Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The reaction of Criegee Intermediates with NO, RO_2, and SO_2, and their fate in the atmosphere.

- Supporting Information -

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Table of content

Loss process contributions with adjusted rates of reactions with H_2O and $(H_2O)_2$

Table S1 : Loss process contributions with the rate of reaction of SCI + H_2O reduced by a factor of 100 compared to the values listed in Table 4. The rates of reaction with $(H_2O)_2$ was likewise scaled down to adhere to the ratios listed in Table 5 (see main text).

Loss path	Boreal forest	Tropical forest	Mega city	Rural Europe
		H_2COO		
H_2O	0.12	0.08	0.14	0.13
$(H_2O)_2$	0.86	0.92	0.60	0.87
NO_2			0.09	
SO_2	0.01		0.05	
CO			0.02	
Carbonyl compounds			0.04	
Hydroxyl compounds	0.01		0.06	
		Anti-CH_3CHOO		
H_2O	0.82	0.78	0.81	0.83
$(H_2O)_2$	0.12	0.18	0.07	0.11
Ester channel	0.06	0.04	0.09	0.06
NO_2			0.01	
SO_2			0.01	
		Syn-CH_3CHOO		
H_2O		0.01		0.01
$(H_2O)_2$	0.07	0.31		0.12
VHP channel	0.11	0.23	0.02	0.22
NO_2	0.02	0.02	0.34	0.26
SO_2	0.20		0.19	0.15
CO	0.04	0.06	0.06	0.05
Carbonyl compounds	0.18	0.06	0.14	0.19
Carboxylic acids	0.15	0.15		
Hydroxyl compounds	0.23	0.14	0.25	
		$(CH_3)_2COO$		
H_2O	0.02	0.03		0.02
$(H_2O)_2$		0.01		
VHP	0.68	0.86	0.25	0.83
NO_2	0.01		0.26	0.07
SO_2	0.08		0.14	0.03
CO	0.01	0.01	0.07	0.01
Carbonyl compounds	0.06	0.02	0.10	0.04
Carboxylic acids	0.05	0.04		
Hydroxyl compounds	0.09	0.03	0.18	
		***Syn*-CH_3-*anti*-(*trans*-$CH{=}CH_2$)-COO**		
H_2O				
$(H_2O)_2$				
VHP	0.08	0.22	0.01	0.16

NO_2	0.02	0.03	0.33	0.34
SO_2	0.23		0.19	0.19
CO	0.04	0.10	0.09	0.07
Carbonyl compounds	0.20	0.10	0.13	0.24
Carboxylic acids	0.17	0.27		
Hydroxyl compounds	0.26	0.26	0.25	
HO_2 and RO_2		0.02		0.01
		***Syn*-CH_3-*anti*-(*cis*-$CH{=}CH_2$)-COO**		
H_2O				
$(H_2O)_2$				
VHP	0.45	0.76	0.11	0.66
NO_2	0.01	0.01	0.30	0.13
SO_2	0.14		0.17	0.09
CO	0.02	0.04	0.08	0.03
Carbonyl compounds	0.12	0.03	0.12	0.09
Carboxylic acids	0.10	0.08		
Hydroxyl compounds	0.16	0.08	0.22	

RRKM Master Equation analysis of the H_2COO and $(CH_3)_2COO$ + SO_2 reactions

To assess the product distribution of the SCI + SO_2 reaction as a function of pressure and SCI substitution, we performed a series of Master Equation analysis on this system. Rate coefficients were obtained in the rigid-rotor harmonic-oscillator approximation using RRKM rate theory, where the energy-specific rate coefficient for H-elimination and H-migration processes was further improved by tunneling corrections using the Eckart formalism. N_2 was used as a bath gas (ε = 48K, σ = 3.9 Å), with ε = 48K, σ=3.9 Å as collision parameters for the **SOZ** and **INT1** intermediates. An exponential energy-down model was used to describe collisional energy loss for these intermediates, using a ΔE_{down} value of 250 cm^{-1}. All other products were considered sinks, and redissociation to the reactants was included in the kinetic model. The master equation was solved by eigenvalue/eigenvector analysis of its matrix representation, followed by Bartis-Widom analysis to obtain a kinetic description of the overall chemistry. All calculations were performed using Mesmer 0.2.

The H_2COO + SO_2 reaction was found to be in the low-pressure regime in atmospheric conditions, with negligible contribution of stabilization of the **SOZ** or **INT1** intermediates up to 100 atm. Direct formation of HCOOH + SO_3 from **SOZ** through **TSisom** is negligible, leaving **TSopen** as the main **SOZ** reaction channel, forming **INT1**. **INT1** in turn decomposes promptly, with 68% going through **TS1**, forming H_2CO + SO_3, 15% forming the formyl sulfinic ester HC(=O)-OS(=O)OH through **TS2**, and 17% of the reaction flux proceeding through **TS3**, forming singlet bisoxy + SO_2. H-elimination through **TS4** has a much smaller contribution of less than 1%. These predictions are in good agreement with the available experimental data. Percival *et al*. reported carbonyl and SO_3 as observable reaction products in the CH_3CHOO + SO_2 reaction. Hatakeyama *et al*. likewise indirectly observed SO_3 formation through its H_2SO_4 hydrolysis product. These latter authors also observed HCOOH and SO_2 as reaction products, where an oxygen exchange occurred between the SCI moiety and the SO_2 reaction partner. This latter observation agrees with our prediction of a sizeable reaction flux through the **SBO** + SO_2 channel, which shows the required oxygen exchange, and where the **SBO** is known to isomerize rapidly to HCOOH. It should be noted that this HCOOH product is formed with a significant energy content ("hot acid"), and is in turn likely to decompose promptly at low pressures such as used in the Advanced Light Source experiments of Welz *et al*. (4 Torr). The formyl sulfinic ester has not been observed to our knowledge. Hatakeyama *et al*. did not observed sulphur-containing compounds other than H_2SO_4, but it is unclear whether the ester would

undergo chemically activated reactions, or what the secondary chemistry of the ester would be under their reaction conditions.

The $(CH_3)_2COO$ + SO_2 **SOZ** adduct has a significantly higher number of degrees of freedom, compared to the H_2COO + SO_2 adduct, leading to a longer lifetime of the nascent **SOZ** at the same internal energy and exit barrier heights. Our M06-2X/aug-cc-pVTZ calculations, and the literature theoretical work by Jiang et al. and Kurtén et al., furthermore suggest that the addition exoergicity for $(CH_3)_2COO$ is less than for H_2COO, reducing the nascent energy content of the **SOZ**, and again increasing the lifetime of the **SOZ**. The increased lifetime will lead to increased collisional energy loss. At this time, we do not have CCSD(T)//M06-2X energies available for this large molecule, so we used the M06-2X energies without adjustments. The main difference is that this latter level of theory overestimates the reaction exoergicity compared to higher-level calculations, and hence will underestimate collisional stabilization. Also, the subsequent reaction chemistry of the **SOZ**, and the ring-openened **INT1** is as yet not fully characterized. It is expected that the lowest reaction channel for the **SOZ** is the ring opening to **INT1**; methyl radical elimination seems to have a higher barrier, while a 1,2-CH_3-migration directly forming an ester and SO_3, i.e. a transformation similar to the ester channel in the ozonolysis, and 1,3-H-migration, forming a vinyl-hydroperoxide + SO_3 directly, are all predicted to have barriers close to or above the free reactants. For **INT1**, the lowest-energy exit channel is again expected to be formation of acetone + SO_3 . Methyl radical elimination or migration are expected to have higher barriers.
At 1 atm., we find that 97% of the nascent **SOZ** is stabilized by collisional energy loss, while only 3% directly forms **INT1** and, through that, acetone + **SO_3** or other products. As explained above, higher-level calculations are expected to yield a slightly lower prompt decomposition contribution. At 4 Torr, a typical pressure in many experimental apparatus, 83% of the nascent **SOZ** is predicted to decompose promptly, with only 17% of collisionally stabilized **SOZ**.

From the above reaction trend, SCI of intermediate size, i.e. *syn*- or *anti*-CH_3CHOO, are predicted to decompose at lower pressures, but undergo significant if not dominant stabilization at the **POZ** stage at atmospheric pressures. SCI with more than two carbons in their substituents, including the many SCI formed from isoprene, monoterpenes and sesquiterpenes, are all expected to be near-completely thermalized at atmospheric pressures.

The stabilized **SOZ** are predicted to have comparatively long thermal lifetimes, of the order of seconds and longer. As such, they are susceptible to undergo secondary reactions with available

coreactants in the atmosphere. For unsaturated **SOZ**, this could involve reactions with the main atmospheric oxidants OH, O_3, and NO_3. The **SOZ** is also expected to form stable complexes with water molecules; these molecules can catalyze or inhibit specific unimolecular reactions of the **SOZ**, possibly inhibiting carbonyl + SO_3 formation in favour of the more stable acid/ester + SO_2 products. If so, the SO_2 and H_2O co-reactants would mostly act as a catalyst in the isomerisation of the SCI formed in the ozonolysis of alkenes. Speculatively, the sulfur-bearing **SOZ** could also be a minor source of organosulfates observed in many aerosols (Hallquist et al.)

References

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Quantum chemical data on CH_2OO + NO

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CH2O2
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33090768
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29641516
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28517619
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28337167
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.28517619
E(PMP3/Aug-CC-pVTZ) (Hartree): -189.28337167
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.63398053
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63398053
E(UHF/Aug-CC-pVTZ) (Hartree): -188.63398053
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -189.28517752
     T1 diagnostic:  0.000001
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -189.33090823
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -189.32926563
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -189.29641531
     T1 diagnostic:  0.042398
     D1 diagnostic:  0.169927
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -189.33614628
E(RHF/AUG-CC-PVTZ) (Hartree): -188.63398063
E(UM052X+HF-M052X/Aug-CC-pVDZ) (Hartree): -189.57322403
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.055305     -0.201474       0.000000
     O       0.000000      0.461914       0.000000
     O      -1.160833     -0.197053       0.000000
     H       0.980834     -1.287699       0.000000
     H       1.974003      0.377649       0.000000
Rotational constants (GHz):   80.1459800   12.7489700   10.9992900
Vibrational harmonic frequencies (cm-1):
      547.9295 (  A')           700.1734 (  A")           953.1161 (  A')
     1017.1748 (  A")          1261.2826 (  A')          1429.8355 (  A')
     1617.2061 (  A')          3194.1947 (  A')          3355.7754 (  A')
Zero-point correction (Hartree): 0.032069

CH2O
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.34281335
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.32541814
E(MP2/Aug-CC-pVTZ) (Hartree): -114.31622683
E(MP3/Aug-CC-pVTZ) (Hartree): -114.32035125
E(RHF/Aug-CC-pVTZ) (Hartree): -113.91392630
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -114.31622674
     T1 diagnostic:  0.000001
E(RHF/AUG-CC-PVTZ) (Hartree): -113.91392637
E(RM052X+HF-M052X/Aug-CC-pVDZ) (Hartree): -114.49822703
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     C       0.000000      0.000000     -0.529092
     O       0.000000      0.000000      0.674025
     H       0.000000      0.942755     -1.108823
     H       0.000000     -0.942755     -1.108823
Rotational constants (GHz):  282.1007400   39.0455800   34.2983500
Vibrational harmonic frequencies (cm-1):
     1233.1451                 1270.5100                 1539.0164
     1857.8363                 3000.2928                 3079.9605
Zero-point correction (Hartree): 0.027294
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NO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -129.72583754
E(CCSD/Aug-CC-pVTZ) (Hartree): -129.70667728
E(MP2/Aug-CC-pVTZ) (Hartree): -129.70233503
E(MP3/Aug-CC-pVTZ) (Hartree): -129.69822927
E(PMP2/Aug-CC-pVTZ) (Hartree): -129.70697179
E(PMP3/Aug-CC-pVTZ) (Hartree): -129.70118248
E(PUHF/Aug-CC-pVTZ) (Hartree): -129.30565632
E(UHF/Aug-CC-pVTZ) (Hartree): -129.29953045
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -129.70767870
     T1 diagnostic:  0.000702
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -129.72596118
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -129.72545464
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -129.70625445
     T1 diagnostic:  0.020700
     D1 diagnostic:  0.048601
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -129.72730031
E(ROHF/AUG-CC-PVTZ) (Hartree): -129.29189210
E(UM052X/Aug-CC-pVDZ) (Hartree): -129.89573917
Point group : C*V
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.532976
     N       0.000000      0.000000      -0.609115
Rotational constants (GHz):    0.0000000   51.8922231   51.8922231
Vibrational harmonic frequencies (cm-1):
     2085.7045 (  SG)
Zero-point correction (Hartree): 0.004752

NO2
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -204.81652837
E(CCSD/Aug-CC-pVTZ) (Hartree): -204.77957582
E(MP2/Aug-CC-pVTZ) (Hartree): -204.79501620
E(MP3/Aug-CC-pVTZ) (Hartree): -204.76823071
E(PMP2/Aug-CC-pVTZ) (Hartree): -204.79880607
E(PMP3/Aug-CC-pVTZ) (Hartree): -204.77004157
E(PUHF/Aug-CC-pVTZ) (Hartree): -204.12171482
E(UHF/Aug-CC-pVTZ) (Hartree): -204.11556105
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -204.80094033
     T1 diagnostic:  0.000632
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -204.81671466
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -204.81569439
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -204.77903318
     T1 diagnostic:  0.024650
     D1 diagnostic:  0.063493
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -204.81977900
E(ROHF/AUG-CC-PVTZ) (Hartree): -204.10670346
E(UM052X/Aug-CC-pVDZ) (Hartree): -205.07639771
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     O       1.093429     -0.138568       0.000000
     N       0.000000      0.316624       0.000000
     O      -1.093429     -0.138477       0.000000
Rotational constants (GHz):  250.4785300   13.2136900   12.5515500
Vibrational harmonic frequencies (cm-1):
      781.1343 (  A')          1482.7239 (  A')          1814.3630 (  A')
Zero-point correction (Hartree): 0.009291
```

CH2O2..NO complex 4-membered ring

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.06173093
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.00730022
E(MP2/Aug-CC-pVTZ) (Hartree): -318.99378259
E(MP3/Aug-CC-pVTZ) (Hartree): -318.98652051
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99784943
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.98899519
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.93909897
E(UHF/Aug-CC-pVTZ) (Hartree): -317.93341682
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.99852147
T1 diagnostic: 0.000422
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.06182568
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05972689
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.00687703
T1 diagnostic: 0.035199
D1 diagnostic: 0.165689
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06840096
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.92583753
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.47468658
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.499783	-0.882598	0.222469
O	1.402759	0.209555	-0.369206
O	0.646683	1.157947	0.199423
H	0.985692	-1.003999	1.173524
H	2.112481	-1.630311	-0.272862
N	-1.363093	-0.439881	-0.219972
O	-2.368844	0.008631	0.082825

Rotational constants (GHz): 11.6649200 2.6315400 2.2550200
Vibrational harmonic frequencies (cm-1):

24.7668	96.8494	112.4996
153.3090	190.5048	549.7414
697.4023	951.2828	1027.1198
1260.8699	1432.5686	1623.5375
2077.0878	3199.1505	3357.6741

Zero-point correction (Hartree): 0.038169

CH2O2..NO complex 5-membered ring

E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.98660245
T1 diagnostic: 0.000497
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05385876
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05165090
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -318.99800824
T1 diagnostic: 0.038275
D1 diagnostic: 0.178233
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06101160
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.91634173
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.47472640
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-1.156142	-0.959265	0.222030
O	-1.187783	0.116364	-0.409880
O	-0.690809	1.201263	0.193504
N	1.717937	0.469954	0.008739
O	1.532150	-0.662285	-0.074386
H	-0.768703	-0.953258	1.238592
H	-1.548463	-1.823561	-0.305837

Rotational constants (GHz): 9.3506200 3.7769800 2.8603500
Vibrational harmonic frequencies (cm-1):

```
       58.6666                 117.0199                 169.1615
      205.2761                 239.2229                 554.2789
      709.3964                 962.7948                1037.4043
     1263.1875                1433.2849                1618.0128
     2010.3582                3200.6367                3360.6738
Zero-point correction (Hartree): 0.038591

SOZ
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.08769669
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.03588388
E(MP2/Aug-CC-pVTZ) (Hartree): -319.02122002
E(MP3/Aug-CC-pVTZ) (Hartree): -319.02391182
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.02450761
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.02596990
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.96438431
E(UHF/Aug-CC-pVTZ) (Hartree): -317.95939684
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.02281560
     T1 diagnostic:  0.000614
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.08777257
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.08666711
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.03570830
     T1 diagnostic:  0.024119
     D1 diagnostic:  0.095493
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.09113610
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.95224765
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.51056396
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.088263      0.175634       0.182735
     O       0.511197     -1.009829      -0.270723
     O      -0.835833     -0.792617       0.189003
     N      -1.117180      0.514780      -0.060032
     O       0.080891      1.152283      -0.108484
     H       1.268563      0.156147       1.263369
     H       1.972082      0.387884      -0.417917
Rotational constants (GHz):    9.1372600    8.8049900    4.8400200
Vibrational harmonic frequencies (cm-1):
      216.2006                 358.8643                 759.4758
      781.1976                 873.9239                 967.1480
      985.4125                1080.5339                1118.9514
     1160.9788                1244.2432                1392.6782
     1521.3725                3133.9536                3252.7535
Zero-point correction (Hartree): 0.042938

ONCH2OO.pc
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.07868829
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.02941689
E(MP2/Aug-CC-pVTZ) (Hartree): -319.00729069
E(MP3/Aug-CC-pVTZ) (Hartree): -319.01365678
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.01022161
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.01542208
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.97003847
E(UHF/Aug-CC-pVTZ) (Hartree): -317.96524874
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.00767470
     T1 diagnostic:  0.000757
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.07869266
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.07788943
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.02920137
     T1 diagnostic:  0.029678
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     D1 diagnostic:  0.136954
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.08258458
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.95833976
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.50152466
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.012402      0.973700       0.114910
     O      -1.005201      0.212391      -0.499439
     O      -1.449263     -0.699268       0.324204
     H       0.174287      1.868068      -0.492893
     H      -0.261108      1.223991       1.144776
     N       1.325422      0.266383       0.197675
     O       1.296272     -0.862990      -0.165398
Rotational constants (GHz):   10.9621900    4.6069200    3.6338900
Vibrational harmonic frequencies (cm-1):
      128.5020                 202.1928                 325.7384
      499.7588                 781.5991                 817.6986
      946.3253                1049.2340                1219.1441
     1284.2390                1350.9978                1442.7633
     1790.8398                3143.6382                3220.4312
Zero-point correction (Hartree): 0.041470

ONCH2OO.tt
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E(UM052X/Aug-CC-pVDZ) (Hartree): -319.49720786
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.022372      0.392914       0.000335
     O       1.103063     -0.493916       0.000336
     H      -0.009898      1.002655       0.908752
     H      -0.009427      1.003198      -0.907708
     N      -1.219612     -0.475929      -0.000229
     O      -2.221583      0.171401      -0.000132
     O       2.204875      0.193536      -0.000385
Rotational constants (GHz):   37.0691600    2.5439400    2.4184500
Vibrational harmonic frequencies (cm-1):
       49.6863                  68.3046                 257.6756
      472.1786                 587.1222                 873.4439
      987.2421                1116.0029                1196.9174
     1284.0605                1352.7356                1443.3698
     1778.5973                3131.8112                3214.2109
Zero-point correction (Hartree): 0.040582

CH2OONO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.05647994
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.00258070
E(MP2/Aug-CC-pVTZ) (Hartree): -318.99439516
E(MP3/Aug-CC-pVTZ) (Hartree): -318.98773375
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99653325
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.98910932
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.92390647
E(UHF/Aug-CC-pVTZ) (Hartree): -317.92070865
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.99484423
     T1 diagnostic:  0.000489
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05650021
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05516447
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.00249789
     T1 diagnostic:  0.023325
     D1 diagnostic:  0.066734
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06034717
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E(ROHF/AUG-CC-PVTZ) (Hartree): -317.91627601
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.47249320
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.827673     -0.578476       0.087057
     O      -1.119087      0.528089      -0.285961
     O       0.102759      0.536748       0.403119
     H      -2.754043     -0.657701      -0.469310
     H      -1.699300     -0.921027       1.108617
     N       1.013160     -0.233060      -0.406718
     O       2.057235     -0.229711       0.093513
Rotational constants (GHz):   21.2624300    3.1472300    2.9962900
Vibrational harmonic frequencies (cm-1):
      108.3845                  192.2054                  231.3009
      401.4093                  488.4808                  570.6460
      643.5528                  806.2298                 1033.1600
     1166.0035                 1214.3747                 1442.9062
     1882.7887                 3206.6696                 3364.2129
Zero-point correction (Hartree): 0.038165

cyc-OOCH2NO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.05941208
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.00517058
E(MP2/Aug-CC-pVTZ) (Hartree): -318.99430060
E(MP3/Aug-CC-pVTZ) (Hartree): -318.99191555
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99863301
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.99442694
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.92221150
E(UHF/Aug-CC-pVTZ) (Hartree): -317.91570991
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.99965607
     T1 diagnostic:  0.000779
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05952532
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05847680
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.00469827
     T1 diagnostic:  0.027329
     D1 diagnostic:  0.106284
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06270556
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.90603115
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.48045249
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.496522      0.975410       0.049290
     O      -1.415107     -0.101039       0.017496
     H      -0.703099      1.742079      -0.699271
     H      -0.322722      1.369881       1.056156
     N       0.605538      0.033759      -0.309661
     O       1.732629      0.022592       0.119235
     O      -0.346749     -1.071644       0.052644
Rotational constants (GHz):   13.2957300    5.3783200    4.0284300
Vibrational harmonic frequencies (cm-1):
      188.0891                  387.3095                  473.5278
      649.3999                  823.9195                  983.4174
     1015.9580                 1095.0846                 1110.9475
     1150.4316                 1341.6548                 1520.8199
     1649.4667                 3134.8728                 3231.0456
Zero-point correction (Hartree): 0.042729

OCH2ONO.mt
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.14134447
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E(CCSD/Aug-CC-pVTZ) (Hartree): -319.09188744
E(MP2/Aug-CC-pVTZ) (Hartree): -319.06912568
E(MP3/Aug-CC-pVTZ) (Hartree): -319.07387370
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.07661422
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.07916748
E(PUHF/Aug-CC-pVTZ) (Hartree): -318.04298538
E(UHF/Aug-CC-pVTZ) (Hartree): -318.03427953
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.07761518
     T1 diagnostic:  0.000554
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.14162490
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.14043723
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.09191963
     T1 diagnostic:  0.022831
     D1 diagnostic:  0.069020
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.14505484
E(ROHF/AUG-CC-PVTZ) (Hartree): -318.02823042
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.56414056
Electronic state : 2-A
Cartesian coordinates (Angs):
     O      -1.869242     -0.666393      -0.178637
     C      -1.178851      0.409103       0.230997
     O       0.114795      0.540831      -0.359280
     N       1.032455     -0.222763       0.371981
     O       2.086525     -0.196603      -0.121749
     H      -1.730527      1.321856      -0.041646
     H      -1.080180      0.360188       1.329127
Rotational constants (GHz):   21.0175100    2.9973800    2.8325000
Vibrational harmonic frequencies (cm-1):
       79.1654                184.5684                352.4494
      516.0257                695.3135                780.0055
      867.5080               1080.5952               1128.0741
     1233.3738               1361.0376               1385.2630
     1859.1252               3045.3450               3105.6521
Zero-point correction (Hartree): 0.040263

OCH2ONO.pc
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E(UM052X/Aug-CC-pVDZ) (Hartree): -319.56308743
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.980521      0.278848       0.399744
     O       1.493958     -0.690809      -0.374081
     O      -1.242807     -0.834396       0.202713
     N      -1.322403      0.257017      -0.219868
     O      -0.135532      0.975165      -0.175726
     H       0.706044     -0.134041       1.381951
     H       1.742697      1.062147       0.535419
Rotational constants (GHz):   11.2204100    4.6621300    3.6825000
Vibrational harmonic frequencies (cm-1):
      125.0470                266.3470                358.7052
      565.7370                674.8910                829.5383
      914.7828                992.2720               1127.8834
     1228.0546               1363.8501               1380.4148
     1794.8429               3065.4894               3113.8758
Zero-point correction (Hartree): 0.040555

OCH2NO2
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.11683965
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.06487713
E(MP2/Aug-CC-pVTZ) (Hartree): -319.05901947
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E(MP3/Aug-CC-pVTZ) (Hartree): -319.05231122
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.06144416
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.05383154
E(PUHF/Aug-CC-pVTZ) (Hartree): -318.00689040
E(UHF/Aug-CC-pVTZ) (Hartree): -318.00301795
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.05922739
     T1 diagnostic:  0.000484
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.11683909
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.11567214
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.06477221
     T1 diagnostic:  0.024248
     D1 diagnostic:  0.088753
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.12067718
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.99749500
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.56150068
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.793983     -0.634478       0.000055
     O       1.830644      0.196291      -0.000061
     H       0.791733     -1.280988      -0.891878
     H       0.791773     -1.280746       0.892166
     N      -0.571483      0.057453      -0.000001
     O      -1.511663     -0.708599      -0.000039
     O      -0.612359      1.258112       0.000023
Rotational constants (GHz):   11.5899200    4.5452900    3.3339700
Vibrational harmonic frequencies (cm-1):
       62.2363                306.3825                519.6828
      556.1448                725.2839                804.3736
      933.9713               1186.5179               1187.5379
     1337.5826               1355.5127               1514.1686
     1766.3918               3062.6733               3115.2981
Zero-point correction (Hartree): 0.041995

TS.SOZ.CH2OO+NO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.05060473
E(CCSD/Aug-CC-pVTZ) (Hartree): -318.99017002
E(MP2/Aug-CC-pVTZ) (Hartree): -318.98449992
E(MP3/Aug-CC-pVTZ) (Hartree): -318.96968053
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99055219
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.97432848
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.90790542
E(UHF/Aug-CC-pVTZ) (Hartree): -317.90048644
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.98847242
     T1 diagnostic:  0.000543
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05101121
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.04922977
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -318.98991518
     T1 diagnostic:  0.035149
     D1 diagnostic:  0.150482
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.05804171
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.89255944
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.46653807
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.848760      0.923723       0.254796
     O       1.077191     -0.151255      -0.380674
     O       0.407743     -1.187137       0.167523
     N      -1.355611     -0.454886       0.043845
     O      -1.157284      0.706993      -0.150401
     H       0.565825      0.865204       1.300904
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     H       1.209691      1.827854      -0.228184
Rotational constants (GHz):    9.4461500    5.9681200    3.9837900
Vibrational harmonic frequencies (cm-1):
     i355.7280                 155.7033                 333.8228
      467.1035                 570.7485                 630.3264
      809.6792                1019.3321                1091.7479
     1247.4930                1406.6190                1568.1983
     1664.8528                3215.2390                3363.7419
Zero-point correction (Hartree): 0.039970

TS.ONCH2OO.CH2OO+NO
-------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.04493089
E(CCSD/Aug-CC-pVTZ) (Hartree): -318.98974828
E(MP2/Aug-CC-pVTZ) (Hartree): -318.94419644
E(MP3/Aug-CC-pVTZ) (Hartree): -318.95117836
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.97538961
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.97948998
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.95822585
E(UHF/Aug-CC-pVTZ) (Hartree): -317.92550656
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.98313964
     T1 diagnostic:  0.000610
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.04884399
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.04728468
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -318.98994459
     T1 diagnostic:  0.045825
     D1 diagnostic:  0.180929
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.05824622
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.89407574
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.46682947
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.479490      1.012985       0.233449
     O      -1.350943      0.219417      -0.295128
     O      -1.298303     -1.016968       0.198588
     H      -0.127746      0.785558       1.235398
     H      -0.455447      2.008418      -0.199894
     N       1.165533     -0.139496      -0.484834
     O       2.061921     -0.189375       0.216245
Rotational constants (GHz):   11.6631900    3.2724300    2.7886100
Vibrational harmonic frequencies (cm-1):
     i364.6947                  63.9586                 134.0172
      283.5691                 411.1760                 571.5077
      759.3350                 857.0840                1055.1748
     1221.6963                1257.9286                1488.9302
     2018.5819                3197.0924                3349.1556
Zero-point correction (Hartree): 0.037975

TS.SOZ.OCH2ONO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.08844984
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.03274177
E(MP2/Aug-CC-pVTZ) (Hartree): -318.99001523
E(MP3/Aug-CC-pVTZ) (Hartree): -318.99998586
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.01378367
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.01826869
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.97965072
E(UHF/Aug-CC-pVTZ) (Hartree): -317.95301059
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.02077365
     T1 diagnostic:  0.000761
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.08921645
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E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.08841287
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.03247187
     T1 diagnostic:  0.037618
     D1 diagnostic:  0.150111
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.09425066
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.93418528
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.50751796
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.084391      0.266479       0.167485
     O       0.668955     -0.969270      -0.273143
     O      -0.821079     -0.811579       0.237741
     N      -1.148266      0.362081      -0.145493
     O      -0.057721      1.149861      -0.058788
     H       1.315971      0.291400       1.238011
     H       1.894300      0.623061      -0.470944
Rotational constants (GHz):    9.3586600    8.3202600    4.7825000
Vibrational harmonic frequencies (cm-1):
     i819.8937                  273.9224                  484.7247
      726.6055                  872.6436                  928.0431
     1022.0343                 1121.6605                 1140.5790
     1147.0149                 1229.4349                 1383.6671
     1520.9732                 3129.5008                 3232.5944
Zero-point correction (Hartree): 0.041493

TS.OCH2ONO.CH2O+NO2
-------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.12127416
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.06066919
E(MP2/Aug-CC-pVTZ) (Hartree): -319.03907927
E(MP3/Aug-CC-pVTZ) (Hartree): -319.03435524
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.04247715
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.03680186
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.98995249
E(UHF/Aug-CC-pVTZ) (Hartree): -317.98508855
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -319.07953885
     T1 diagnostic:  0.001031
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.12448476
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.12361991
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.06144995
     T1 diagnostic:  0.033393
     D1 diagnostic:  0.129811
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.12937146
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.94354959
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.54272647
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.187171      0.352244       0.262092
     O       1.231679     -0.793776      -0.282102
     O      -1.031672     -0.922032       0.174683
     N      -1.259291      0.208601      -0.097433
     O      -0.346675      1.070394      -0.144258
     H       1.109644      0.434931       1.355759
     H       1.755713      1.154710      -0.232873
Rotational constants (GHz):   10.0330600    5.5132200    3.8230600
Vibrational harmonic frequencies (cm-1):
     i865.1722                  191.5003                  255.7189
      348.7258                  473.5595                  792.9952
      968.2333                 1041.3423                 1194.5803
     1312.4643                 1380.1369                 1520.1196
     1648.6578                 3050.0205                 3134.9665
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Zero-point correction (Hartree): 0.039442

TS.OCH2ONO_cc.initrot
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E(UM052X/Aug-CC-pVDZ) (Hartree): -319.53892941
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.188222     -0.371788       0.000076
     O      -1.089773      0.991163      -0.000090
     O       1.155672      0.828977       0.000080
     N       1.262685     -0.342095      -0.000064
     O       0.136664     -1.054088      -0.000035
     H      -1.664865     -0.751414       0.912166
     H      -1.665094     -0.751605      -0.911813
Rotational constants (GHz):   10.0306600    5.7941200    3.7643700
Vibrational harmonic frequencies (cm-1):
     i433.6471                288.0537                309.3065
      465.3750                694.6365                837.3492
      943.3748                960.2526               1166.6872
     1172.3471               1395.5015               1543.4698
     1751.2137               3088.7928               3150.4072
Zero-point correction (Hartree): 0.040476

TS.OCH2ONO_tt.initrot
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E(UM052X/Aug-CC-pVDZ) (Hartree): -319.55989686
Electronic state : 2-A
Cartesian coordinates (Angs):
     O      -2.207193     -0.322292      -0.000081
     C      -1.105070      0.419925       0.000051
     O       0.081631     -0.405001       0.000089
     N       1.196427      0.412929      -0.000060
     O       2.182537     -0.215187      -0.000018
     H      -1.100115      1.064954      -0.896922
     H      -1.100256      1.064838       0.897109
Rotational constants (GHz):   37.8649600    2.6192300    2.4889100
Vibrational harmonic frequencies (cm-1):
     i100.4325                195.6167                255.0880
      474.0343                717.9306                780.2465
      873.9054               1110.7376               1175.7239
     1185.1759               1356.6595               1389.9631
     1838.7951               3017.3189               3061.4021
Zero-point correction (Hartree): 0.039714

TS.cyc-OOCH2NO.ONCH2OO
----------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.05545499
E(CCSD/Aug-CC-pVTZ) (Hartree): -318.99091123
E(MP2/Aug-CC-pVTZ) (Hartree): -318.98926186
E(MP3/Aug-CC-pVTZ) (Hartree): -318.97071903
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99491693
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.97485895
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.88794342
E(UHF/Aug-CC-pVTZ) (Hartree): -317.88077246
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.99961581
     T1 diagnostic:  0.000732
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05614835
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05519703
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -318.99100911
     T1 diagnostic:  0.045380
     D1 diagnostic:  0.201664
```

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E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06441401
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.87163960
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.47044099
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.312106      0.972596       0.134732
     O      -1.385289      0.147822      -0.116510
     H      -0.346081      1.901129      -0.439813
     H      -0.084419      1.097889       1.197398
     N       0.738326     -0.059463      -0.382845
     O       1.792412     -0.138299       0.119951
     O      -0.765266     -1.061818       0.135801
Rotational constants (GHz):   12.8050200    4.8121000    3.7375500
Vibrational harmonic frequencies (cm-1):
     i601.6999                281.2359                 371.0445
      529.8233                673.2382                 775.4199
      950.8771               1063.9356                1103.1972
     1214.4394               1283.1314                1497.8346
     1814.5257               3134.8578                3233.0483
Zero-point correction (Hartree): 0.040840

TS.CH2OONO.CH2O+NO2
-------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.05578459
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.00069211
E(MP2/Aug-CC-pVTZ) (Hartree): -318.98418909
E(MP3/Aug-CC-pVTZ) (Hartree): -318.97971969
E(PMP2/Aug-CC-pVTZ) (Hartree): -318.99333973
E(PMP3/Aug-CC-pVTZ) (Hartree): -318.98591733
E(PUHF/Aug-CC-pVTZ) (Hartree): -317.92650842
E(UHF/Aug-CC-pVTZ) (Hartree): -317.91548142
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -318.99312335
     T1 diagnostic:  0.000421
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -319.05600359
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -319.05476951
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -319.00055233
     T1 diagnostic:  0.026480
     D1 diagnostic:  0.069019
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -319.06006565
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.90768416
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.47140072
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.818145      0.539093       0.172292
     O      -1.171350     -0.505090      -0.340219
     H      -2.288307      1.206062      -0.541029
     H      -1.819118      0.677767       1.247854
     O       0.148665     -0.639423       0.310670
     N       0.967637      0.314373      -0.321409
     O       2.053040      0.229639       0.093210
Rotational constants (GHz):   19.9901000    3.1944700    2.9882500
Vibrational harmonic frequencies (cm-1):
     i342.4488                110.7066                 197.7847
      328.8803                444.3390                 496.2932
      549.0504                610.9990                 940.5377
     1142.7363               1194.8756                1467.0807
     1852.7738               3205.1766                3360.4974
Zero-point correction (Hartree): 0.036227

TS.OCH2NO2.CH2O+NO2
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```

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -319.12111565
E(CCSD/Aug-CC-pVTZ) (Hartree): -319.06254650
E(MP2/Aug-CC-pVTZ) (Hartree): -319.04427293
E(MP3/Aug-CC-pVTZ) (Hartree): -319.03966075
E(PMP2/Aug-CC-pVTZ) (Hartree): -319.05307354
E(PMP3/Aug-CC-pVTZ) (Hartree): -319.04615542
E(PUHF/Aug-CC-pVTZ) (Hartree): -318.00117884
E(UHF/Aug-CC-pVTZ) (Hartree): -317.99106486
E(ROHF/AUG-CC-PVTZ) (Hartree): -317.94518078
E(UM052X/Aug-CC-pVDZ) (Hartree): -319.54528443
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.021439	-0.566053	0.265593
O	1.805377	0.259810	-0.282022
H	0.902543	-1.584308	-0.130748
H	0.908040	-0.473839	1.364072
N	-0.651640	0.047217	0.019616
O	-1.427856	-0.841367	-0.168784
O	-0.799738	1.222051	0.080281

Rotational constants (GHz): 10.6706600 4.2238800 3.1999300
Vibrational harmonic frequencies (cm-1):

i1140.0792	110.7231	249.3143
375.3375	525.2692	687.8054
902.1533	1030.4412	1172.9351
1360.1025	1437.7646	1492.4684
1816.2273	2981.1469	3130.7366

Zero-point correction (Hartree): 0.039349

Quantum chemical data on $CH_2OO + RO_2$

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CH2O2
-----
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -189.28461405
     T1 diagnostic:  0.000001
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -189.33059401
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -189.32897960
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -189.29649251
     T1 diagnostic:  0.041941
     D1 diagnostic:  0.167600
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -189.33566407
E(RHF/AUG-CC-PVTZ) (Hartree): -188.63545484
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.57546372
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.057192     -0.186724       0.000000
     O       0.000000      0.458901       0.000000
     O      -1.164431     -0.209976       0.000000
     H       1.006139     -1.269491       0.000000
     H       1.966157      0.398436       0.000000
Rotational constants (GHz):   81.1979300   12.6778000   10.9656800
Vibrational harmonic frequencies (cm-1):
      537.7503 (  A')           697.5723 (  A")           930.1710 (  A')
     1022.3957 (  A")          1261.0787 (  A')          1433.3936 (  A')
     1630.8711 (  A')          3141.7356 (  A')          3292.7088 (  A')
Zero-point correction (Hartree): 0.031775


E(UM052X+HF-M052X/Aug-CC-pVDZ) (Hartree): -189.57322403
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.055305     -0.201474       0.000000
     O       0.000000      0.461914       0.000000
     O      -1.160833     -0.197053       0.000000
     H       0.980834     -1.287699       0.000000
     H       1.974003      0.377649       0.000000
Rotational constants (GHz):   80.1459800   12.7489700   10.9992900
Vibrational harmonic frequencies (cm-1):
      547.9295 (  A')           700.1734 (  A")           953.1161 (  A')
     1017.1748 (  A")          1261.2826 (  A')          1429.8355 (  A')
     1617.2061 (  A')          3194.1947 (  A')          3355.7754 (  A')
Zero-point correction (Hartree): 0.032069

CH3O2
-----
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -189.90725379
     T1 diagnostic:  0.001014
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -189.96048406
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -189.96015358
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -189.93388906
     T1 diagnostic:  0.034531
     D1 diagnostic:  0.139667
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -189.96314477
E(ROHF/AUG-CC-PVTZ) (Hartree): -189.27411192
E(UM062X/Aug-CC-pVTZ) (Hartree): -190.20981111
Point group : CS
Electronic state : 2-A"
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Cartesian coordinates (Angs):
     C      -0.987497     -0.480576       0.000000
     O       0.000000      0.561551       0.000000
     O       1.199179      0.067204       0.000000
     H      -0.859473     -1.084492       0.894432
     H      -0.859473     -1.084492      -0.894432
     H      -1.949500      0.022404       0.000000
Rotational constants (GHz):   53.5982600   11.5647700   10.1270600
Vibrational harmonic frequencies (cm-1):
      131.9529 (  A")           512.7257 (  A')           979.3410 (  A')
     1146.3194 (  A")          1201.5411 (  A')          1294.9750 (  A')
     1458.0924 (  A')          1485.2020 (  A")          1494.9064 (  A')
     3087.8942 (  A')          3178.9216 (  A")          3195.3531 (  A')
Zero-point correction (Hartree): 0.043666


E(UM052X+HF-M052X/Aug-CC-pVDZ) (Hartree): -190.20987927
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):
     C      -0.987902     -0.486640       0.000000
     O       0.000000      0.565619       0.000000
     O       1.197727      0.069199       0.000000
     H      -0.849504     -1.088381       0.900758
     H      -0.849504     -1.088381      -0.900758
     H      -1.955393      0.018057       0.000000
Rotational constants (GHz):   52.9321100   11.5552700   10.1050300
Vibrational harmonic frequencies (cm-1):
      132.2670 (  A")           508.8175 (  A')           966.9108 (  A')
     1143.6845 (  A")          1200.4673 (  A')          1288.2294 (  A')
     1448.8573 (  A')          1475.1542 (  A")          1484.9905 (  A')
     3127.6431 (  A')          3227.2125 (  A")          3240.5317 (  A')
Zero-point correction (Hartree): 0.043843

complex
-------
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -379.20232508
     T1 diagnostic:  0.000788
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -379.30154640
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -379.29965532
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -379.24027017
     T1 diagnostic:  0.038419
     D1 diagnostic:  0.156319
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -379.30920146
E(ROHF/AUG-CC-PVTZ) (Hartree): -377.91305190
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.79734062
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.904175      0.786126      -0.168534
     O      -1.339129     -0.354734       0.506360
     O      -0.891192     -1.230930      -0.337426
     H      -2.726482      0.440499      -0.790129
     H      -1.116814      1.259693      -0.747021
     H      -2.251402      1.444531       0.621657
     C       1.628439     -0.835742       0.241935
     O       1.663827      0.217559      -0.404029
     O       1.129984      1.329070       0.170965
     H       1.197167     -0.828613       1.236033
     H       2.044033     -1.706127      -0.247910
Rotational constants (GHz):    5.5587400    2.3516100    1.8083000
Vibrational harmonic frequencies (cm-1):
```

```
       30.3591                  54.6089                 104.0771
      124.9182                 155.5029                 167.0084
      210.0045                 513.1296                 533.2790
      704.3476                 900.5040                 967.3066
     1063.5060                1146.7372                1203.0406
     1258.8412                1308.8256                1437.5622
     1452.7742                1478.7543                1494.0028
     1644.4899                3087.0219                3144.4374
     3186.1323                3198.3733                3291.5904
Zero-point correction (Hartree): 0.077141


TS.CH3O2+CH2OO
--------------
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -379.19914754
     T1 diagnostic:  0.000980
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -379.29962223
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -379.29779187
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -379.23565256
     T1 diagnostic:  0.042868
     D1 diagnostic:  0.186939
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -379.30887582
E(ROHF/AUG-CC-PVTZ) (Hartree): -377.89761117
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.79591735
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.750489     -0.728005      0.381548
     O      -1.198993      0.192754     -0.572315
     O      -0.755496      1.273253      0.017942
     H      -2.647040     -0.283546      0.809316
     H      -1.007047     -0.933537      1.145849
     H      -1.979322     -1.626786     -0.181802
     C       1.429661      0.879878      0.023857
     O       1.388494     -0.288774      0.478755
     O       1.131360     -1.270422     -0.412242
     H       1.388815      1.023120     -1.046759
     H       1.646648      1.655018      0.743838
Rotational constants (GHz):    5.4460500    2.8182200    2.1214600
Vibrational harmonic frequencies (cm-1):
     i317.7840                 78.2390                 118.2019
      175.4008                 191.3138                 249.9005
      308.4532                 514.0921                 545.5739
      749.3986                 900.9432                 977.4638
     1007.8161                1156.8760                1186.1435
     1237.5207                1255.2934                1362.6432
     1457.9899                1477.9910                1488.1110
     1525.6996                3084.6256                3161.5705
     3177.2270                3201.9877                3313.0296
Zero-point correction (Hartree): 0.077238


E(UM052X/Aug-CC-pVDZ) (Hartree): -379.79439391
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.769089     -0.761085      0.367870
     O      -1.233700      0.202069     -0.567570
     O      -0.826074      1.274488      0.049871
     H      -2.700431     -0.356711      0.771638
     H      -1.027795     -0.931195      1.148593
     H      -1.936449     -1.665967     -0.216407
     C       1.477093      0.890092     -0.000142
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     O       1.439978     -0.276579       0.471002
     O       1.162781     -1.264392      -0.397027
     H       1.368136      1.019277      -1.072368
     H       1.704644      1.675863       0.711973
Rotational constants (GHz):    5.4285900    2.6862000    2.0347800
Vibrational harmonic frequencies (cm-1):
     i112.7802                  72.0941                 103.7946
      158.6977                 175.5894                 215.0173
      268.2290                 511.5063                 549.8546
      713.8111                 942.9980                 961.3072
     1000.0920                1150.4548                1192.6017
     1249.5631                1259.7843                1347.6539
     1451.4010                1469.9797                1481.8689
     1521.0762                3132.0676                3215.3120
     3234.1444                3256.3953                3378.4935
Zero-point correction (Hartree): 0.077489

CH3OOCH2OO.pmm
--------------
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -379.28163637
     T1 diagnostic:  0.000675
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -379.37232337
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -379.37137194
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -379.31597329
     T1 diagnostic:  0.025489
     D1 diagnostic:  0.131080
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -379.37614501
E(ROHF/AUG-CC-PVTZ) (Hartree): -377.99613426
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.87324686
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.843378      0.875793       0.004754
     O       1.409598     -0.433248      -0.314753
     O       0.394979     -0.765483       0.632247
     C      -0.758629     -0.988575      -0.078662
     O      -1.310728      0.236713      -0.602025
     O      -1.788581      0.975732       0.357330
     H       2.231730      0.911049       1.022237
     H       1.034055      1.595137      -0.118368
     H       2.642295      1.080497      -0.705312
     H      -0.585467     -1.604840      -0.958987
     H      -1.473255     -1.414865       0.621491
Rotational constants (GHz):    6.5948600    2.5831300    2.1528800
Vibrational harmonic frequencies (cm-1):
       70.2345                  88.2531                 165.3625
      236.8732                 313.6120                 460.3035
      513.9439                 662.6000                 902.9542
      933.2627                1086.5635                1145.8837
     1167.9870                1189.3282                1232.3171
     1259.6245                1325.2686                1415.3997
     1462.1400                1474.1717                1478.6904
     1518.2979                3062.2351                3106.6998
     3140.4332                3161.6727                3184.0131
Zero-point correction (Hartree): 0.081463


E(UM052X/Aug-CC-pVDZ) (Hartree): -379.87181605
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.836555      0.884104       0.005216
     O       1.411263     -0.437302      -0.312277
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     O       0.397421     -0.767053       0.635713
     C      -0.757137     -0.990486      -0.085400
     O      -1.304113      0.245724      -0.605546
     O      -1.791845      0.965513       0.362532
     H       2.216767      0.918867       1.030607
     H       1.015491      1.594175      -0.129619
     H       2.642825      1.086240      -0.704892
     H      -0.572684     -1.601606      -0.971859
     H      -1.480711     -1.414435       0.613487
Rotational constants (GHz):    6.5689900    2.5855800    2.1558600
Vibrational harmonic frequencies (cm-1):
       70.3221                  90.1056                 163.2061
      225.1235                 312.6415                 458.5626
      515.1701                 661.6999                 897.8779
      922.0080                1071.0806                1137.1495
     1161.6968                1181.8004                1228.0874
     1254.2939                1321.0023                1408.4266
     1450.9447                1467.9789                1470.4584
     1507.1968                3107.5754                3159.9926
     3194.9171                3211.1748                3245.3410
Zero-point correction (Hartree): 0.081777

CH3OOCH2OO.b
------------
E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -379.28108404
     T1 diagnostic:  0.000687
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -379.37174583
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -379.37078992
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -379.31517200
     T1 diagnostic:  0.025637
     D1 diagnostic:  0.132175
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -379.37561756
E(ROHF/AUG-CC-PVTZ) (Hartree): -377.99439107
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.87280701
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.799158     -0.781499      -0.290744
     O       1.208578      0.143732       0.602951
     O       0.513413      1.100711      -0.193080
     H       2.482168     -0.272398      -0.970576
     H       1.038361     -1.325616      -0.850062
     H       2.352828     -1.464206       0.350935
     C      -0.823753      0.984742       0.108287
     O      -1.388765     -0.184662      -0.516698
     O      -1.509669     -1.171743       0.324457
     H      -1.004393      0.897395       1.177777
     H      -1.309851      1.841062      -0.354365
Rotational constants (GHz):    5.9225800    2.8877100    2.2274800
Vibrational harmonic frequencies (cm-1):
       64.6104                 116.9737                 127.5663
      229.2406                 361.9395                 472.4855
      519.8171                 594.6544                 895.3275
      946.4117                1085.3806                1132.4733
     1176.9505                1193.3947                1230.2919
     1268.2440                1336.3571                1408.0499
     1460.8377                1470.9242                1479.1338
     1519.0149                3060.6162                3105.5615
     3138.5954                3161.0179                3184.5846
Zero-point correction (Hartree): 0.081423
```

CH3OOCH2OO.a

E(RHF-RMP2/AUG-CC-PVTZ) (Hartree): -379.28041691
T1 diagnostic: 0.000722
E(RHF-UCCSD(T)/AUG-CC-PVTZ) (Hartree): -379.37116948
E(RHF-UCCSD-T/AUG-CC-PVTZ) (Hartree): -379.37027797
E(RHF-UCCSD/AUG-CC-PVTZ) (Hartree): -379.31479227
T1 diagnostic: 0.026498
D1 diagnostic: 0.137955
E(RHF-UCCSD[T]/AUG-CC-PVTZ) (Hartree): -379.37505516
E(ROHF/AUG-CC-PVTZ) (Hartree): -377.99388331
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.87230489
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-2.007222	-0.843634	-0.148400
O	-1.387627	0.196691	0.584723
O	-0.619012	0.953739	-0.349975
H	-1.261844	-1.514494	-0.574584
H	-2.643977	-0.432081	-0.931115
H	-2.614385	-1.369816	0.585695
C	0.688342	0.870872	0.043426
O	1.195798	-0.439095	-0.327607
O	2.357530	-0.640923	0.212221
H	1.240387	1.618148	-0.523901
H	0.819588	0.971516	1.118845

Rotational constants (GHz): 8.0032600 2.1594900 1.8665100
Vibrational harmonic frequencies (cm-1):

46.7422	80.3069	153.1533
234.0607	327.1543	422.8215
487.6509	599.8172	898.8178
994.0993	1088.1754	1116.7451
1184.9672	1196.4158	1232.5826
1289.0849	1305.5025	1413.5277
1461.4169	1478.7510	1487.6609
1519.3048	3061.6054	3101.9137
3140.4345	3161.3593	3177.0118

Zero-point correction (Hartree): 0.081242

CH3OOCH2OO.ppt

E(UM062X/Aug-CC-pVTZ) (Hartree): -379.87017399
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-2.472041	-0.273481	0.309870
O	-1.253293	-0.491994	-0.370806
O	-0.566170	0.757833	-0.365764
C	0.582599	0.591106	0.359416
O	1.533485	-0.152090	-0.443909
O	2.567307	-0.462370	0.274104
H	-3.056770	0.498702	-0.189315
H	-2.295504	0.000731	1.351761
H	-2.992588	-1.227672	0.260607
H	0.997581	1.582742	0.532095
H	0.433309	0.028708	1.280137

Rotational constants (GHz): 12.2320100 1.7406700 1.6767700
Vibrational harmonic frequencies (cm-1):

26.4389	51.7516	141.3578
235.7153	328.2544	417.2087
473.9955	622.5649	901.4940
1008.5109	1087.7305	1115.6468

```
     1181.4887                 1189.8520                 1238.7693
     1286.4223                 1304.4217                 1415.4627
     1459.6687                 1479.3552                 1481.7937
     1515.8314                 3051.5878                 3092.8993
     3126.5309                 3162.5133                 3167.9409
Zero-point correction (Hartree): 0.081024


CH3OOCH2OO.ppm
--------------
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.87036404
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -2.256912     -0.420443      0.273561
     O      -1.058928     -0.405972     -0.474963
     O      -0.512708      0.902233     -0.337915
     C       0.613164      0.798442      0.447987
     O       1.687689      0.176299     -0.276650
     O       1.904248     -1.041307      0.128817
     H      -2.954468      0.326981     -0.103675
     H      -2.060567     -0.251587      1.334456
     H      -2.662802     -1.419651      0.129823
     H       0.927231      1.820972      0.648612
     H       0.450691      0.205262      1.347182
Rotational constants (GHz):    8.0388200    2.2309700    1.9355900
Vibrational harmonic frequencies (cm-1):
       46.6212                   78.5721                  125.7031
      231.7909                  353.7063                  464.1066
      539.3355                  596.4217                  899.9751
      960.5767                 1084.1715                 1129.3027
     1175.5564                 1189.0679                 1233.6807
     1262.1621                 1335.4525                 1407.9937
     1457.9892                 1471.3238                 1479.7616
     1516.6079                 3049.2087                 3094.0205
     3123.5208                 3161.7272                 3172.9267
Zero-point correction (Hartree): 0.081197


CH3OOCH2OO.ptm
--------------
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.86427684
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -2.507232      0.216394     -0.313322
     O      -1.525115     -0.450434      0.454651
     O      -0.317402     -0.377924     -0.292421
     C       0.544086      0.389215      0.509015
     O       1.728058      0.556873     -0.251211
     O       2.509491     -0.481749     -0.138461
     H      -2.630280     -0.269894     -1.280375
     H      -2.248379      1.267503     -0.452360
     H      -3.422964      0.132334      0.268528
     H       0.139751      1.388810      0.671158
     H       0.780486     -0.126528      1.438436
Rotational constants (GHz):   14.5090300    1.6572600    1.6273800
Vibrational harmonic frequencies (cm-1):
       44.7606                   66.0286                  116.0197
      219.9599                  343.3259                  401.6430
      480.6489                  593.2866                  972.6317
     1022.8988                 1096.9560                 1138.4649
     1171.4663                 1186.8655                 1230.2427
```

1239.6683	1294.9656	1423.0372
1460.3664	1478.5659	1513.2696
1520.0915	3054.2881	3083.5100
3129.7071	3156.1323	3161.8807

Zero-point correction (Hartree): 0.081104

complex2

E(UM062X/Aug-CC-pVTZ) (Hartree): -569.46154607
Electronic state : 2-A
Cartesian coordinates (Angs):

C	3.167975	0.766447	0.061250
O	2.410588	-0.140730	-0.714861
O	1.828697	-1.070395	0.196824
H	3.937453	0.238443	0.624472
H	2.526494	1.334421	0.735301
H	3.630064	1.431280	-0.665972
C	0.462956	-0.956110	0.081958
O	0.015246	0.250665	0.751958
O	-0.228913	1.216555	-0.084674
H	0.120691	-0.896850	-0.947267
H	0.027403	-1.782299	0.634588
C	-2.815030	0.989264	0.109717
O	-2.799757	-0.055599	-0.552852
O	-2.411075	-1.195040	0.074458
H	-2.543851	0.951454	1.158108
H	-3.111939	1.882299	-0.423600

Rotational constants (GHz): 3.7233400 0.7626700 0.6796900
Vibrational harmonic frequencies (cm-1):

30.0074	45.5014	63.6293
101.2025	111.6745	128.7002
141.9426	162.6748	212.1043
229.3544	363.0996	476.9081
517.6577	535.4191	587.7523
705.5056	889.5826	909.1686
927.0569	1061.6894	1088.6905
1128.4564	1173.5101	1192.1694
1230.0450	1259.0309	1268.7361
1335.0008	1397.9447	1434.5564
1455.3511	1460.7316	1478.3287
1519.3981	1630.9799	3058.4621
3132.5478	3134.0371	3145.1070
3159.7241	3216.4572	3293.3116

Zero-point correction (Hartree): 0.114804

E(UM052X/Aug-CC-pVDZ) (Hartree): -569.45705594
Electronic state : 2-A
Cartesian coordinates (Angs):

C	3.179369	0.747956	0.109357
O	2.404173	-0.107773	-0.720937
O	1.826685	-1.084266	0.142260
H	3.954000	0.171698	0.624981
H	2.539580	1.268413	0.828397
H	3.635133	1.459300	-0.584522
C	0.455899	-0.957516	0.031380
O	0.016629	0.228810	0.755047
O	-0.245705	1.216843	-0.049405
H	0.120679	-0.839529	-0.999369
H	0.015434	-1.807560	0.550554

C	-2.779836	1.014268	0.051436
O	-2.770512	-0.077053	-0.554742
O	-2.456511	-1.174501	0.160196
H	-2.571133	1.019057	1.118283
H	-3.024358	1.883899	-0.550723

Rotational constants (GHz): 3.7243500 0.7639400 0.6810900
Vibrational harmonic frequencies (cm-1):

33.0679	42.9819	63.0652
105.2680	109.3952	125.9576
139.8802	164.0719	210.3657
225.1603	358.9970	476.8301
518.8779	545.2522	585.2545
703.1822	882.9664	915.4533
935.1246	1034.0626	1074.3123
1119.7366	1168.8671	1184.8904
1224.8333	1256.1803	1262.8190
1329.3720	1390.2184	1397.4217
1449.1449	1455.1796	1467.0506
1507.7519	1559.1475	3104.0494
3184.2670	3187.7065	3202.6419
3209.1743	3279.3593	3365.2556

Zero-point correction (Hartree): 0.115172

TS.CH3OOCH2OO+CH2OO

E(ROHF/AUG-CC-PVTZ) (Hartree): -566.61909293
E(UM062X/Aug-CC-pVTZ) (Hartree): -569.46024409
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-3.030020	0.798400	-0.104192
O	-2.294773	-0.054178	0.751617
O	-1.777361	-1.104037	-0.062808
H	-3.835765	0.248920	-0.590889
H	-2.380773	1.260128	-0.848087
H	-3.444368	1.558639	0.555209
C	-0.403284	-1.031296	-0.012288
O	0.077790	0.041706	-0.851962
O	0.263795	1.150068	-0.173915
H	-0.029556	-0.854413	0.993002
H	-0.025450	-1.944762	-0.460334
C	2.479277	1.105908	0.079792
O	2.534857	-0.020528	0.629700
O	2.494766	-1.091025	-0.189862
H	2.530109	1.163532	-0.998570
H	2.517376	1.953835	0.747644

Rotational constants (GHz): 3.5811800 0.8397100 0.7453800
Vibrational harmonic frequencies (cm-1):

i309.8713	43.5158	63.7552
82.8038	119.8430	132.4095
173.5600	210.9661	222.8622
304.3262	374.6084	468.2930
511.2891	545.4490	606.5628
748.1901	882.9467	902.5698
940.8215	1010.1268	1087.0832
1125.4563	1167.5502	1188.6506
1199.6997	1245.4923	1254.3266
1328.0384	1361.2935	1401.7396
1458.2402	1461.7056	1478.4973
1518.1052	1523.4782	3059.0248
3126.7621	3135.1787	3159.3105
3159.8085	3211.4020	3311.9935

Zero-point correction (Hartree): 0.114609

E(UM052X/Aug-CC-pVDZ) (Hartree): -569.45698934
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-3.116056	0.753431	-0.140627
O	-2.345211	-0.059042	0.736136
O	-1.795008	-1.100614	-0.066411
H	-3.907531	0.158241	-0.606793
H	-2.476762	1.212639	-0.900547
H	-3.549975	1.518006	0.509265
C	-0.420033	-0.989630	0.014268
O	0.035358	0.124983	-0.801618
O	0.264793	1.190139	-0.081357
H	-0.072006	-0.803021	1.030927
H	-0.004403	-1.885460	-0.445086
C	2.608473	1.071217	0.060464
O	2.629964	-0.070015	0.589396
O	2.497077	-1.117605	-0.240567
H	2.565539	1.140930	-1.022130
H	2.715041	1.905775	0.745099

Rotational constants (GHz): 3.6649300 0.8025700 0.7146400
Vibrational harmonic frequencies (cm-1):

i78.8388	42.3303	60.1715
85.4707	112.8202	126.3502
160.6846	187.6022	218.4254
263.7104	364.1020	474.4108
514.7443	549.9278	594.1610
709.8567	884.0413	917.2741
948.2580	1001.1688	1073.5021
1119.3778	1167.3157	1184.0014
1211.5435	1246.7342	1255.0056
1327.5476	1349.1474	1397.2811
1449.3456	1457.8312	1467.4547
1507.8168	1520.7350	3103.7029
3180.8199	3187.8774	3208.5529
3212.8895	3277.0424	3376.3617

Zero-point correction (Hartree): 0.115042

CH3OOCH2OOCH2OO

E(ROHF/AUG-CC-PVTZ) (Hartree): -566.71500746
E(UM062X/Aug-CC-pVTZ) (Hartree): -569.53837299
Electronic state : 2-A
Cartesian coordinates (Angs):

C	2.768425	0.960034	-0.041441
O	2.149967	-0.052342	-0.810457
O	1.823548	-1.109470	0.088203
H	3.664677	0.575449	0.445500
H	2.077700	1.366122	0.697392
H	3.039595	1.728489	-0.763202
C	0.442126	-1.193671	0.156753
O	-0.140433	-0.235100	1.010288
O	-0.393828	0.957001	0.269903
H	-0.003759	-1.125410	-0.834262
H	0.238013	-2.148675	0.639997
C	-1.762334	1.113359	0.213346
O	-2.339336	0.219421	-0.755483
O	-2.791568	-0.867788	-0.197466
H	-2.241206	0.913648	1.169585

```
     H      -1.931124      2.118262      -0.166871
Rotational constants (GHz):    3.3683700    0.9153000    0.8189000
Vibrational harmonic frequencies (cm-1):
       36.9118                  59.7335                  97.4790
      102.9343                 134.5664                 145.5741
      225.3887                 322.4432                 409.4573
      428.3414                 487.2776                 518.9317
      598.6216                 650.7791                 879.1377
      911.4276                 951.1170                1054.4394
     1082.6764                1126.6894                1135.8472
     1166.6573                1188.1048                1195.1161
     1237.7063                1258.2677                1333.5881
     1342.1462                1403.3893                1421.4795
     1455.0144                1461.4660                1468.6197
     1478.6143                1517.1766                3058.4515
     3097.4980                3109.4955                3134.6620
     3156.2366                3166.8011                3189.7610
Zero-point correction (Hartree): 0.118920


E(UM052X/Aug-CC-pVDZ) (Hartree): -569.53518586
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       2.812415      0.940128       0.003422
     O       2.187165     -0.056650      -0.795569
     O       1.836614     -1.118547       0.086827
     H       3.702172      0.528057       0.489810
     H       2.111015      1.333703       0.744745
     H       3.097268      1.720325      -0.707792
     C       0.446839     -1.182886       0.125614
     O      -0.136875     -0.210456       0.975023
     O      -0.393383      0.967659       0.215955
     H       0.023255     -1.091255      -0.876778
     H       0.219303     -2.139823       0.603715
     C      -1.768845      1.119161       0.181705
     O      -2.355814      0.175585      -0.743723
     O      -2.877297     -0.840436      -0.118183
     H      -2.230188      0.941459       1.155214
     H      -1.948549      2.111870      -0.236004
Rotational constants (GHz):    3.4661100    0.8933800    0.7995000
Vibrational harmonic frequencies (cm-1):
       36.6601                  54.6648                  85.1885
      100.4420                 122.0945                 143.9635
      214.6930                 317.0115                 405.5570
      434.9046                 486.6485                 526.4123
      590.6093                 646.4767                 875.8053
      906.7598                 940.7045                1039.8437
     1067.1596                1116.7753                1123.9921
     1162.7085                1182.5376                1190.6333
     1233.2495                1256.3348                1330.6953
     1340.0865                1397.9305                1414.3532
     1448.9620                1451.5591                1467.6900
     1469.3449                1507.1660                3102.8676
     3150.8673                3160.6795                3188.0125
     3205.9347                3229.1894                3250.0851
Zero-point correction (Hartree): 0.119324
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Quantum chemical data on CH_2OO and $(CH_3)_2COO + SO_2$

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CH2O2
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059345
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649234
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(PMP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(UHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -189.16882447
E(CCSD/Aug-CC-pVDZ) (Hartree): -189.14423973
     T1 diagnostic:  0.043994
E(MP2/Aug-CC-pVDZ) (Hartree): -189.12365394
E(MP3/Aug-CC-pVDZ) (Hartree): -189.12767115
E(PMP2/Aug-CC-pVDZ) (Hartree): -189.12365394
E(PMP3/Aug-CC-pVDZ) (Hartree): -189.12767115
E(PUHF/Aug-CC-pVDZ) (Hartree): -188.58838987
E(RHF/Aug-CC-pVDZ) (Hartree): -188.58838987
E(UHF/Aug-CC-pVDZ) (Hartree): -188.58838987
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.57546372
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.057192     -0.186724       0.000000
     O       0.000000      0.458901       0.000000
     O      -1.164431     -0.209976       0.000000
     H       1.006139     -1.269491       0.000000
     H       1.966157      0.398436       0.000000
Rotational constants (GHz):   81.1979300   12.6778000   10.9656800
Vibrational harmonic frequencies (cm-1):
      537.7503 (  A')           697.5723 (  A")           930.1710 (  A')
     1022.3957 (  A")          1261.0787 (  A')          1433.3936 (  A')
     1630.8711 (  A')          3141.7356 (  A')          3292.7088 (  A')
Zero-point correction (Hartree): 0.031775


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -189.33059345
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -189.29649234
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -189.28461281
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -189.28352075
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -189.28461281
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -189.28352075
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -188.63545474
E(RHF/Aug-CC-pV(T+d)Z) (Hartree): -188.63545474
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -188.63545474
E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -189.57546372
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -189.57546372
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.057192     -0.186724       0.000000
     O       0.000000      0.458901       0.000000
     O      -1.164431     -0.209976       0.000000
     H       1.006139     -1.269491       0.000000
     H       1.966157      0.398436       0.000000
Rotational constants (GHz):   81.1980300   12.6778000   10.9656800
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Vibrational harmonic frequencies (cm-1):
      537.7497 (  A')          697.5720 (  A")          930.1719 (  A')
     1022.3947 (  A")         1261.0783 (  A')         1433.3936 (  A')
     1630.8708 (  A')         3141.7376 (  A')         3292.7116 (  A')
Zero-point correction (Hartree): 0.031775

CH2O
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.34256392
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.32534423
E(MP2/Aug-CC-pVTZ) (Hartree): -114.31597943
E(MP3/Aug-CC-pVTZ) (Hartree): -114.32041589
E(RHF/Aug-CC-pVTZ) (Hartree): -113.91460270
E(RM062X/Aug-CC-pVTZ) (Hartree): -114.49898473
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     H       0.000000      0.938502      -1.105299
     C       0.000000      0.000000      -0.525504
     H       0.000000     -0.938502      -1.105299
     O       0.000000      0.000000       0.670453
Rotational constants (GHz):  284.6635300   39.4631100   34.6583900
Vibrational harmonic frequencies (cm-1):
     1219.4936                1275.7091                1540.1761
     1872.8789                2960.1527                3028.2997
Zero-point correction (Hartree): 0.027103


SO2
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -547.99003145
E(CCSD/Aug-CC-pVTZ) (Hartree): -547.95428493
E(MP2/Aug-CC-pVTZ) (Hartree): -547.96330170
E(MP3/Aug-CC-pVTZ) (Hartree): -547.94481517
E(RHF/Aug-CC-pVTZ) (Hartree): -547.29142735
E(RM062X/Aug-CC-pVTZ) (Hartree): -548.61955231
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     O       1.230985     -0.370228       0.000000
     S       0.000000      0.370022       0.000000
     O      -1.230985     -0.369815       0.000000
Rotational constants (GHz):   57.7087400   10.4255700    8.8303000
Vibrational harmonic frequencies (cm-1):
      539.8562 (  A')          1240.9142 (  A')         1424.5802 (  A')
Zero-point correction (Hartree): 0.007302


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -548.00544813
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -547.97032327
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -547.97818658
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -547.96118083
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -547.97818658
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -547.96118083
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -547.30884047
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -547.30884047
E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -548.63510930
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     O       1.226922     -0.362184       0.000000
```

```
     S       0.000000      0.362186       0.000000
     O      -1.226922     -0.362188       0.000000
Rotational constants (GHz):   60.2328200   10.4947300    8.9374900
Vibrational harmonic frequencies (cm-1):
      540.2232 (  A')          1254.8776 (  A')          1454.8194 (  A')
Zero-point correction (Hartree): 0.007404

SO3
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -623.08766433
E(CCSD/Aug-CC-pVTZ) (Hartree): -623.04175588
E(MP2/Aug-CC-pVTZ) (Hartree): -623.05818283
E(MP3/Aug-CC-pVTZ) (Hartree): -623.03156981
E(RHF/Aug-CC-pVTZ) (Hartree): -622.14683752
E(RM062X/Aug-CC-pVTZ) (Hartree): -623.81059265
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       0.701824      1.241863       0.000006
     S      -0.000018      0.000009      -0.000010
     O       0.724682     -1.228680       0.000006
     O      -1.426470     -0.013202       0.000006
Rotational constants (GHz):   10.3524500   10.3508100    5.1758200
Vibrational harmonic frequencies (cm-1):
      506.0320                  528.9374                  530.2308
     1109.7634                 1428.5436                 1430.1780
Zero-point correction (Hartree): 0.012607


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -623.11151442
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -623.06638180
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -623.08198665
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -623.05646642
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -623.08198665
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -623.05646642
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -622.17326266
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -622.17326266
E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -623.83456232
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.362584     -0.384076       0.000023
     S       0.000008     -0.000022      -0.000035
     O      -1.013944     -0.987933       0.000023
     O      -0.348655      1.372052       0.000023
Rotational constants (GHz):   10.5108700   10.5100800    5.2552400
Vibrational harmonic frequencies (cm-1):
      519.5979                  540.6917                  541.3334
     1133.2096                 1457.9092                 1458.7568
Zero-point correction (Hartree): 0.012875

HCOOH
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.51743385
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.48985472
E(MP2/Aug-CC-pVTZ) (Hartree): -189.48637779
E(MP3/Aug-CC-pVTZ) (Hartree): -189.48384082
E(RHF/Aug-CC-pVTZ) (Hartree): -188.84524735
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.76956179
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.420998       0.000000
```

```
     O       1.151972      0.110123       0.000000
     O      -1.023295     -0.440188       0.000000
     H      -0.656022     -1.335776       0.000000
     H      -0.373391      1.450309       0.000000
Rotational constants (GHz):   78.0147100   12.2112900   10.5586000
Vibrational harmonic frequencies (cm-1):
      646.8647 (  A')           667.6500 (  A")          1069.9055 (  A")
     1161.8122 (  A')          1320.7674 (  A')          1407.4975 (  A')
     1864.7893 (  A')          3118.6782 (  A')          3782.8701 (  A')
Zero-point correction (Hartree): 0.034266


HSO3
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -623.67727034
E(CCSD/Aug-CC-pVTZ) (Hartree): -623.63357394
E(MP2/Aug-CC-pVTZ) (Hartree): -623.63613804
E(MP3/Aug-CC-pVTZ) (Hartree): -623.62196310
E(PMP2/Aug-CC-pVTZ) (Hartree): -623.64066369
E(PMP3/Aug-CC-pVTZ) (Hartree): -623.62433747
E(PUHF/Aug-CC-pVTZ) (Hartree): -622.73577263
E(UHF/Aug-CC-pVTZ) (Hartree): -622.72912633
E(UM062X/Aug-CC-pVTZ) (Hartree): -624.40252518
Electronic state : 2-A
Cartesian coordinates (Angs):
     O      -0.256760      1.406152      -0.186859
     O      -1.085551     -0.930052      -0.107908
     S       0.125156      0.076481       0.256729
     O       1.330346     -0.576808      -0.199675
     H      -1.906767     -0.418028      -0.152119
Rotational constants (GHz):    9.3151400    8.9850100    4.8839000
Vibrational harmonic frequencies (cm-1):
      307.7863                  431.1816                  435.4668
      536.8557                  815.0731                 1122.6265
     1136.9222                 1337.2053                 3803.6256
Zero-point correction (Hartree): 0.022615


H2SO3
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -624.33102164
E(CCSD/Aug-CC-pVTZ) (Hartree): -624.28911492
E(MP2/Aug-CC-pVTZ) (Hartree): -624.28612318
E(MP3/Aug-CC-pVTZ) (Hartree): -624.28042127
E(RHF/Aug-CC-pVTZ) (Hartree): -623.35782454
E(RM062X/Aug-CC-pVTZ) (Hartree): -625.05879539
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.243063     -0.741859       0.155757
     O      -1.242097     -0.743497       0.155617
     S       0.000091      0.109488      -0.440245
     O      -0.001106      1.361867       0.312549
     H      -1.474066     -0.382367       1.025876
     H       1.473727     -0.381536       1.026664
Rotational constants (GHz):    8.6260000    7.8521800    4.9659600
Vibrational harmonic frequencies (cm-1):
      204.9841                  356.1396                  443.6911
      461.2983                  505.3561                  817.6957
      827.3365                 1106.8130                 1127.3227
     1266.4254                 3748.3408                 3751.8636
Zero-point correction (Hartree): 0.033301
```

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CO
--
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16172649
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14439487
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14174840
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13823018
E(RHF/Aug-CC-pVTZ) (Hartree): -112.78216037
E(RM062X/Aug-CC-pVTZ) (Hartree): -113.32023229
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
     C       0.000000      0.000000      -0.640803
     O       0.000000      0.000000       0.480603
Rotational constants (GHz):    0.0000000   58.6148167   58.6148167
Vibrational harmonic frequencies (cm-1):
     2260.4092 (  SG)
Zero-point correction (Hartree): 0.005150


HCO
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.69212284
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.67456505
E(MP2/Aug-CC-pVTZ) (Hartree): -113.66827745
E(MP3/Aug-CC-pVTZ) (Hartree): -113.66790340
E(PMP2/Aug-CC-pVTZ) (Hartree): -113.67079349
E(PMP3/Aug-CC-pVTZ) (Hartree): -113.66926734
E(PUHF/Aug-CC-pVTZ) (Hartree): -113.29918713
E(UHF/Aug-CC-pVTZ) (Hartree): -113.29521840
E(UM062X/Aug-CC-pVTZ) (Hartree): -113.84942760
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     H      -0.864084      1.211618       0.000000
     C       0.061720      0.580840       0.000000
     O       0.061720     -0.587082       0.000000
Rotational constants (GHz):  720.9556400   45.4308400   42.7377300
Vibrational harmonic frequencies (cm-1):
     1105.0720 (  A')          2001.1708 (  A')          2719.5282 (  A')
Zero-point correction (Hartree): 0.013272


H2dioxirane
-----------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.37251453
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.34263386
E(MP2/Aug-CC-pVTZ) (Hartree): -189.33731410
E(MP3/Aug-CC-pVTZ) (Hartree): -189.33664162
E(RHF/Aug-CC-pVTZ) (Hartree): -188.68359343
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.62310852
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.731759       0.000000
     O       0.732234     -0.436574       0.000000
     O      -0.732240     -0.436315       0.000000
     H       0.000022      1.296279       0.927921
     H       0.000022      1.296279      -0.927921
Rotational constants (GHz):   28.8814600   26.7572300   15.3541300
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Vibrational harmonic frequencies (cm-1):
      909.7412 (  A')           953.6802 (  A')          1056.3705 (  A")
     1185.6085 (  A")          1279.4511 (  A')          1373.1126 (  A')
     1557.8367 (  A')          3106.0701 (  A')          3205.4059 (  A")
Zero-point correction (Hartree): 0.033323


H2bisoxy
--------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.35006665
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.32804226
E(MP2/Aug-CC-pVTZ) (Hartree): -189.29304900
E(MP3/Aug-CC-pVTZ) (Hartree): -189.31925724
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.31713328
E(PMP3/Aug-CC-pVTZ) (Hartree): -189.34314484
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.76296452
E(RHF/Aug-CC-pVTZ) (Hartree): -188.56723935
E(UHF/Aug-CC-pVTZ) (Hartree): -188.73870155
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.60299579
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.388948       0.000000
     O       1.164159     -0.280543       0.000000
     O      -1.164165     -0.280465       0.000000
     H       0.000025      1.077190       0.872695
     H       0.000025      1.077190      -0.872695
Rotational constants (GHz):   62.3361700   11.2581500   10.1223300
Vibrational harmonic frequencies (cm-1):
      589.7484 (  A')           593.2123 (  A")           861.3307 (  A")
      958.9701 (  A')          1138.4808 (  A')          1224.6031 (  A')
     1292.3454 (  A')          2901.9537 (  A')          2931.9502 (  A")
Zero-point correction (Hartree): 0.028460


H2bisoxy.SO2_complex
--------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.34647824
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.28785977
E(MP2/Aug-CC-pVTZ) (Hartree): -737.26206190
E(MP3/Aug-CC-pVTZ) (Hartree): -737.26956923
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.28702408
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.29430411
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.05596699
E(RHF/Aug-CC-pVTZ) (Hartree): -735.85993289
E(UHF/Aug-CC-pVTZ) (Hartree): -736.03081104
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.23027850
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.097188      0.197303       0.186592
     O       1.255777      1.247638       0.145752
     O       1.895673     -0.840673      -0.642069
     O      -0.687930     -0.824507       0.924682
     S      -1.228037     -0.264372      -0.287593
     O      -2.235665      0.749593      -0.150052
     H       3.129679      0.573891       0.026341
     H       2.112947     -0.184172       1.229099
Rotational constants (GHz):    5.9713900    1.6255900    1.4670000
Vibrational harmonic frequencies (cm-1):
       46.9624                   62.2309                   92.4520
      107.6173                  130.0179                  159.8590
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```
      542.8119                  592.3078                  604.7513
      915.9357                  953.1754                 1125.7409
     1229.2400                 1241.2545                 1284.4391
     1414.9340                 2915.4100                 2946.4111
Zero-point correction (Hartree): 0.037283


E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.19519664
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.24527773
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.097188      0.197303       0.186592
     O       1.255777      1.247638       0.145752
     O       1.895673     -0.840673      -0.642069
     O      -0.687930     -0.824507       0.924682
     S      -1.228037     -0.264372      -0.287593
     O      -2.235665      0.749593      -0.150052
     H       3.129679      0.573891       0.026341
     H       2.112947     -0.184172       1.229099
Rotational constants (GHz):    5.9713872    1.6255879    1.4669954

OCHOSO2
-------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -736.83706529
E(CCSD/Aug-CC-pVTZ) (Hartree): -736.77292446
E(MP2/Aug-CC-pVTZ) (Hartree): -736.77848976
E(MP3/Aug-CC-pVTZ) (Hartree): -736.75659543
E(PMP2/Aug-CC-pVTZ) (Hartree): -736.78319067
E(PMP3/Aug-CC-pVTZ) (Hartree): -736.75907704
E(PUHF/Aug-CC-pVTZ) (Hartree): -735.49766972
E(UHF/Aug-CC-pVTZ) (Hartree): -735.49080241
E(UM062X/Aug-CC-pVTZ) (Hartree): -737.72404654
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.657276      0.242642      -0.023171
     O       0.548381     -0.598788       0.063266
     O       2.734331     -0.228050      -0.080834
     O      -0.938173      1.400255      -0.189975
     S      -0.956333      0.022031       0.263094
     O      -1.848985     -0.962300      -0.296048
     H       1.393233      1.302724      -0.041758
Rotational constants (GHz):    8.4923900    1.9312700    1.6174500
Vibrational harmonic frequencies (cm-1):
       86.5612                  123.3506                  211.9382
      373.7503                  440.3390                  516.9503
      565.7589                  846.6309                 1018.7163
     1048.5884                 1144.7599                 1333.0952
     1407.2320                 1920.3003                 3159.5603
Zero-point correction (Hartree): 0.032344


SOZ_H2
------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.38754958
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.32237079
E(MP2/Aug-CC-pVTZ) (Hartree): -737.32006656
E(MP3/Aug-CC-pVTZ) (Hartree): -737.30981448
E(RHF/Aug-CC-pVTZ) (Hartree): -735.99877923
E(RM062X/Aug-CC-pVTZ) (Hartree): -738.27402617
Electronic state : 1-A
Cartesian coordinates (Angs):
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```
     C      -1.540046     -0.528227       0.110275
     O      -1.228634      0.774411       0.506030
     O      -0.246147      1.144814      -0.462234
     O      -0.301298     -1.176893      -0.146272
     S       0.897772     -0.082032      -0.406199
     O       1.657181      0.010397       0.813566
     H      -2.137459     -0.533025      -0.802408
     H      -2.035447     -1.006922       0.951221
Rotational constants (GHz):    6.0999800    3.1804900    2.6470800
Vibrational harmonic frequencies (cm-1):
      139.4758                  293.1813                  395.3431
      484.8045                  601.1843                  678.9773
      736.5851                  761.7108                  942.7998
     1026.3188                 1100.0067                 1153.1992
     1260.4274                 1313.5481                 1411.3702
     1521.6605                 3092.6416                 3186.9403
Zero-point correction (Hartree): 0.045792


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.40097612
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.33618437
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.33326400
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.32372599
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.33326400
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.32372599
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.01358691
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.01358692
E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.28710343
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.539196     -0.528623       0.110809
     O      -1.230996      0.775987       0.501410
     O      -0.237167      1.137975      -0.461519
     O      -0.296573     -1.169911      -0.149648
     S       0.893925     -0.080942      -0.400486
     O       1.652255      0.007719       0.808322
     H      -2.138521     -0.540446      -0.800410
     H      -2.029250     -1.006911       0.954816
Rotational constants (GHz):    6.1605600    3.1986300    2.6613100
Vibrational harmonic frequencies (cm-1):
      137.6542                  289.8734                  396.6069
      487.1188                  608.7314                  684.1430
      736.7230                  768.5847                  937.4660
     1021.2992                 1099.8024                 1151.2483
     1254.4042                 1328.9190                 1406.2453
     1522.9297                 3084.3613                 3175.9517
Zero-point correction (Hartree): 0.045773

SOZ_H2.b
--------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.38661797
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.32106385
E(MP2/Aug-CC-pVTZ) (Hartree): -737.31883037
E(MP3/Aug-CC-pVTZ) (Hartree): -737.30830238
E(RHF/Aug-CC-pVTZ) (Hartree): -735.99641427
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -737.01606177
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.97017361
     T1 diagnostic:  0.020652
E(MP2/Aug-CC-pVDZ) (Hartree): -736.95441906
E(MP3/Aug-CC-pVDZ) (Hartree): -736.95109929
E(RHF/Aug-CC-pVDZ) (Hartree): -735.86957994
```

E(RM062X/Aug-CC-pVTZ) (Hartree): -738.27290870
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.336629	-0.662570	0.412963
O	1.565636	0.642624	-0.016234
O	0.266244	1.216719	0.007430
O	0.262392	-1.117724	-0.403189
S	-0.891276	0.036793	-0.425881
O	-1.722489	-0.075632	0.747438
H	1.044146	-0.692338	1.463761
H	2.222235	-1.248820	0.188996

Rotational constants (GHz): 6.3915200 3.0934400 2.5333700
Vibrational harmonic frequencies (cm-1):

126.1046	325.0864	379.4990
470.8143	590.2067	667.3954
743.2753	766.7666	944.3923
1018.3951	1113.6121	1176.3786
1267.4247	1306.9058	1396.6377
1522.4123	3113.1058	3208.7369

Zero-point correction (Hartree): 0.045876

E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.39975086
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.33459491
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.33174363
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.32193232
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.33174363
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.32193232
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.01096785
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.01096785
E(RM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.28574478
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.334513	-0.665256	0.409232
O	1.564145	0.643579	-0.007296
O	0.260409	1.211427	0.000254
O	0.257656	-1.107615	-0.411617
S	-0.888979	0.037576	-0.419664
O	-1.712497	-0.078788	0.746226
H	1.040644	-0.706864	1.459252
H	2.218236	-1.251646	0.179435

Rotational constants (GHz): 6.4413800 3.1140100 2.5513000
Vibrational harmonic frequencies (cm-1):

111.7100	319.5083	370.6367
470.7589	591.4319	669.7387
743.7145	777.1958	941.4553
1014.9687	1114.2536	1171.0093
1264.8592	1320.1800	1396.9651
1520.4913	3089.8474	3194.1196

Zero-point correction (Hartree): 0.045752

OCH2OSO2.singlet

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.36710360
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.30725074
E(MP2/Aug-CC-pVTZ) (Hartree): -737.29205639
E(MP3/Aug-CC-pVTZ) (Hartree): -737.29068594
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.32524094
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.32350955
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.06678162
E(RHF/Aug-CC-pVTZ) (Hartree): -735.86129215

E(UHF/Aug-CC-pVTZ) (Hartree): -736.03320439
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.25460215
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.666281	-0.112030	0.468404
O	-0.399330	-0.786599	0.386020
O	-2.275355	0.068601	-0.696294
O	0.751572	1.420708	0.264853
S	0.825610	0.063691	-0.250604
O	1.997408	-0.760228	-0.064231
H	-2.270682	-0.754039	1.122710
H	-1.535747	0.867314	0.953752

Rotational constants (GHz): 7.1034400 2.1156000 1.8447300
Vibrational harmonic frequencies (cm-1):

66.1441	98.7492	258.3848
370.8456	463.0314	521.2687
624.0097	733.3177	847.1769
982.2362	1122.2652	1139.2954
1211.2566	1327.3708	1361.5593
1385.2161	2994.7329	3050.3573

Zero-point correction (Hartree): 0.042276

E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.38602385
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.32673928
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.31157956
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.31041470
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.34265797
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.34118622
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.08566823
E(RHF/Aug-CC-pV(T+d)Z) (Hartree): -735.88393380
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.05424529
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.27289302
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.663769	-0.110013	0.468101
O	-0.392397	-0.779281	0.384648
O	-2.273980	0.067861	-0.695879
O	0.753127	1.410766	0.259328
S	0.825052	0.062905	-0.244526
O	1.986088	-0.756577	-0.069685
H	-2.265186	-0.756603	1.120390
H	-1.535739	0.868055	0.956129

Rotational constants (GHz): 7.1932400 2.1261700 1.8566100
Vibrational harmonic frequencies (cm-1):

60.0746	93.0289	257.7087
377.3376	470.4561	532.1606
624.2640	736.0920	834.4091
978.9193	1124.1375	1155.3359
1210.0767	1355.3720	1357.1959
1386.2142	2985.9071	3038.4014

Zero-point correction (Hartree): 0.042322

OCH2OSO2.triplet

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.36698554
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.30717421
E(MP2/Aug-CC-pVTZ) (Hartree): -737.29199935
E(MP3/Aug-CC-pVTZ) (Hartree): -737.29066266
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.29738074
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.29360206

E(PUHF/Aug-CC-pVTZ) (Hartree): -736.04133782
E(UHF/Aug-CC-pVTZ) (Hartree): -736.03323629
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.25458568
Electronic state : 3-A
Cartesian coordinates (Angs):

C	-1.658891	-0.241585	0.453312
O	-0.375695	-0.866777	0.277832
O	-2.220905	0.206452	-0.662441
O	0.643340	1.399308	0.349774
S	0.822444	0.087334	-0.249720
O	2.032422	-0.680764	-0.064410
H	-2.277911	-1.019017	0.918860
H	-1.561146	0.605425	1.150754

Rotational constants (GHz): 7.1599600 2.1695600 1.8723600
Vibrational harmonic frequencies (cm-1):

72.8342	95.1755	258.1895
366.8841	461.0644	530.7100
629.7946	735.9933	840.4807
987.1747	1119.4222	1139.6178
1204.0652	1325.8477	1350.9100
1387.7743	2996.7831	3059.6886

Zero-point correction (Hartree): 0.042288

OCHOSO2H

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.49719253
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.43485759
E(MP2/Aug-CC-pVTZ) (Hartree): -737.43565506
E(MP3/Aug-CC-pVTZ) (Hartree): -737.42155257
E(RHF/Aug-CC-pVTZ) (Hartree): -736.12609444
E(RM062X/Aug-CC-pVTZ) (Hartree): -738.38681601
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.770993	-0.397914	0.258544
O	-0.495368	-0.776217	0.495648
O	-2.099854	0.468590	-0.487691
O	0.759057	1.363353	0.421322
S	0.717400	-0.003221	-0.421662
O	1.880421	-0.775172	-0.043191
H	-2.450581	-1.013518	0.858176
H	1.244098	1.208107	1.248446

Rotational constants (GHz): 6.6365500 2.2828800 1.9525800
Vibrational harmonic frequencies (cm-1):

78.1739	176.8771	213.8384
318.4693	365.1827	460.0337
495.4170	615.7074	820.4303
848.8033	1064.3416	1124.7849
1159.5236	1299.4010	1403.2080
1860.3674	3111.9564	3744.4898

Zero-point correction (Hartree): 0.043652

cycCH2OSO2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.45425488
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.39278453
E(MP2/Aug-CC-pVTZ) (Hartree): -737.39686638
E(MP3/Aug-CC-pVTZ) (Hartree): -737.38166615
E(RHF/Aug-CC-pVTZ) (Hartree): -736.08310705
E(RM062X/Aug-CC-pVTZ) (Hartree): -738.34111250

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Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.693884      0.000000      -0.000163
     O      -0.736974     -0.000005      -1.067464
     O      -0.737053      0.000002       1.067509
     O       1.178906     -1.237380       0.000011
     S       0.478863      0.000000       0.000006
     O       1.178903      1.237382       0.000005
     H      -2.284382      0.911531       0.000197
     H      -2.284386     -0.911528       0.000203
Rotational constants (GHz):    5.8017400    3.3605600    3.0705900
Vibrational harmonic frequencies (cm-1):
      148.2181                315.5734                462.3757
      491.7343                511.6144                726.4902
      730.4324                933.3777               1028.9415
     1111.0473               1156.4125               1167.2524
     1275.5362               1400.3797               1461.4152
     1556.0821               3126.1332               3205.4059
Zero-point correction (Hartree): 0.047405


SOZ_H2.TSisom
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.33128007
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.25223409
E(MP2/Aug-CC-pVTZ) (Hartree): -737.26409922
E(MP3/Aug-CC-pVTZ) (Hartree): -737.23165622
E(RHF/Aug-CC-pVTZ) (Hartree): -735.90063778
E(RM062X/Aug-CC-pVTZ) (Hartree): -738.20739406
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.322120     -0.598669       0.316105
     O      -0.611446     -1.046394      -0.674718
     O      -1.605889      0.696145       0.259819
     O       0.131506      1.301968      -0.083093
     S       0.983369      0.085483      -0.370628
     O       1.567491     -0.483490       0.821655
     H      -2.504144     -0.497718       0.131758
     H      -1.150333     -1.023826       1.312354
Rotational constants (GHz):    5.7147700    2.9239600    2.4266600
Vibrational harmonic frequencies (cm-1):
    i1220.5517                144.2004                284.3730
      332.1612                416.9629                470.1871
      537.2677                576.2062                731.4285
      886.0170               1006.0144               1201.9086
     1258.6419               1300.5986               1332.3928
     1437.7543               2413.9856               3075.6098
Zero-point correction (Hartree): 0.039653


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.33720663
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.26038212
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.21295133
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.21332336
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.29550690
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.28877225
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.01685312
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -735.93091508
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.22097713
Electronic state : 1-A
Cartesian coordinates (Angs):
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     C      -1.321287     -0.600142       0.310765
     O      -0.601829     -1.035213      -0.681858
     O      -1.610385      0.693386       0.265962
     O       0.136205      1.296031      -0.086554
     S       0.981267      0.088712      -0.362127
     O       1.560447     -0.487878       0.815704
     H      -2.500273     -0.516378       0.119918
     H      -1.147776     -1.032763       1.303486
Rotational constants (GHz):    5.7631900    2.9354000    2.4384700
Vibrational harmonic frequencies (cm-1):
    i1201.7939                143.3151                285.2865
      322.8310                411.1429                466.5634
      532.5822                578.1301                728.3506
      885.1224               1022.9226               1198.4388
     1256.7034               1320.3329               1329.6627
     1429.4637               2428.5693               3057.3070
Zero-point correction (Hartree): 0.039633

SOZ_H2.TSopen
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.35338046
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.28497682
E(MP2/Aug-CC-pVTZ) (Hartree): -737.24518833
E(MP3/Aug-CC-pVTZ) (Hartree): -737.25192808
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.29504597
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.29945261
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.04311824
E(RHF/Aug-CC-pVTZ) (Hartree): -735.92428423
E(UHF/Aug-CC-pVTZ) (Hartree): -735.99183259
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -736.98062310
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.93097022
     T1 diagnostic:  0.051242
E(MP2/Aug-CC-pVDZ) (Hartree): -736.87814585
E(MP3/Aug-CC-pVDZ) (Hartree): -736.89022685
E(PMP2/Aug-CC-pVDZ) (Hartree): -736.92495416
E(PMP3/Aug-CC-pVDZ) (Hartree): -736.93483233
E(PUHF/Aug-CC-pVDZ) (Hartree): -735.90658241
E(RHF/Aug-CC-pVDZ) (Hartree): -735.79273071
E(UHF/Aug-CC-pVDZ) (Hartree): -735.85843867
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.23275716
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.597307     -0.458968      -0.022594
     O      -1.432727      0.683698       0.662173
     O       0.006454      1.199293      -0.464820
     O      -0.326001     -1.126584      -0.221491
     S       0.870941     -0.032985      -0.352175
     O       1.737776     -0.162373       0.792294
     H      -2.067505     -0.333444      -0.999796
     H      -2.167731     -1.137264       0.624907
Rotational constants (GHz):    6.1847300    2.9151700    2.5048300
Vibrational harmonic frequencies (cm-1):
     i883.4211                143.4705                297.3223
      399.2127                471.6906                516.1148
      614.6303                740.6618                903.7150
      921.7921               1034.4937               1135.7507
     1198.3679               1296.7800               1383.2838
     1462.2590               3049.8059               3124.8864
Zero-point correction (Hartree): 0.042589
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E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.37025953
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.30183222
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.26333663
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.26892567
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.31475432
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.31779287
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.05976794
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.00680526
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.24909383
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.595411     -0.464026      -0.012581
     O      -1.425080      0.691202       0.649456
     O       0.001326      1.186179      -0.468475
     O      -0.314586     -1.122296      -0.222778
     S       0.865554     -0.032443      -0.346048
     O       1.731490     -0.154678       0.784986
     H      -2.076320     -0.360387      -0.986805
     H      -2.145288     -1.139620       0.653539
Rotational constants (GHz):    6.2590700    2.9450900    2.5260900
Vibrational harmonic frequencies (cm-1):
     i921.1177                146.6100                 289.6120
      401.6877                483.3483                 533.2592
      616.9810                751.7118                 889.1355
      947.6664               1039.6837                1137.0978
     1203.0512               1319.9485                1376.0270
     1461.7171               3036.3658                3110.4818
Zero-point correction (Hartree): 0.042703

OCH2OSO2.singlet.TSox
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.36067448
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.28116878
E(MP2/Aug-CC-pVTZ) (Hartree): -737.27260215
E(MP3/Aug-CC-pVTZ) (Hartree): -737.24520722
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.30036552
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.26805216
E(PUHF/Aug-CC-pVTZ) (Hartree): -735.96535285
E(RHF/Aug-CC-pVTZ) (Hartree): -735.93214702
E(UHF/Aug-CC-pVTZ) (Hartree): -735.93554121
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -736.98070766
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.92228334
     T1 diagnostic:  0.055818
E(MP2/Aug-CC-pVDZ) (Hartree): -736.90059593
E(MP3/Aug-CC-pVDZ) (Hartree): -736.88063782
E(PMP2/Aug-CC-pVDZ) (Hartree): -736.92738973
E(PMP3/Aug-CC-pVDZ) (Hartree): -736.90261845
E(PUHF/Aug-CC-pVDZ) (Hartree): -735.82600878
E(RHF/Aug-CC-pVDZ) (Hartree): -735.79393350
E(UHF/Aug-CC-pVDZ) (Hartree): -735.79720172
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.23714035
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.785798     -0.299547      -0.131010
     O       1.690969      0.501157       0.831172
     O      -1.725690     -0.406841       0.837554
     O       0.302828     -0.997175      -0.500685
     S      -0.863338     -0.027841      -0.253220
     O      -0.417481      1.334909      -0.440101
     H       2.214399     -1.283596       0.132907
     H       2.079205      0.069928      -1.118851
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Rotational constants (GHz):    5.8333900    2.5040400    2.2691600
Vibrational harmonic frequencies (cm-1):
    i1361.0849                  94.6331                 153.3229
      183.9509                 372.5079                 446.7985
      495.5931                 605.7370                 798.6638
      921.9332                1097.4835                1154.4708
     1236.9576                1353.4145                1369.2256
     1423.1216                2927.6241                3064.0111
Zero-point correction (Hartree): 0.040322


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.36929646
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.30572901
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.28862100
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.28485036
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.31654554
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.31248642
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.05693188
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.02871835
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.25701720
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.776102     -0.296808      -0.144917
     O       1.698049      0.491291       0.833524
     O      -1.719277     -0.415204       0.826065
     O       0.302894     -0.983714      -0.496113
     S      -0.861268     -0.025542      -0.248371
     O      -0.426754      1.329362      -0.429341
     H       2.225850     -1.276060       0.099112
     H       2.058539      0.091711      -1.128751
Rotational constants (GHz):    5.9175300    2.5151600    2.2809700
Vibrational harmonic frequencies (cm-1):
    i1400.0682                  94.2734                 151.5840
      186.5720                 378.1552                 456.5419
      506.9930                 615.2426                 804.4324
      932.9099                1098.8362                1176.1418
     1246.7424                1358.7775                1386.7320
     1416.2553                2932.1566                3062.0345
Zero-point correction (Hartree): 0.040561

OCH2OSO2.singlet.14Hshift
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.34096784
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.27347083
E(MP2/Aug-CC-pVTZ) (Hartree): -737.25869390
E(MP3/Aug-CC-pVTZ) (Hartree): -737.24812234
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.29651240
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.28536614
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.01319379
E(RHF/Aug-CC-pVTZ) (Hartree): -735.88236660
E(UHF/Aug-CC-pVTZ) (Hartree): -735.97484635
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -736.96292049
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.91492314
     T1 diagnostic:  0.037680
E(MP2/Aug-CC-pVDZ) (Hartree): -736.88709464
E(MP3/Aug-CC-pVDZ) (Hartree): -736.88306197
E(PMP2/Aug-CC-pVDZ) (Hartree): -736.92372952
E(PMP3/Aug-CC-pVDZ) (Hartree): -736.91913192
E(PUHF/Aug-CC-pVDZ) (Hartree): -735.87363101
E(RHF/Aug-CC-pVDZ) (Hartree): -735.74749689
E(UHF/Aug-CC-pVDZ) (Hartree): -735.83648370
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E(UM062X/Aug-CC-pVTZ) (Hartree): -738.22719807
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.628299     -0.085592       0.516260
     O      -0.263794     -0.874316      -0.378200
     O      -2.619957     -0.010794      -0.159168
     O       0.422843      1.371932       0.019394
     S       0.972556      0.017115      -0.315781
     O       2.046077     -0.489184       0.518139
     H      -1.561742     -0.657379       1.450459
     H      -0.910700      0.915986       0.503165
Rotational constants (GHz):    7.9929400    1.9308600    1.7212900
Vibrational harmonic frequencies (cm-1):
     i602.2600                  66.7928                 169.0057
      292.3870                 402.9507                 455.2004
      494.4296                 544.7975                 777.3838
      881.8458                 964.1136                1087.5074
     1156.2963                1252.1249                1269.6770
     1611.6970                1763.9623                3028.6531
Zero-point correction (Hartree): 0.036949


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.36014410
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.29339432
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.27767255
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.26811686
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.31218296
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.30216742
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.03416840
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -735.99921724
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.24583403
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.644556     -0.084905       0.522949
     O      -0.249871     -0.860874      -0.396956
     O      -2.628659     -0.007391      -0.163189
     O       0.444096      1.365812       0.015152
     S       0.972635      0.018230      -0.303537
     O       2.037895     -0.496592       0.513879
     H      -1.582835     -0.689204       1.436724
     H      -0.939673      0.899309       0.531075
Rotational constants (GHz):    8.0570900    1.9224200    1.7176200
Vibrational harmonic frequencies (cm-1):
     i521.6327                  59.5258                 167.5780
      185.5445                 364.9847                 456.0449
      507.5609                 551.7952                 811.7205
      890.3257                 978.1610                1085.1672
     1183.4565                1272.4622                1300.2936
     1620.1045                1847.3874                3028.7524
Zero-point correction (Hartree): 0.037159

OCH2OSO2.singlet.TSbisoxy
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.33857283
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.27756417
E(MP2/Aug-CC-pVTZ) (Hartree): -737.25020226
E(MP3/Aug-CC-pVTZ) (Hartree): -737.25623620
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.29069654
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.29608189
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.05328834
E(RHF/Aug-CC-pVTZ) (Hartree): -735.85141162
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E(UHF/Aug-CC-pVTZ) (Hartree): -736.01231487
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -736.97165305
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.92899487
     T1 diagnostic:  0.031133
E(MP2/Aug-CC-pVDZ) (Hartree): -736.89110602
E(MP3/Aug-CC-pVDZ) (Hartree): -736.90132712
E(PMP2/Aug-CC-pVDZ) (Hartree): -736.92752143
E(PMP3/Aug-CC-pVDZ) (Hartree): -736.93718916
E(PUHF/Aug-CC-pVDZ) (Hartree): -735.91935624
E(RHF/Aug-CC-pVDZ) (Hartree): -735.72431171
E(UHF/Aug-CC-pVDZ) (Hartree): -735.88252494
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.22224201
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.839938      0.070157       0.402079
     O      -0.808155     -0.818859       0.439762
     O      -2.664438      0.057101      -0.647953
     O       1.087864      1.358134       0.288098
     S       1.075194      0.054681      -0.325966
     O       2.102631     -0.878413       0.035733
     H      -2.420754     -0.149882       1.326285
     H      -1.485929      1.110341       0.551572
Rotational constants (GHz):    6.9698000    1.5904100    1.4303600
Vibrational harmonic frequencies (cm-1):
     i324.9621                  60.4777                  75.4619
      147.4461                 212.2548                 255.5535
      534.1052                 591.0347                 671.5684
      935.7559                1047.8853                1128.4529
     1219.4231                1250.1470                1301.5467
     1404.0956                2894.0285                2946.9518
Zero-point correction (Hartree): 0.037991


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.35430759
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.29390433
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.26564057
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.27288902
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.30581069
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.31242126
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.07064849
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -736.03000381
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.23798198
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.841159      0.067968       0.401897
     O      -0.810981     -0.822043       0.443961
     O      -2.655985      0.063252      -0.656235
     O       1.084757      1.349740       0.291442
     S       1.079107      0.057973      -0.320346
     O       2.094931     -0.876484       0.025099
     H      -2.432386     -0.157745       1.318052
     H      -1.488152      1.106641       0.561963
Rotational constants (GHz):    6.9886400    1.5942200    1.4352600
Vibrational harmonic frequencies (cm-1):
     i317.2794                  54.2924                  69.5705
      139.7619                 211.8262                 246.9922
      535.2555                 589.9794                 658.8565
      935.6031                1030.5355                1129.6182
     1233.8012                1249.7131                1301.0977
     1434.6324                2880.1588                2928.3333
Zero-point correction (Hartree): 0.037886
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OCH2OSO2.singlet.Helim
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.32555896
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.26036964
E(MP2/Aug-CC-pVTZ) (Hartree): -737.25417133
E(MP3/Aug-CC-pVTZ) (Hartree): -737.23802286
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.31346017
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.29589334
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.02755285
E(RHF/Aug-CC-pVTZ) (Hartree): -735.84366747
E(UHF/Aug-CC-pVTZ) (Hartree): -735.96724805
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -736.94794432
E(CCSD/Aug-CC-pVDZ) (Hartree): -736.90242507
     T1 diagnostic:  0.028158
E(MP2/Aug-CC-pVDZ) (Hartree): -736.88423902
E(MP3/Aug-CC-pVDZ) (Hartree): -736.87454598
E(PMP2/Aug-CC-pVDZ) (Hartree): -736.94170898
E(PMP3/Aug-CC-pVDZ) (Hartree): -736.93064722
E(PUHF/Aug-CC-pVDZ) (Hartree): -735.88747444
E(RHF/Aug-CC-pVDZ) (Hartree): -735.70812248
E(UHF/Aug-CC-pVDZ) (Hartree): -735.82901831
E(UM062X/Aug-CC-pVTZ) (Hartree): -738.21320323
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.624934      0.209843      -0.074342
     O      -0.494959     -0.641375      -0.177155
     O      -2.689928     -0.284184       0.131880
     O       0.866215      1.397626       0.149483
     S       0.991941      0.011739      -0.277166
     O       1.878750     -0.913190       0.384855
     H      -1.168516      0.865490       1.427515
     H      -1.433563      1.216611      -0.459313
Rotational constants (GHz):    7.9664200    1.9218900    1.6310300
Vibrational harmonic frequencies (cm-1):
     i982.1014                  81.1304                 126.7991
      217.0665                 377.9145                 436.3822
      501.2621                 541.0617                 551.4999
      579.6280                 836.4240                 954.6326
     1086.3401                1127.6122                1318.6657
     1376.1755                1779.1105                3086.8944
Zero-point correction (Hartree): 0.034124


E(CCSD(T)/Aug-CC-pV(T+d)Z) (Hartree): -737.34443583
E(CCSD/Aug-CC-pV(T+d)Z) (Hartree): -737.27988943
E(MP2/Aug-CC-pV(T+d)Z) (Hartree): -737.27382468
E(MP3/Aug-CC-pV(T+d)Z) (Hartree): -737.25786896
E(PMP2/Aug-CC-pV(T+d)Z) (Hartree): -737.33035000
E(PMP3/Aug-CC-pV(T+d)Z) (Hartree): -737.31307874
E(PUHF/Aug-CC-pV(T+d)Z) (Hartree): -736.04601365
E(UHF/Aug-CC-pV(T+d)Z) (Hartree): -735.98854645
E(UM062X/Aug-CC-pV(T+d)Z) (Hartree): -738.23149977
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.623837      0.213376      -0.071003
     O      -0.487341     -0.633999      -0.166558
     O      -2.688487     -0.285696       0.120075
     O       0.872376      1.388108       0.143133
     S       0.987443      0.010735      -0.270321
     O       1.873086     -0.909808       0.372634
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     H      -1.183811      0.856171       1.443368
     H      -1.429337      1.222989      -0.446492
Rotational constants (GHz):    8.0964500    1.9299100    1.6382100
Vibrational harmonic frequencies (cm-1):
     i982.9430                84.3173                127.0439
      217.3890                384.0912               444.5563
      510.4490                547.5279               557.6359
      578.5280                847.1148               951.7147
     1085.6268               1149.0319              1350.9956
     1377.4303               1782.4374              3087.9433
Zero-point correction (Hartree): 0.034364

cycCH2OSO2.TSox
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -737.40746969
E(CCSD/Aug-CC-pVTZ) (Hartree): -737.34143408
E(MP2/Aug-CC-pVTZ) (Hartree): -737.34999170
E(MP3/Aug-CC-pVTZ) (Hartree): -737.32605051
E(PMP2/Aug-CC-pVTZ) (Hartree): -737.34999170
E(PMP3/Aug-CC-pVTZ) (Hartree): -737.32605051
E(PUHF/Aug-CC-pVTZ) (Hartree): -736.02879444
E(RHF/Aug-CC-pVTZ) (Hartree): -736.02879444
E(UHF/Aug-CC-pVTZ) (Hartree): -736.02879444
E(RM062X/Aug-CC-pVTZ) (Hartree): -738.29052069
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.848495      0.000019      -0.017500
     O      -1.078431     -0.000142      -1.019765
     O      -0.328661      0.000022       1.286682
     O       1.135116     -1.239364      -0.268946
     S       0.546533      0.000013       0.098615
     O       1.134981      1.239420      -0.269069
     H      -2.278703      0.934217       0.347910
     H      -2.278900     -0.934033       0.348050
Rotational constants (GHz):    5.2182800    3.0017300    2.9160200
Vibrational harmonic frequencies (cm-1):
     i528.4572               i125.0000                222.9737
      318.1533                439.8518                447.4253
      539.7501                574.3084                599.2040
     1024.6585               1224.6906               1243.1489
     1328.8148               1444.1335               1462.0895
     1616.4372               3095.9719               3202.4907
Zero-point correction (Hartree): 0.042793


cycCH2OSO2.12Hshift
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E(UM062X/Aug-CC-pVTZ) (Hartree): -738.20589173
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.721786      0.298850       0.067204
     O      -0.953759      0.278930       1.094037
     O      -1.324662     -0.563182      -0.880304
     O       1.411931      1.207073      -0.298214
     S       0.692903     -0.024325      -0.142329
     O       1.361535     -1.183257       0.360032
     H      -2.153117      1.251089      -0.265744
     H      -2.562969     -0.571500      -0.064630
Rotational constants (GHz):    5.5656200    2.5019400    2.2847800
Vibrational harmonic frequencies (cm-1):
    i1360.1916                91.6497                140.0516
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      193.1498                282.5972                431.8377
      471.5041                551.9223                764.0325
      892.1341               1165.4498               1228.8055
     1230.9819               1348.7122               1428.5337
     1458.8274               2293.8747               3067.3285
Zero-point correction (Hartree): 0.038823
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