tt      5.65 0.00444
```

TS.HMVKB02.HO2elim

Conformer	Erel	%
TS.HMVKB02.HO2elim.cZm	0.00	95.1
TS.HMVKB02.HO2elim.mEc	2.23	3.24
TS.HMVKB02.HO2elim.cEc	3.29	0.723
TS.HMVKB02.HO2elim.mEt	3.81	0.362
TS.HMVKB02.HO2elim.mZt	4.12	0.19
TS.HMVKB02.HO2elim.cEt	4.30	0.181
TS.HMVKB02.HO2elim.pEt	4.50	0.101
TS.HMVKB02.HO2elim.pZl	4.88	0.0572
TS.HMVKB02.HO2elim.pZt	5.15	0.0356
TS.HMVKB02.HO2elim.mZh	7.44	0.000766
TS.HMVKB02.HO2elim.mZc	7.86	0.000462

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

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HMVKAO2.mpmmt
-----
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
H      -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

HMVKAO2.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

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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
    H      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

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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

 HMVKAO2.hpmpp

 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 3765.7256
 Zero-point correction (Hartree): 0.115027

 HMVKAO2.hpmpt

 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

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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): 0.1115081

HMVKAO2.hptp
-----
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): 0.1115486

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): 0.1115176

HMVKAO2.htm
-----
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

```

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

HMVKAO2.htm

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

HMVKAO2.htm

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 -0.222286 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
 261.2693 312.2695 391.9313

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

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.mmmmt

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 1.15753800 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

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

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HMVKAO2.mmpt

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

HMVKAO2.mmmtm

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

HMVKAO2.mptt
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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

HMVKAO2.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

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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

HMVKAO2.mtmt

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	1.9335852	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

HMVKAO2.mtm

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	1.933232	-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	2950.2555
2982.3242	3001.1129	3050.2723
3062.8517	3093.4871	3649.4865

Zero-point correction (Hartree): 0.115046

HMVKAO2.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

HMVKAO2.tppp
-----
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

HMVKBO2.hmmm
-----
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

HMVKBO2.hmmmt
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.36228035
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.75274738
E(CCSD/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
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
    O      0.193985      1.772848     -0.519474
    C     -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
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
Zero-point correction (Hartree): 0.115715

HMVKBO2.hptm
-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38560665
Electronic state : 2-A
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

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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

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HMVKBO2.hptt

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

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HMVKBO2.ltmm

E(UM062X/Aug-CC-pVTZ) (Hartree): -457.38275007

Electronic state : 2-A

Cartesian coordinates (Angs):

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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      0.176661    -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    -1.090585
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

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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.ltmp
-----
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   -1.378298
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.pmmmp
-----
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

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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.pppmm

 E(UVQ6Z/X/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
 HMVKBO2.pppmp

 E(UVQ6Z/X/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

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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.ppmmt
-----
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
-----
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
-----
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

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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.pppt

 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

 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

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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
-----
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
-----
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
-----
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

HMVKBO2.ptmt
-----
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
  H      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       998.9983
 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

HMVKBO2.ptpp
-----
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      0.2029239   -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

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

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.HMVKA02.14HshiftCH2OH.dtsl

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)
 i2103.8767 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

 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): 3.3842900 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

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

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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

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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

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
C      -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

TS.HMVKB02.15HshiftCH3.bis.pn
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IRC pathway available
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31237540
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.70300785
E(CCSD/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

TS.HMVKB02.15HshiftOH.t
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IRC pathway available
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31841429
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -456.70991292
E(CCSD/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
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

TS.HMVKBO2.15HshiftOH.bis.c
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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
 TS.HMVKB02.15HshiftOH.bis.t

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -456.31690208
 E(CCSD/Aug-CC-pVDZ) (Hartree): -456.26077363
 T1 diagnostic: 0.037093
 E(MP2/Aug-CC-pVDZ) (Hartree): -456.1580528
 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
 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 -1.472204
 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
 TS.HMVKB02.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): -456.69491482

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