

Theoretical study of the Reactions of Criegee Intermediates with Ozone, Alkylhydroperoxides, and Carbon Monoxide

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- Supporting Information -

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Table S1

Table S1: Additional relative energies for the CH₂OO + CO reaction, based on CCSD(T) geometries obtained with the cc-pVDZ and cc-pVTZ basis sets, and single point energies at these levels of theory and at the CCSD(T)/aug-cc-pVTZ level.. Scaled M06-2X/aVTZ ZPE-corrections are used through-out.

Geometry	CCSD(T)/cc-pVDZ	CCSD(T)/cc-pVDZ	CCSD(T)/cc-pVTZ	CCSD(T)/cc-pVTZ
Single point energy	CCSD(T)/cc-pVDZ	CCSD(T)/aug-cc-pVTZ	CCSD(T)/cc-pVTZ	CCSD(T)/aug-cc-pVTZ
CH ₂ OO + CO	0.0	0.0	0.0	0.0
TS1	12.3	9.9	10.8	10.1
TS2	13.3	11.9	13.7	12.0

This section discusses some additional calculations related to the CI + CO reaction, which do not influence the conclusions in the main paper, but could be useful in future investigations on this reaction attempting to reconcile the experimental and theoretical results.

A) Formic Acid Anhydride

A first set of calculations relate to the formation of formic acid anhydride (FAA, HC(=O)OC(=O)H) in the CI + CO reaction. Su et al. (1980) observed the formation of FAA in their ethene ozonolysis experiments, and observed an increase in the yield of FAA upon addition of CO. They invoke the reaction of CH₂OO + CO as the source of FAA, and note that it anti-correlates with an observed unknown species X, and that both FAA and X formation can be suppressed by scavenging of the CI by SO₂. The high yields of FAA in the experiments without CO added, and the complex rearrangements needed to obtain FAA from CH₂OO + CO directly lead us to believe that FAA is not formed in the CH₂OO + CO reaction, but rather from an intermediate formed later in the ozonolysis reaction sequence, such as e.g. the dioxirane or the singlet bis-oxy intermediate which already have both oxygen atoms attached to the carbon, as needed for FAA formation.

We have attempted to characterize pathways leading to FAA in the CH₂OO + CO system; as mentioned in the main paper, the only candidate found is the reaction through **TS5** (see main text), a complex reaction with a high barrier which involves O- and H-transfer from CH₂OO to the CO moiety, forming transient HC[•]O + OCHO[•] radical moieties. IRC calculations on this reaction then finds that the OCHO[•] H-atom migrates back to the HC[•]O moiety, forming H₂CO + CO₂ as final products. A dynamical study that incorporates the kinematic movements of the moieties could likewise yield a radical-radical recombination reaction forming FAA (-115.4 kcal/mol below the reactants), or even a non-reactive separation of the HC[•]O + OCHO[•] radical fragments (-19.5 kcal/mol below the reactants). **TS5** is, in this respect, reminiscent of the 1,3-H-migration **TSa** in FAA, forming CH₂O + CO₂ (see figure S-1). Here, too, the reaction proceeds through transient HC[•]O + OCHO[•] radical moieties, but with a breaking C–O bond rather than a breaking O–O bond as in **TS5**.

In the course of these studies, we also characterized some high-energy transition states linking FAA to the cyclic form of FAA, and to the H₂CO + CO₂ products (see figure S-1). **TSb** is a ring opening TS, while **TSa** is a 1,2-H-migration with fragmentation.

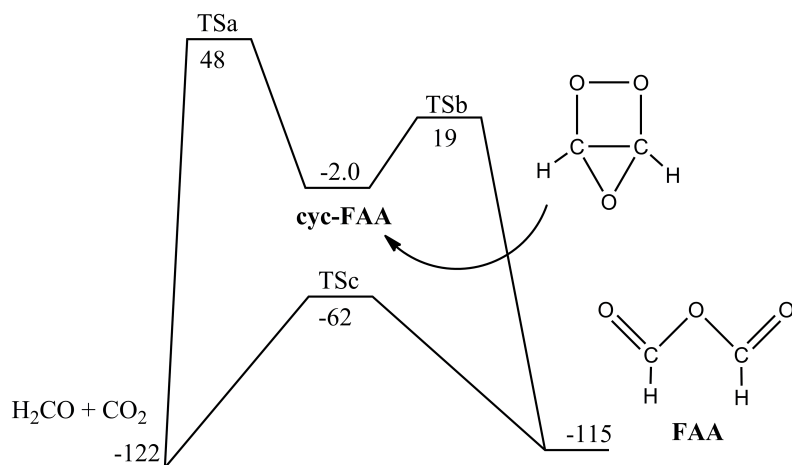


Figure S-1: M06-2X/aug-cc-pVTZ calculations on the interconversion of formic acid anhydride and H₂CO + CO₂ (kcal/mol, energies relative to CH₂OO + CO).

These results are shown here in an effort to be complete, but they have no bearing on the CI + CO reaction as we were unable to find a link between this PES and the CI + CO PES. In particular, we attempted to find an H-migration + ring closure pathway connecting **cyc-FAA** to the cyclic adduct formed in the $\text{CH}_2\text{OO} + \text{CO}$ reaction, but were unsuccessful. H-migration in the cyclic adduct instead forms the OOCH-CHO substituted carbonyl oxide, of which we characterized three conformers: *anti-trans*- CHOCHOO at 1.3 kcal/mol above the $\text{CH}_2\text{OO} + \text{CO}$ energy level, and two *syn*-forms at 2.7 and 9.0 kcal/mol above $\text{CH}_2\text{OO} + \text{CO}$, where the most stable *syn*-conformer has an H-bond between the aldehyde H-atom and the oxide O-atom. The 1,2-H-migration in the cycloadduct forms the most stable *syn*-form only, with a TS 24 kcal/mol above $\text{CH}_2\text{OO} + \text{CO}$, i.e. 68 kcal/mol above the cycloadduct and hence with a negligible reaction flux compared to **TS6**. (see Figure S-2)

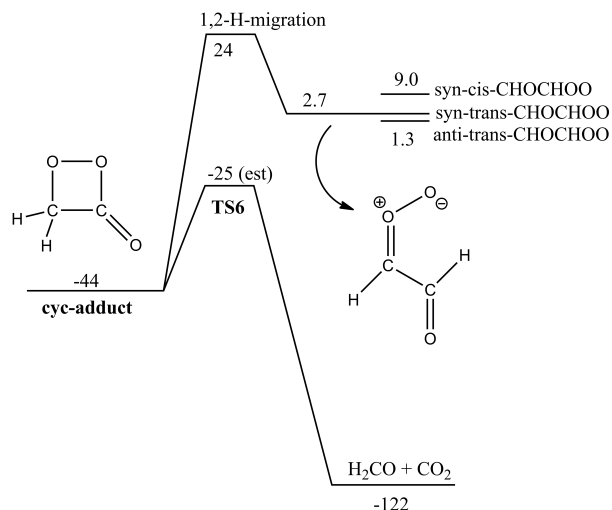


Figure S-2: M06-2X/aug-cc-pVTZ calculations on the reactions of the cycloadduct (kcal/mol, energies relative to $\text{CH}_2\text{OO} + \text{CO}$).

B) The decomposition of the cyclic adduct

The cyclic adduct formed in the CI+ CO reactions readily falls apart to $\text{CH}_2\text{O} + \text{CO}_2$ by breaking the O–O bond. The wavefunction of this transition state **TS6** is strongly multi-reference (T1 diagnostic above 0.088), and can not be reliably characterized on the M06-2X level of theory. We have characterized this TS also at the BLYP/aug-cc-pVTZ level of theory, which includes no Hartree-Fock exchange and is thus better suited to describe multi-reference systems. **TS6** is thus calculated at an energy of -21.2 kcal/mol relative to $\text{CH}_2\text{OO} + \text{CO}$, close to the M06-2X energy of -25 kcal/mol. The wavefunction, however, shows a strong spin contamination ($S^2 = 0.4036$ prior to annihilation, 0.0069 after), reducing the reliability of the predictions due to the mixing of the singlet and triplet PES. An UCCSD(T)/aug-cc-pVTZ single point calculation on the BLYP geometry yields a relative energy of -10.4 kcal/mol but again the broken symmetry UHF reference wavefunction has a spin contamination exceeding $S^2 = 1$ before annihilation (and still 0.1714 after), making these calculations unreliable.

A transient $\cdot\text{OCH}_2\text{C(=O)O}\cdot$ structure formed formally in the decomposition of the cycloadduct can be isolated at the BLYP level of theory, but its singlet wavefunction also shows very strong spin contamination ($S^2 > 1$ prior to annihilation), and could be an artifact of the methodology caused by mixing of the singlet wavefunction with the triplet potential energy surface where this intermediate is more stable due to higher barriers to decomposition.

We conclude that the characterization of **TS6** requires the application of (computationally costly) multi-reference quantum chemical methods; as this TS is currently not critical to our understanding of the CI + CO chemistry, we opted to postpone such calculations until a later date.

C) BLYP/aug-cc-pVTZ calculations on the CH₂OO + CO transition states

We re-optimized several of the initial CH₂OO + CO transition states using the BLYP functional. This functional includes no Hartree-Fock exchange and is thus better suited to describe multi-reference systems. The lowest TS, **TS1**, for cycloaddition of CO onto the CI, was predicted with a barrier to reaction of 7.79 kcal/mol, compared to the M06-2X value of 8.69 kcal/mol. CCSD(T)/aug-cc-pVTZ single-point calculations, however, increased the barrier to 9.99 kcal/mol, directly comparable to the CCSD(T) calculations on M06-2X and CCSD(T) geometries (see main text). The BLYP energy barriers for **TS2** and **TS3** entrance channels, 7.3 and 8.8 kcal/mol, respectively, were likewise somewhat below the M06-2X values. CCSD(T) calculations on these BLYP geometries, however, again resulted in higher energy barriers of 11.3 and 13.5 kcal/mol respectively, significantly higher than the cycloaddition channel **TS1**, and in line with the relative energies of the CCSD(T)//M06-2X and CCSD(T)//CCSD(T) barriers listed in the main text. Given the large energy differences between the BLYP and the CCSD(T)/BLYP values, it would be necessary to perform IRCMax calculations to obtain reliable CCSD(T)/BLYP energy barriers. However, as the BLYP, M06-2X, and CCSD(T) geometries all yield similar barrier height for CCSD(T) energies, this aspect was not investigated further.

Compared to the CCSD(T) benchmark calculations listed in the main paper, the BLYP TS energies were thus found to be less reliable than the M06-2X values. However, the geometries optimized using BLYP were of slightly better quality than the M06-2X geometries, i.e. CCSD(T)/aug-cc-pVTZ single point calculations on these geometries returns absolute energies that are closer to the CCSD(T)/aug-cc-pVTZ geometry values.

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*****
CH2OO + O3
*****

CH2O2
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -189.16882449
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -189.37915916
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059354
E(CCSD/Aug-CC-pVDZ) (Hartree): -189.14423971
  T1 diagnostic: 0.043994
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.34290813
  T1 diagnostic: 0.040884
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649231
  T1 diagnostic: 0.041942
E(MP2/Aug-CC-pVDZ) (Hartree): -189.12365394
E(MP2/Aug-CC-pVQZ) (Hartree): -189.33750956
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461284
E(PMP2/Aug-CC-pVDZ) (Hartree): -189.12365394
E(PMP2/Aug-CC-pVQZ) (Hartree): -189.33750956
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.28461284
E(PUHF/Aug-CC-pVDZ) (Hartree): -188.58838987
E(PUHF/Aug-CC-pVQZ) (Hartree): -188.64753905
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(ROHF/Aug-CC-pVDZ) (Hartree): -188.58838987
E(ROHF/Aug-CC-pVQZ) (Hartree): -188.64753905
E(ROHF/Aug-CC-pVTZ) (Hartree): -188.63545474
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

CH2O
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -114.24391147
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.34257265
E(CCSD/Aug-CC-pVDZ) (Hartree): -114.23211277
  T1 diagnostic: 0.016180
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.32534873
  T1 diagnostic: 0.015270
E(MP2/Aug-CC-pVDZ) (Hartree): -114.21760744
E(MP2/Aug-CC-pVTZ) (Hartree): -114.31598817
E(PMP2/Aug-CC-pVDZ) (Hartree): -114.21760744
E(PMP2/Aug-CC-pVTZ) (Hartree): -114.31598817
E(PUHF/Aug-CC-pVDZ) (Hartree): -113.88576298
E(PUHF/Aug-CC-pVTZ) (Hartree): -113.91458960
E(ROHF/Aug-CC-pVDZ) (Hartree): -113.88576298
E(ROHF/Aug-CC-pVTZ) (Hartree): -113.91458961
E(RM062X/Aug-CC-pVTZ) (Hartree): -114.49897007
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):

```

C	0.000067	0.525524	0.000000
O	0.000067	-0.670583	0.000000
H	-0.938823	1.104753	0.000000
H	0.937882	1.106772	0.000000

Rotational constants (GHz): 284.7542300 39.4477400 34.6478800
 Vibrational harmonic frequencies (cm-1):
 1213.8279 (A'') 1273.4992 (A') 1539.9496 (A')
 1868.6291 (A') 2944.7283 (A') 3014.8572 (A')
 Zero-point correction (Hartree): 0.027009

O3

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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.96813033
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -225.21050793
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -225.15298425
 E(CCSD/Aug-CC-pVDZ) (Hartree): -224.93176919
 T1 diagnostic: 0.027517
 E(CCSD/Aug-CC-pVQZ) (Hartree): -225.15977939
 T1 diagnostic: 0.026385
 E(CCSD/Aug-CC-pVTZ) (Hartree): -225.10489180
 T1 diagnostic: 0.026586
 E(MP2/Aug-CC-pVDZ) (Hartree): -224.95574979
 E(MP2/Aug-CC-pVQZ) (Hartree): -225.19957423
 E(MP2/Aug-CC-pVTZ) (Hartree): -225.13809543
 E(PMP2/Aug-CC-pVDZ) (Hartree): -224.95574979
 E(PMP2/Aug-CC-pVQZ) (Hartree): -225.19957423
 E(PMP2/Aug-CC-pVTZ) (Hartree): -225.13809543
 E(PUHF/Aug-CC-pVDZ) (Hartree): -224.29476823
 E(PUHF/Aug-CC-pVQZ) (Hartree): -224.36449970
 E(PUHF/Aug-CC-pVTZ) (Hartree): -224.34937878
 E(ROHF/Aug-CC-pVDZ) (Hartree): -224.29476823
 E(ROHF/Aug-CC-pVQZ) (Hartree): -224.36449970
 E(ROHF/Aug-CC-pVTZ) (Hartree): -224.34937878
 E(UM062X/Aug-CC-pVTZ) (Hartree): -225.41041563
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 O 1.068215 -0.222465 0.000000
 O 0.000000 0.444791 0.000000
 O -1.068215 -0.222326 0.000000
 Rotational constants (GHz): 106.4709600 13.8448500 12.2517100
 Vibrational harmonic frequencies (cm-1):
 743.4824 (A') 1092.2611 (A') 1238.7702 (A')
 Zero-point correction (Hartree): 0.007004

complex.CH200+O3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -414.14510680
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -414.59604616
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.49061814
 E(CCSD/Aug-CC-pVDZ) (Hartree): -414.08320927
 T1 diagnostic: 0.036382
 E(CCSD/Aug-CC-pVQZ) (Hartree): -414.50830867
 T1 diagnostic: 0.034178
 E(CCSD/Aug-CC-pVTZ) (Hartree): -414.40764670
 T1 diagnostic: 0.034859
 E(MP2/Aug-CC-pVDZ) (Hartree): -414.08826639
 E(MP2/Aug-CC-pVQZ) (Hartree): -414.54453305
 E(MP2/Aug-CC-pVTZ) (Hartree): -414.43072369
 E(PMP2/Aug-CC-pVDZ) (Hartree): -414.08826639
 E(PMP2/Aug-CC-pVQZ) (Hartree): -414.54453305
 E(PMP2/Aug-CC-pVTZ) (Hartree): -414.43072369
 E(PUHF/Aug-CC-pVDZ) (Hartree): -412.88623511
 E(PUHF/Aug-CC-pVQZ) (Hartree): -413.01348401

E(PUHF/Aug-CC-pVTZ) (Hartree): -412.98662896
 E(ROHF/Aug-CC-pVDZ) (Hartree): -412.88623511
 E(ROHF/Aug-CC-pVQZ) (Hartree): -413.01348401
 E(ROHF/Aug-CC-pVTZ) (Hartree): -412.98662896
 E(UM062X/Aug-CC-pVTZ) (Hartree): -414.99441523
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.337210	0.796707	0.627688
O	1.641871	-0.007819	-0.267924
O	1.059839	-1.221477	-0.243443
O	-0.966033	1.006046	-0.575482
O	-1.381139	-0.172827	-0.405209
O	-1.664820	-0.482749	0.774682
H	0.660894	0.477873	1.413389
H	1.798103	1.772489	0.559492

 Rotational constants (GHz): 6.1837200 2.4947400 2.1849500
 Vibrational harmonic frequencies (cm-1):

66.9163	82.2719	109.0898
138.2766	205.4938	226.1759
546.4164	711.7394	759.5289
930.0132	1037.1989	1106.0692
1243.6659	1262.8713	1427.5775
1600.6944	3138.6088	3291.3483

 Zero-point correction (Hartree): 0.040743

cyc-CO5H2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.55794430
 E(CCSD/Aug-CC-pVTZ) (Hartree): -414.49035514
 T1 diagnostic: 0.018787
 E(MP2/Aug-CC-pVTZ) (Hartree): -414.48312904
 E(MP3/Aug-CC-pVTZ) (Hartree): -414.47792290
 E(RHF/Aug-CC-pVTZ) (Hartree): -413.09991546
 E(RM062X/Aug-CC-pVTZ) (Hartree): -415.07928260
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.266074	0.000873	0.208765
O	0.622077	-1.150146	-0.279580
O	-0.672470	-1.104939	0.285313
O	-1.285610	-0.001516	-0.303125
O	-0.673952	1.104769	0.284790
O	0.620041	1.150812	-0.279522
H	1.255926	0.001208	1.299164
H	2.266945	0.001707	-0.214761

 Rotational constants (GHz): 5.7445500 5.6029000 3.1476100
 Vibrational harmonic frequencies (cm-1):

369.2805	383.2205	536.0985
581.9988	612.0527	798.0573
825.2624	935.1807	939.1342
994.5629	1045.8298	1079.8264
1189.0445	1317.4347	1408.9287
1482.1411	3095.0572	3185.0720

 Zero-point correction (Hartree): 0.047336

O2.triplet

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -150.01964278
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -150.14022210
 E(CCSD/Aug-CC-pVDZ) (Hartree): -150.00658871
 T1 diagnostic: 0.017878
 E(CCSD/Aug-CC-pVTZ) (Hartree): -150.12032829
 T1 diagnostic: 0.017459
 E(MP2/Aug-CC-pVDZ) (Hartree): -150.01791249
 E(MP2/Aug-CC-pVTZ) (Hartree): -150.13640826

E(PMP2/Aug-CC-pVDZ) (Hartree): -150.01791249
 E(PMP2/Aug-CC-pVTZ) (Hartree): -150.13640826
 E(PUHF/Aug-CC-pVDZ) (Hartree): -149.62284252
 E(PUHF/Aug-CC-pVTZ) (Hartree): -149.65772956
 E(ROHF/Aug-CC-pVDZ) (Hartree): -149.62284252
 E(ROHF/Aug-CC-pVTZ) (Hartree): -149.65772956
 E(UM062X/Aug-CC-pVTZ) (Hartree): -150.32479538
 Point group : D*H
 Electronic state : 3-SGG
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.594925
 O 0.000000 0.000000 -0.594925
 Rotational constants (GHz): 0.0000000 44.6355303 44.6355303
 Vibrational harmonic frequencies (cm-1):
 1754.4579 (SGG)
 Zero-point correction (Hartree): 0.003997

 O3
 --
 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -224.96813033
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -225.21050793
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -225.15298425
 E(CCSD/Aug-CC-pVDZ) (Hartree): -224.93176919
 T1 diagnostic: 0.027517
 E(CCSD/Aug-CC-pVQZ) (Hartree): -225.15977939
 T1 diagnostic: 0.026385
 E(CCSD/Aug-CC-pVTZ) (Hartree): -225.10489180
 T1 diagnostic: 0.026586
 E(MP2/Aug-CC-pVDZ) (Hartree): -224.95574979
 E(MP2/Aug-CC-pVQZ) (Hartree): -225.19957423
 E(MP2/Aug-CC-pVTZ) (Hartree): -225.13809543
 E(PMP2/Aug-CC-pVDZ) (Hartree): -224.95574979
 E(PMP2/Aug-CC-pVQZ) (Hartree): -225.19957423
 E(PMP2/Aug-CC-pVTZ) (Hartree): -225.13809543
 E(PUHF/Aug-CC-pVDZ) (Hartree): -224.29476823
 E(PUHF/Aug-CC-pVQZ) (Hartree): -224.36449970
 E(PUHF/Aug-CC-pVTZ) (Hartree): -224.34937878
 E(ROHF/Aug-CC-pVDZ) (Hartree): -224.29476823
 E(ROHF/Aug-CC-pVQZ)
 (Hartree): -224.36449970
 E(ROHF/Aug-CC-pVTZ) (Hartree): -224.34937878
 E(UM062X/Aug-CC-pVTZ) (Hartree): -225.41041563
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 O 1.068215 -0.222465 0.000000
 O 0.000000 0.444791 0.000000
 O -1.068215 -0.222326 0.000000
 Rotational constants (GHz): 106.4709600 13.8448500 12.2517100
 Vibrational harmonic frequencies (cm-1):
 743.4824 (A') 1092.2611 (A') 1238.7702 (A')
 Zero-point correction (Hartree): 0.007004

 OCH2O.triplet.a

 E(UM062X/Aug-CC-pVTZ) (Hartree): -264.74783209
 Electronic state : 3-A
 Cartesian coordinates (Angs):
 C -0.653460 0.506933 0.266514
 O 0.627096 0.406979 -0.412104
 O 1.414667 -0.426402 0.191394
 O -1.358046 -0.604870 -0.133195
 H -0.461014 0.517697 1.339442
 H -1.087970 1.435048 -0.107280

Rotational constants (GHz): 22.0202600 6.2739200 5.5470200
 Vibrational harmonic frequencies (cm-1):
 153.2539 401.9883 547.4104
 780.9686 1069.0821 1166.4963
 1244.5026 1318.8063 1378.5832
 1529.8144 3067.5476 3143.6996
 Zero-point correction (Hartree): 0.036000

OOCH2O.triplet.b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -264.20006599
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.41995128
 E(CCSD/Aug-CC-pVDZ) (Hartree): -264.17680797
 T1 diagnostic: 0.032615
 E(CCSD/Aug-CC-pVTZ) (Hartree): -264.38543847
 T1 diagnostic: 0.031604
 E(MP2/Aug-CC-pVDZ) (Hartree): -264.13500403
 E(MP2/Aug-CC-pVTZ) (Hartree): -264.35277845
 E(PMP2/Aug-CC-pVDZ) (Hartree): -264.13500403
 E(PMP2/Aug-CC-pVTZ) (Hartree): -264.35277845
 E(PUHF/Aug-CC-pVDZ) (Hartree): -263.47404491
 E(PUHF/Aug-CC-pVTZ) (Hartree): -263.53687144
 E(ROHF/Aug-CC-pVDZ) (Hartree): -263.47404491
 E(ROHF/Aug-CC-pVTZ) (Hartree): -263.53687144
 E(UM062X/Aug-CC-pVTZ) (Hartree): -264.76493916

Electronic state : 3-A

Cartesian coordinates (Angs):

O	1.394475	-0.488889	0.145109
O	0.680754	0.491691	-0.325062
C	-0.649156	0.457902	0.237605
H	-1.113813	1.404218	-0.069187
H	-0.544420	0.429110	1.332392
O	-1.381083	-0.575394	-0.156152

Rotational constants (GHz): 22.5409200 6.2791400 5.4204500
 Vibrational harmonic frequencies (cm-1):
 111.8450 397.6785 624.5703
 833.4899 927.4494 1138.2247
 1193.0832 1259.3176 1355.5853
 1379.7775 2984.7389 3045.1585

Zero-point correction (Hartree): 0.034744

OOCH2O00.triplet.trans

E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07602915

Electronic state : 3-A

Cartesian coordinates (Angs):

C	0.649428	0.898627	0.006081
O	1.451346	-0.121589	-0.602958
O	2.120705	-0.781329	0.299457
O	-2.377027	-0.572319	0.064496
O	-1.438939	0.061460	-0.416319
O	-0.443416	0.369936	0.656620
H	1.242541	1.402598	0.766395
H	0.359539	1.556369	-0.813244

Rotational constants (GHz): 10.1629500 1.9645200 1.8682900
 Vibrational harmonic frequencies (cm-1):
 51.3837 87.8829 158.3656
 295.4656 411.1341 532.2314
 621.6282 758.9081 954.7686
 1091.0839 1175.7031 1246.8955
 1316.9581 1381.0358 1415.8794
 1463.2433 3095.0977 3171.5154

Zero-point correction (Hartree): 0.043807

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OOCH2000.ppp
-----
E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07635751
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.390266      0.149700      0.819912
  O      1.235958     -0.680344      0.009990
  O     -0.369557      0.998632      0.062659
  H     -0.207940     -0.545043      1.408738
  H      1.011516      0.793954      1.440522
  O      2.194799      0.019500     -0.526758
  O     -1.548113      0.255565     -0.569812
  O     -1.906233     -0.736742      0.052830
Rotational constants (GHz):   9.0098100   2.2478600   2.1294500
Vibrational harmonic frequencies (cm-1):
  16.3693           74.4237           154.6690
  311.5749          468.7547           472.1550
  628.6633          741.3744           947.4216
 1082.4147          1143.2787          1243.7285
 1307.9650          1386.0069          1429.2597
 1452.7068          3100.5478          3165.7761
Zero-point correction (Hartree): 0.043575

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OOCH2000.mpp
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -414.21020260
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.55134435
E(CCSD/Aug-CC-pVDZ) (Hartree): -414.09931200
  T1 diagnostic: 0.036819
E(CCSD/Aug-CC-pVTZ) (Hartree): -414.41951264
  T1 diagnostic: 0.035276
E(MP2/Aug-CC-pVDZ) (Hartree): -414.18053557
E(MP2/Aug-CC-pVTZ) (Hartree): -414.52320666
E(PMP2/Aug-CC-pVDZ) (Hartree): -414.18053557
E(PMP2/Aug-CC-pVTZ) (Hartree): -414.52320666
E(PUHF/Aug-CC-pVDZ) (Hartree): -412.82349532
E(PUHF/Aug-CC-pVTZ) (Hartree): -412.92169918
E(ROHF/Aug-CC-pVDZ) (Hartree): -412.82349532
E(ROHF/Aug-CC-pVTZ) (Hartree): -412.92169918
E(UM062X/Aug-CC-pVDZ) (Hartree): -414.98197248
E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07692523
E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07692561
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.516537      0.818671      0.488870
  O      1.642040      0.114125     -0.051071
  O     -0.464027      1.005370     -0.454453
  H      0.149310      0.272186      1.358387
  H      0.882996      1.810293      0.747335
  O      1.380001     -1.159422     -0.135963
  O     -1.338213     -0.230179     -0.543786
  O     -1.736242     -0.604208      0.555406
Rotational constants (GHz):   6.7876800   2.8652200   2.3624800
Vibrational harmonic frequencies (cm-1):
  67.6699           85.5963           140.3564
 347.7766           439.4704           515.6713
 614.5771           728.1926           955.6213
1079.1214           1151.5819          1241.4201
1323.0782           1370.0261          1413.3602
1461.3619           3094.7054          3167.0857
Zero-point correction (Hartree): 0.043733

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OOCH2000.tmm
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E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07594297
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.402440	0.587819	0.515840
O	-1.262140	0.039023	-0.515149
O	0.713755	1.087859	-0.067799
H	-0.912308	1.429886	0.984801
H	-0.208926	-0.210805	1.234130
O	-2.257132	-0.592065	0.027360
O	1.724454	-0.052165	-0.369004
O	1.523047	-1.075901	0.260346

 Rotational constants (GHz): 8.0752200 2.3417100 2.0054900
 Vibrational harmonic frequencies (cm-1):

47.6459	67.8785	145.3401
370.3863	398.9415	429.1383
535.8769	741.4986	1003.4140
1061.9200	1162.1094	1265.2437
1296.6857	1384.1282	1444.2513
1464.5814	3080.5601	3141.5754

 Zero-point correction (Hartree): 0.043379

OOCH2000.mpt

 E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07613914
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.754119	0.914125	0.297248
O	1.655349	0.026577	-0.378844
O	-0.502256	0.886288	-0.265136
H	0.737236	0.636619	1.351122
H	1.144850	1.915511	0.127760
O	1.547187	-1.185901	0.085585
O	-1.223824	-0.265658	0.373600
O	-2.277305	-0.465916	-0.223001

 Rotational constants (GHz): 8.0040700 2.3929600 1.9780800
 Vibrational harmonic frequencies (cm-1):

54.8104	72.7318	139.9419
315.5866	441.0240	484.5611
616.9366	733.5626	956.3152
1095.5645	1180.8194	1247.8687
1327.9137	1387.5163	1416.0481
1462.2820	3096.6890	3174.2749

 Zero-point correction (Hartree): 0.043751

OOCH2000.ppt

 E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07606639
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.650495	0.901199	0.006787
O	-1.453535	-0.117774	-0.603175
O	0.441928	0.371959	0.657082
H	-0.361368	1.559793	-0.812113
H	-1.242774		
1.404965	0.768002		
O	-2.110311	-0.788118	0.300675
O	1.433097	0.054961	-0.418636
O	2.377210	-0.567523	0.064479

 Rotational constants (GHz): 10.1202400 1.9706600 1.8731800
 Vibrational harmonic frequencies (cm-1):

51.7680	90.4262	158.7357
294.5972	410.1936	529.6402
622.5327	758.9611	954.6489
1090.7727	1176.3999	1246.3056

1316.1138	1381.6369	1416.1380
1463.6342	3094.9427	3170.7635

Zero-point correction (Hartree): 0.043805

OOCH2000.tpt

E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07539287

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.621813	0.722551	0.234770
O	1.352943	-0.340492	-0.421520
O	-0.637866	0.775268	-0.296829
H	0.628305	0.512087	1.304706
H	1.108693	1.668471	0.001903
O	2.514365	-0.484825	0.137731
O	-1.408633	-0.318133	0.389264
O	-2.504293	-0.446299	-0.148049

Rotational constants (GHz): 12.9639100 1.7739900 1.6594500

Vibrational harmonic frequencies (cm-1):

51.2159	65.0098	156.5873
318.9946	380.0786	440.0767
593.7525	745.4244	1017.7585
1075.4826	1181.9270	1279.2032
1295.0382	1384.2327	1416.3365
1477.3537	3087.2215	3159.4512

Zero-point correction (Hartree): 0.043570

TS.CH200+O3.a

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -414.13908883

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.48431110

E(CCSD/Aug-CC-pVDZ) (Hartree): -414.07464243

T1 diagnostic: 0.040288

E(CCSD/Aug-CC-pVTZ) (Hartree): -414.39857782

T1 diagnostic: 0.038861

E(MP2/Aug-CC-pVDZ) (Hartree): -414.08112789

E(MP2/Aug-CC-pVTZ) (Hartree): -414.42331796

E(PMP2/Aug-CC-pVDZ) (Hartree): -414.08112789

E(PMP2/Aug-CC-pVTZ) (Hartree): -414.42331796

E(PUHF/Aug-CC-pVDZ) (Hartree): -412.87107684

E(PUHF/Aug-CC-pVTZ) (Hartree): -412.97160090

E(ROHF/Aug-CC-pVDZ) (Hartree): -412.87107684

E(ROHF/Aug-CC-pVTZ) (Hartree): -412.97160090

E(UM062X/Aug-CC-pVTZ) (Hartree): -414.98724498

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.104713	1.042683	-0.328373
O	1.390965	-0.172364	-0.488402
O	1.921573	-0.822658	0.542047
O	-1.506229	-1.104847	-0.211483
O	-1.805961	0.117410	-0.156746
O	-1.086343	0.817804	0.634205
H	1.351197	1.516751	0.611677
H	0.708487	1.544395	-1.198400

Rotational constants (GHz): 6.4363200 2.1643600 1.8463300

Vibrational harmonic frequencies (cm-1):

i217.0439	41.2544	43.9639
93.8369	170.0431	253.8863
549.7613	712.8566	734.6456
847.9761	1006.3166	1050.1355
1211.1376	1258.1761	1288.2811
1500.5993	3156.1072	3313.3123

Zero-point correction (Hartree): 0.039258

TS.CH200+O3.b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -414.14496914
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -414.59524811
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.48999098
E(CCSD/Aug-CC-pVDZ) (Hartree): -414.08213672
T1 diagnostic: 0.037217
E(CCSD/Aug-CC-pVQZ) (Hartree): -414.50654125
T1 diagnostic: 0.035111
E(CCSD/Aug-CC-pVTZ) (Hartree): -414.40605568
T1 diagnostic: 0.035774
E(MP2/Aug-CC-pVDZ) (Hartree): -414.08852474
E(MP2/Aug-CC-pVQZ) (Hartree): -414.54418801
E(MP2/Aug-CC-pVTZ) (Hartree): -414.43054682
E(PMP2/Aug-CC-pVDZ) (Hartree): -414.08852474
E(PMP2/Aug-CC-pVQZ) (Hartree): -414.54418801
E(PMP2/Aug-CC-pVTZ) (Hartree): -414.43054682
E(PUHF/Aug-CC-pVDZ) (Hartree): -412.88297649
E(PUHF/Aug-CC-pVQZ) (Hartree): -413.00956670
E(PUHF/Aug-CC-pVTZ) (Hartree): -412.98280666
E(ROHF/Aug-CC-pVDZ) (Hartree): -412.88297649
E(ROHF/Aug-CC-pVQZ) (Hartree): -413.00956670
E(ROHF/Aug-CC-pVTZ) (Hartree): -412.98280666
E(UM062X/Aug-CC-pVTZ) (Hartree): -414.99431514

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.337895	0.950104	0.295032
O	-1.270177	-0.288032	0.456508
O	-1.173570	-1.040851	-0.649478
O	1.519984	-0.621013	0.752400
O	0.985765	1.054237	-0.445289
O	1.290358	-0.176634	-0.396791
H	-1.423629	1.340373	-0.710574
H	-1.367886	1.537340	1.201575

Rotational constants (GHz): 5.8976000 2.8035100 2.4024500

Vibrational harmonic frequencies (cm-1):

i99.4001	77.6727	133.5830
148.6445	273.8598	317.4853
548.7315	710.8606	757.6748
919.6993	1011.6317	1091.1339
1228.8265	1259.3663	1379.5146
1538.9145	3153.5661	3307.8653

Zero-point correction (Hartree): 0.040686

TS.cyc-CO5H2.OOCH2000

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -414.19975247
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -414.54563680
E(CCSD/Aug-CC-pVDZ) (Hartree): -414.13887246
T1 diagnostic: 0.027660
E(CCSD/Aug-CC-pVTZ) (Hartree): -414.46410691
T1 diagnostic: 0.026207
E(MP2/Aug-CC-pVDZ) (Hartree): -414.12641908
E(MP2/Aug-CC-pVTZ) (Hartree): -414.47017437
E(PMP2/Aug-CC-pVDZ) (Hartree): -414.12641908
E(PMP2/Aug-CC-pVTZ) (Hartree): -414.47017437
E(PUHF/Aug-CC-pVDZ) (Hartree): -412.93844513
E(PUHF/Aug-CC-pVTZ) (Hartree): -413.03794595
E(ROHF/Aug-CC-pVDZ) (Hartree): -412.93844513
E(ROHF/Aug-CC-pVTZ) (Hartree): -413.03794595
E(UM062X/Aug-CC-pVTZ) (Hartree): -415.05182650

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.812699	0.958939	0.207575
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O	1.298308	-0.268799	-0.324996
O	0.634285	-1.265251	0.274848
O	-1.054910	-0.920005	-0.298181
O	-1.301573	0.182828	0.320936
O	-0.469934	1.221658	-0.266191
H	0.827331	0.897210	1.295874
H	1.447065	1.745716	-0.192652
Rotational constants (GHz): 5.7372000 4.9252500 2.9371200			
Vibrational harmonic frequencies (cm-1):			
i732.1011	301.4551	364.7423	
459.9248	496.0813	569.5410	
723.6256	822.5741	977.2572	
1000.8469	1063.4364	1121.3502	
1183.6131	1316.8599	1402.9672	
1472.3551	3095.6759	3183.6494	
Zero-point correction (Hartree): 0.044552			

TS.OOCH2O.CH2O+O2.triplet

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -264.18928237
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.41036254
E(CCSD/Aug-CC-pVDZ) (Hartree): -264.16280043
T1 diagnostic: 0.053855
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.36366494
T1 diagnostic: 0.056801
E(MP2/Aug-CC-pVDZ) (Hartree): -264.12231989
E(MP2/Aug-CC-pVTZ) (Hartree): -264.36925271
E(PMP2/Aug-CC-pVDZ) (Hartree): -264.12231989
E(PMP2/Aug-CC-pVTZ) (Hartree): -264.36925271
E(PUHF/Aug-CC-pVDZ) (Hartree): -263.44928957
E(PUHF/Aug-CC-pVTZ) (Hartree): -263.45388625
E(ROHF/Aug-CC-pVDZ) (Hartree): -263.44928957
E(ROHF/Aug-CC-pVTZ) (Hartree): -263.45388625
E(UM062X/Aug-CC-pVDZ) (Hartree): -264.69275227
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.75411400
Electronic state : 3-A
Cartesian coordinates (Angs):

O	1.377946	-0.500335	0.125657
O	0.765995	0.524562	-0.242441
C	-0.805265	0.485112	0.175252
H	-1.185690	1.391769	-0.312219
H	-0.649359	0.608254	1.259076
O	-1.310611	-0.638064	-0.133012

Rotational constants (GHz): 21.5515800 6.2863200 5.2201000
Vibrational harmonic frequencies (cm-1):

i2805.8788	188.0044	309.5356
556.9903	900.1711	995.4066
1120.7676	1323.5723	1388.5637
1443.0836	2944.7324	3042.9442

Zero-point correction (Hartree): 0.032381

TS.OOCH2OOO.OOCH2O+O2.b

E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07315819
Electronic state : 1-A
Cartesian coordinates (Angs):

O	-2.312118	-0.416338	-0.227874
O	1.413379	-1.255337	0.044457
O	1.717672	-0.042007	-0.312141
C	0.821394	0.907816	0.306068
H	1.312847	1.875654	0.185694
H	0.730931	0.626936	1.358393
O	-0.378545	0.968566	-0.322406
O	-1.311906	-0.248570	0.395402

Rotational constants (GHz):	7.5119400	2.3571400	1.9244800
Vibrational harmonic frequencies (cm-1):			
i561.1021			
	57.3568	70.7205	
135.9617		258.7894	437.2108
514.8418		627.7291	924.1311
1086.9936		1159.7557	1238.3792
1313.4979		1393.1827	1444.7318
1576.2853		3059.9588	3125.3485

Zero-point correction (Hartree): 0.041975

TS.OOCH2OOO.OOCH2O+O2.triplet

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -414.21394164

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -414.16271051

T1 diagnostic: 0.038989

E(MP2/Aug-CC-pVDZ) (Hartree): -414.12531565

E(PMP2/Aug-CC-pVDZ) (Hartree): -414.12531565

E(PUHF/Aug-CC-pVDZ) (Hartree): -413.01038284

E(ROHF/Aug-CC-pVDZ) (Hartree): -413.01038284

E(UM062X/Aug-CC-pVTZ) (Hartree): -415.07233020

Electronic state : 3-A

Cartesian coordinates (Angs):

C	-0.678834	0.894144	0.077594
O	-1.451872	-0.206085	0.604180
O	-2.157908	-0.763869	-0.336056
O	2.423690	-0.573712	-0.114526
O	1.550132	0.026586	0.429761
O	0.356515	0.479032	-0.692763
H	-1.336472	1.494856	-0.554808
H	-0.354976	1.444658	0.964485

Rotational constants (GHz):	9.6096100	1.8727500	1.7864600
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Vibrational harmonic frequencies (cm-1):

i584.0924	43.4023	78.5136
141.9594	251.3278	401.0280
535.2689	641.6094	928.4342
1073.9925	1163.0293	1243.6082
1296.5740	1396.3318	1446.0065
1573.6540	3059.2482	3123.2157

Zero-point correction (Hartree): 0.041912

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*****
syn-CH3CHOO + O3
*****

CH3CHO2s
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.39106506
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.59065166
E(CCSD/Aug-CC-pVDZ) (Hartree): -228.36107891
  T1 diagnostic: 0.036890
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.54908138
  T1 diagnostic: 0.035105
E(MP2/Aug-CC-pVDZ) (Hartree): -228.32874471
E(MP2/Aug-CC-pVTZ) (Hartree): -228.52797758
E(PMP2/Aug-CC-pVDZ) (Hartree): -228.32874471
E(PMP2/Aug-CC-pVTZ) (Hartree): -228.52797758
E(PUHF/Aug-CC-pVDZ) (Hartree): -227.64668973
E(PUHF/Aug-CC-pVTZ) (Hartree): -227.70288046
E(ROHF/Aug-CC-pVDZ) (Hartree): -227.64668973
E(ROHF/Aug-CC-pVTZ) (Hartree): -227.70288046
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.90272701
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.471417      0.702258      0.000009
  O     -0.770016      0.584690      0.000003
  O     -1.269067     -0.677676      0.000002
  C      1.348246     -0.472175     -0.000015
  H      0.807438      1.732755      0.000032
  H      1.095834     -1.089417     -0.866318
  H      1.095907     -1.089400      0.866323
  H      2.395505     -0.190547     -0.000045
Rotational constants (GHz):  17.8489200   7.2532700   5.3217500
Vibrational harmonic frequencies (cm-1):
  216.1377      321.0560      471.8577
  683.1234      781.1765      928.5602
  998.9468      1068.7093     1112.1445
  1361.4043     1410.3805     1440.5155
  1464.6823     1647.0242     3053.7590
  3098.7604     3190.5974     3206.8169
Zero-point correction (Hartree): 0.060270

complex.CH3CHO2s+O3
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36784194
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -453.75159562
E(CCSD/Aug-CC-pVDZ) (Hartree): -453.30077271
  T1 diagnostic: 0.032911
E(CCSD/Aug-CC-pVTZ) (Hartree): -453.66133934
  T1 diagnostic: 0.031422
E(MP2/Aug-CC-pVDZ) (Hartree): -453.29404093
E(MP2/Aug-CC-pVTZ) (Hartree): -453.67505366
E(MP3/Aug-CC-pVDZ) (Hartree): -453.26793172
E(MP3/Aug-CC-pVTZ) (Hartree): -453.63603814
E(RHF/Aug-CC-pVDZ) (Hartree): -451.94472989
E(RHF/Aug-CC-pVTZ) (Hartree): -452.05498466
E(UM062X/Aug-CC-pVTZ) (Hartree): -454.32169609
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -1.814606     -0.016298      0.506294
  O     -1.302495     -1.027185     -0.012126
  O     -0.480339     -0.820869     -1.079350
  O      1.244014     -0.260251      1.116170
  O      2.021794     -0.229758      0.128214
  O      1.910174      0.766983     -0.626284

```

C	-1.563553	1.329985	-0.014571	
H	-2.452207	-0.246314	1.352819	
H	-1.819097	1.337600	-1.077505	
H	-0.486761	1.515383	0.022374	
H	-2.118168	2.079864	0.538987	
Rotational constants (GHz):	4.2206000	1.6113700	1.5291200	
Vibrational harmonic frequencies (cm-1):				
56.0577	72.8427		83.6935	
98.9319	140.4636		163.5776	
215.0875	325.7346		469.8725	
682.0889	753.0662		783.2781	
921.8197	1000.2328		1076.7887	
1102.1288	1112.8347		1247.7952	
1362.7094	1411.4253		1443.8027	
1466.6415	1653.8930		3054.9396	
3104.2124	3185.7296		3200.4417	
Zero-point correction (Hartree):	0.068778			

complex.CH3CHO2s+O3.b

E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31822703

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.354973	-0.043208	0.757427	
O	0.713324	-1.029045	0.345690	
O	-1.018916	1.248276	-0.263089	
O	-1.760431	0.239059	-0.375034	
O	-1.997276	-0.384224	0.685285	
H	1.397990	0.002774	1.840883	
C	2.017223	0.944761	-0.109427	
H	1.908183	0.658191	-1.149198	
H	3.067672	1.013763	0.178411	
H	1.568757	1.924538	0.064536	
O	0.541327	-1.200139	-0.995681	
Rotational constants (GHz):	4.0744000	1.8612500	1.6058800	
Vibrational harmonic frequencies (cm-1):				
i130.6130	23.9589		79.1982	
112.0098	114.6901		139.9909	
169.1006	338.9637		453.5321	
653.5840	759.0672		824.6597	
898.9765	934.2171		1075.0701	
1112.4123	1162.7889		1252.4699	
1365.4302	1419.7912		1440.6838	
1474.5294	1657.9219		3067.2758	
3123.6567	3186.8350		3206.6189	
Zero-point correction (Hartree):	0.068453			

TS.CH3CHO2s+O3.a

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36097256

E(CCSD/Aug-CC-pVDZ) (Hartree): -453.28970300

T1 diagnostic: 0.038396

E(MP2/Aug-CC-pVDZ) (Hartree): -453.28538701

E(PMP2/Aug-CC-pVDZ) (Hartree): -453.28538701

E(PUHF/Aug-CC-pVDZ) (Hartree): -451.92338316

E(ROHF/Aug-CC-pVDZ) (Hartree): -451.92338316

E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31342729

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.982911	-0.398413	0.659595
O	0.839854	0.862490	0.573062
O	1.389840	1.455803	-0.487849
O	-2.107342	0.822889	-0.196156
O	-2.008563	-0.374712	0.185461

O	-1.018095	-1.023238	-0.321242
C	1.791849	-1.142771	-0.311604
H	0.581732	-0.802807	1.578611
H	2.810426	-0.745382	-0.291689
H	1.409807	-0.946371	-1.314103
H	1.783918	-2.204186	-0.086969
Rotational constants (GHz):	4.1360600	1.8012500	1.4133300
Vibrational harmonic frequencies (cm-1):			
i397.3974	40.6347		51.9448
111.2823	136.7457		208.9676
241.3176	326.8425		421.3983
679.7110	726.5276		777.9200
881.3071	986.4933		1044.9787
1065.2710	1126.9791		1215.8049
1301.9997	1387.0702		1448.4415
1469.9358	1507.1569		3058.8034
3117.2203	3189.5432		3229.4911
Zero-point correction (Hartree):	0.067784		

TS.CH3CHO2s+O3.b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36511194
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -453.74694042
 E(CCSD/Aug-CC-pVDZ) (Hartree): -453.29421341
 T1 diagnostic: 0.036827
 E(CCSD/Aug-CC-pVTZ) (Hartree): -453.65279234
 T1 diagnostic: 0.035553
 E(MP2/Aug-CC-pVDZ) (Hartree): -453.29069735
 E(MP2/Aug-CC-pVTZ) (Hartree): -453.67007305
 E(PMP2/Aug-CC-pVDZ) (Hartree): -453.29069735
 E(PMP2/Aug-CC-pVTZ) (Hartree): -453.67007305
 E(PUHF/Aug-CC-pVDZ) (Hartree):
 -451.92900378
 E(PUHF/Aug-CC-pVTZ) (Hartree): -452.03752995
 E(ROHF/Aug-CC-pVDZ) (Hartree): -451.92900378
 E(ROHF/Aug-CC-pVTZ) (Hartree): -452.03752995
 E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31839365
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.145504	-0.227318	0.706854
O	0.605970	0.918312	0.617080
O	0.612112	1.476931	-0.601153
O	-2.203212	0.360107	0.242735
O	-0.809342	-1.254628	0.061709
O	-1.462318	-0.311742	-0.521106
H	1.097897	-0.629828	1.709875
C	1.941404	-0.797619	-0.389753
H	2.801698	-0.141821	-0.556094
H	1.362634	-0.789802	-1.310734
H	2.270647	-1.800767	-0.139766
Rotational constants (GHz):	4.2347400	2.0950700	1.6817100
Vibrational harmonic frequencies (cm-1):			
i337.2908	66.4130		112.8110
129.6982	154.2741		216.6229
325.0448	345.6827		450.2366
678.3998	735.3996		805.5392
906.8221	982.9098		1051.4578
1081.6087	1130.5895		1214.2381
1333.3115	1393.6992		1450.0865
1469.8346	1524.8200		3056.3841
3135.6706	3193.7018		3228.0843
Zero-point correction (Hartree):	0.068740		

```

*****
anti-CH3CHOO + O3
*****

CH3CHO2a
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.38520130
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.58475551
E(CCSD/Aug-CC-pVDZ) (Hartree): -228.35603807
  T1 diagnostic: 0.036580
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.54410227
  T1 diagnostic: 0.034770
E(MP2/Aug-CC-pVDZ) (Hartree): -228.32228609
E(MP2/Aug-CC-pVTZ) (Hartree): -228.52150948
E(PMP2/Aug-CC-pVDZ) (Hartree): -228.32228609
E(PMP2/Aug-CC-pVTZ) (Hartree): -228.52150948
E(PUHF/Aug-CC-pVDZ) (Hartree): -227.64577921
E(PUHF/Aug-CC-pVTZ) (Hartree): -227.70219095
E(ROHF/Aug-CC-pVDZ) (Hartree): -227.64577921
E(ROHF/Aug-CC-pVTZ) (Hartree): -227.70219095
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.89710572
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -0.370039    0.399961    -0.000016
  O     0.566461   -0.412338    -0.000016
  O     1.839494    0.076289    0.000014
  H    -0.096126    1.452422   -0.000002
  C    -1.762517   -0.093270    0.000005
  H    -2.286708    0.287505    0.878116
  H    -1.782679   -1.179231    0.000001
  H    -2.286786    0.287547   -0.878036
Rotational constants (GHz):  50.1860100    4.4801100    4.2196900
Vibrational harmonic frequencies (cm-1):
  167.6530          268.3336          329.1509
  566.4967          883.5010          901.6039
  986.5165         1094.5197         1168.6110
  1362.4820        1421.7142        1467.7291
  1469.4722        1672.6658        3064.4357
  3120.6224        3166.0899        3183.3546
Zero-point correction (Hartree): 0.059904

complex.CH3CHO2a+O3
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36375732
E(CCSD/Aug-CC-pVDZ) (Hartree): -453.29685347
  T1 diagnostic: 0.032848
E(MP2/Aug-CC-pVDZ) (Hartree): -453.28945251
E(PMP2/Aug-CC-pVDZ) (Hartree): -453.28945251
E(PUHF/Aug-CC-pVDZ) (Hartree): -451.94354549
E(ROHF/Aug-CC-pVDZ) (Hartree): -451.94354549
E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31746942
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -1.193758   -0.011949    0.424838
  O    -1.013429    0.959719   -0.331826
  O     0.047470    1.770743   -0.061342
  O     0.850102   -1.049082   -0.731584
  O     1.732786   -0.228425   -0.357612
  O     2.026686   -0.267087    0.858503
  H    -0.521039   -0.098774    1.275092
  C    -2.295673   -0.952887    0.148308
  H    -2.828676   -0.665519   -0.753241
  H    -2.980556   -0.977647    0.997177
  H    -1.882064   -1.955989    0.032972

```

Rotational constants (GHz):	3.8934100	1.8532400	1.4739600
Vibrational harmonic frequencies (cm-1):			
59.8003	79.2842		115.6231
134.6370	138.9451		207.3188
244.6694	298.4435		338.0953
570.1583	760.3055		894.3536
912.3241	989.8175		1091.1347
1110.2106	1174.6423		1243.6006
1363.5249	1420.1545		1464.7809
1469.2618	1640.7650		3066.8349
3126.1452	3164.2070		3183.5243
Zero-point correction (Hartree): 0.068943			

complex.CH3CHO2a+O3.b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36401383
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -453.74656349
E(CCSD/Aug-CC-pVDZ) (Hartree): -453.29732198
T1 diagnostic: 0.032557
E(CCSD/Aug-CC-pVTZ) (Hartree): -453.65687603
T1 diagnostic: 0.031152
E(MP2/Aug-CC-pVDZ) (Hartree): -453.29016337
E(MP2/Aug-CC-pVTZ) (Hartree): -453.67019976
E(PMP2/Aug-CC-pVDZ) (Hartree): -453.29016337
E(PMP2/Aug-CC-pVTZ) (Hartree): -453.67019976
E(PUHF/Aug-CC-pVDZ) (Hartree): -451.94446676
E(PUHF/Aug-CC-pVTZ) (Hartree): -452.05356406
E(ROHF/Aug-CC-pVDZ) (Hartree): -451.94446676
E(ROHF/Aug-CC-pVTZ) (Hartree): -452.05356406
E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31781824
Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.289815	0.063469	-0.362170
O	0.752914	0.888594	0.401351
O	-0.010736	1.861109	-0.171438
O	-1.490657	-0.514375	1.057875
O	-1.047132	-0.829788	-0.992961
O	-1.698857	-0.182394	-0.130056
C	2.054367	-1.059656	0.211123
H	1.167086	0.240563	-1.427021
H	2.050925	-1.008969	1.296059
H	3.077589	-1.044998	-0.166298
H	1.595060	-1.994638	-0.114624

Rotational constants (GHz):	3.4728300	2.1085100	1.6874200
Vibrational harmonic frequencies (cm-1):			
49.3537	90.9940		134.5617
137.5111	150.6466		233.1150
284.5394	312.8701		338.2377
569.0224	766.2615		890.1564
909.0388	987.4836		1088.2145
1114.5365	1172.3741		1246.0654
1358.2029	1417.5782		1462.2227
1468.1477	1633.6239		3067.0331
3127.1003	3175.7628		3187.0565
Zero-point correction (Hartree): 0.069192			

TS.CH3CHO2a+O3.a

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.35708240
E(CCSD/Aug-CC-pVDZ) (Hartree): -453.28738416
T1 diagnostic: 0.036173
E(MP2/Aug-CC-pVDZ) (Hartree): -453.28287460
E(PMP2/Aug-CC-pVDZ) (Hartree): -453.28287460
E(PUHF/Aug-CC-pVDZ) (Hartree): -451.92487555

E(ROHF/Aug-CC-pVDZ) (Hartree): -451.92487555
 E(UM062X/Aug-CC-pVTZ) (Hartree): -454.30915609
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.025160	0.598455	-0.394694
O	-1.406213	-0.196010	0.502394
O	-1.987368	-1.338199	0.112176
O	1.839244	-0.277422	0.990144
O	1.923676	-0.192444	-0.266246
O	0.957429	-0.721122	-0.910462
H	-1.257664	0.323064	-1.417712
C	-0.407212	1.877728	0.010308
H	-0.198703	1.876689	1.077127
H	-1.079576	2.703919	-0.229885
H	0.516032	2.040814	-0.547260

 Rotational constants (GHz): 3.5984000 1.8037800 1.4811500
 Vibrational harmonic frequencies (cm-1):

i248.2236	26.9880	61.9808
84.3796	146.2296	198.0009
238.4096	275.9085	339.6708
571.8357	733.8353	830.7757
913.1434	931.5701	1068.4116
1085.5217	1167.3282	1217.5295
1311.0188	1408.2403	1459.5095
1465.9448	1521.3153	3061.5351
3119.1454	3171.3237	3192.0819

 Zero-point correction (Hartree): 0.067437

TS.CH3CHO2s+O3.a

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -453.36097256
 E(CCSD/Aug-CC-pVDZ) (Hartree): -453.28970300
 T1 diagnostic: 0.038396
 E(MP2/Aug-CC-pVDZ) (Hartree): -453.28538701
 E(PMP2/Aug-CC-pVDZ) (Hartree): -453.28538701
 E(PUHF/Aug-CC-pVDZ) (Hartree): -451.92338316
 E(ROHF/Aug-CC-pVDZ) (Hartree): -451.92338316
 E(UM062X/Aug-CC-pVTZ) (Hartree): -454.31342729
 Electronic state : 1-A
 Cartesian
 coordinates (Angs):

C	0.982911	-0.398413	0.659595
O	0.839854	0.862490	0.573062
O	1.389840	1.455803	-0.487849
O	-2.107342	0.822889	-0.196156
O	-2.008563	-0.374712	0.185461
O	-1.018095	-1.023238	-0.321242
C	1.791849	-1.142771	-0.311604
H	0.581732	-0.802807	1.578611
H	2.810426	-0.745382	-0.291689
H	1.409807	-0.946371	-1.314103
H	1.783918	-2.204186	-0.086969

 Rotational constants (GHz): 4.1360600 1.8012500 1.4133300
 Vibrational harmonic frequencies (cm-1):

i397.3974	40.6347	51.9448
111.2823	136.7457	208.9676
241.3176	326.8425	421.3983
679.7110	726.5276	777.9200
881.3071	986.4933	1044.9787
1065.2710	1126.9791	1215.8049
1301.9997	1387.0702	1448.4415
1469.9358	1507.1569	3058.8034
3117.2203	3189.5432	3229.4911

 Zero-point correction (Hartree): 0.067784


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*****
(CH3)2COO + O3
*****

diMeCO2
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -267.60813740
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.84500747
E(CCSD/Aug-CC-pVDZ) (Hartree): -267.57299559
  T1 diagnostic: 0.031837
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.79627234
  T1 diagnostic: 0.030244
E(MP2/Aug-CC-pVDZ) (Hartree): -267.52824243
E(MP2/Aug-CC-pVTZ) (Hartree): -267.76526821
E(PMP2/Aug-CC-pVDZ) (Hartree): -267.52824243
E(PMP2/Aug-CC-pVTZ) (Hartree): -267.76526821
E(PUHF/Aug-CC-pVDZ) (Hartree): -266.70129407
E(PUHF/Aug-CC-pVTZ) (Hartree): -266.76658097
E(ROHF/Aug-CC-pVDZ) (Hartree): -266.70129407
E(ROHF/Aug-CC-pVTZ) (Hartree): -266.76658097
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.22346276
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.22346276
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.371023      0.018452      -0.000027
  O       0.558598     -0.817600     -0.000024
  O       1.839016     -0.328582      0.000021
  C      -0.054287      1.456041     -0.000027
  C      -1.752455     -0.524533      0.000001
  H       0.577833      1.668419     -0.865255
  H       0.577302      1.668413      0.865633
  H      -0.955030      2.062056     -0.000193
  H      -1.739071     -1.610392     -0.000038
  H      -2.287778     -0.159336     -0.877977
  H      -2.287572     -0.159472      0.878172
Rotational constants (GHz):   8.9511500   4.3735300   3.0465400
Vibrational harmonic frequencies (cm-1):
  161.9148      207.9997      291.0494
  329.8758      366.3996      493.5235
  609.7889      827.3699      925.0890
  952.8522      989.4152     1085.5992
 1102.0388     1316.0864     1393.9569
 1411.7327     1442.1700     1466.9935
 1474.3193     1486.7861     1653.9857
 3059.3241     3065.3017     3110.0176
 3121.6801     3182.2214     3183.6485
Zero-point correction (Hartree): 0.088190

complex.diMeCOO+O3
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -492.58592853
E(CCSD/Aug-CC-pVDZ) (Hartree): -492.51356859
  T1 diagnostic: 0.029989
E(MP2/Aug-CC-pVDZ) (Hartree): -492.49465773
E(PMP2/Aug-CC-pVDZ) (Hartree): -492.49465773
E(PUHF/Aug-CC-pVDZ) (Hartree): -490.99956003
E(ROHF/Aug-CC-pVDZ) (Hartree): -490.99956003
E(UM062X/Aug-CC-pVTZ) (Hartree): -493.64297944
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -1.481246     -0.081034     -0.045690
  O      -0.888511     -0.076554      1.054633
  O       0.154359     -0.960229      1.206063
  O       1.309008      1.251187     -0.214111

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O	2.291420	0.531427	0.100885
O	2.413584	-0.539775	-0.540520
C	-1.070045	-1.023330	-1.098919
C	-2.587388	0.895679	-0.201800
H	-1.086189	-2.032341	-0.681348
H	-0.022392	-0.829586	-1.339893
H	-1.704647	-0.936817	-1.975536
H	-2.365646	1.555875	-1.042053
H	-2.717388	1.480348	0.703886
H	-3.510536	0.366178	-0.442195
Rotational constants (GHz):	3.3455200	1.1612700	1.1244200
Vibrational harmonic frequencies (cm-1):			
42.5359	56.2292		89.1493
96.3114	134.7534		154.5544
174.0714	208.9334		306.2506
332.6513	369.7642		493.8324
608.3518	753.0709		827.6978
922.8626	951.3373		991.4378
1087.2843	1101.9531		1103.6857
1248.4847	1316.5299		1391.9574
1411.3949	1444.6472		1467.4025
1474.3947	1487.9278		1658.5355
3062.3207	3065.9567		3117.5025
3123.1397	3182.7424		3184.1207
Zero-point correction (Hartree):	0.096694		

complex.diMeCOO+O3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -492.58592853

E(CCSD/Aug-CC-pVDZ) (Hartree): -492.51356859

T1 diagnostic: 0.029989

E(MP2/Aug-CC-pVDZ) (Hartree): -492.49465773

E(PMP2/Aug-CC-pVDZ) (Hartree): -492.49465773

E(PUHF/Aug-CC-pVDZ) (Hartree): -490.99956003

E(ROHF/Aug-CC-pVDZ) (Hartree): -490.99956003

E(UM062X/Aug-CC-pVTZ) (Hartree): -493.64297944

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.481246	-0.081034	-0.045690
O	-0.888511	-0.076554	1.054633
O	0.154359	-0.960229	1.206063
O	1.309008	1.251187	-0.214111
O	2.291420	0.531427	0.100885
O	2.413584	-0.539775	-0.540520
C	-1.070045	-1.023330	-1.098919
C	-2.587388	0.895679	-0.201800
H	-1.086189	-2.032341	-0.681348
H	-0.022392	-0.829586	-1.339893
H	-1.704647	-0.936817	-1.975536
H	-2.365646	1.555875	-1.042053
H	-2.717388	1.480348	0.703886
H	-3.510536	0.366178	-0.442195
Rotational constants (GHz):	3.3455200	1.1612700	1.1244200
Vibrational harmonic frequencies (cm-1):			
42.5359	56.2292		89.1493
96.3114	134.7534		154.5544
174.0714	208.9334		306.2506
332.6513	369.7642		493.8324
608.3518	753.0709		827.6978
922.8626	951.3373		991.4378
1087.2843	1101.9531		1103.6857
1248.4847	1316.5299		1391.9574
1411.3949	1444.6472		1467.4025
1474.3947	1487.9278		1658.5355

3062.3207	3065.9567	3117.5025
3123.1397	3182.7424	3184.1207
Zero-point correction (Hartree): 0.096694		

TS.diMeCOO+O3.a

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -492.57936075

E(CCSD/Aug-CC-pVDZ) (Hartree): -492.50211672

T1 diagnostic: 0.035157

E(MP2/Aug-CC-pVDZ) (Hartree): -492.48791373

E(PMP2/Aug-CC-pVDZ) (Hartree): -492.48791373

E(PUHF/Aug-CC-pVDZ) (Hartree): -490.97374681

E(ROHF/Aug-CC-pVDZ) (Hartree): -490.97374681

E(UM062X/Aug-CC-pVTZ) (Hartree): -493.63390916

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.921552	0.425928	-0.207627
O	0.854885	-0.725527	-0.752798
O	1.473073	-1.732312	-0.125027
O	-2.331513	-0.701706	-0.428837
O	-2.051949	0.252288	0.349241
O	-1.010830	0.066365	1.081351
C	1.740613	0.606157	1.003594
C	0.342285	1.534814	-1.006615
H	2.773710	0.343366	0.759291
H	1.423034	-0.106658	1.764020
H	1.675082	1.627845	1.364595
H	-0.299100	1.144051	-1.792885
H	1.152402	2.110018	-1.460961
H	-0.221155	2.207123	-0.361613

Rotational constants (GHz): 2.7804000 1.4544900 1.2876100

Vibrational harmonic frequencies (cm-1):

i440.5600	26.9605	64.8608
107.1825	129.0328	183.6272
218.5172	240.0595	276.7818
333.4750	369.2357	424.1813
621.1736	725.3932	
	795.8071	
886.1279	942.1803	993.8788
1024.8593	1081.5749	1127.5629
1220.3073	1321.6379	1385.6353
1412.4631	1431.0152	1450.4175
1475.2235	1489.2020	1503.3925
3058.2332	3062.0790	3122.7747
3130.0674	3172.9378	3186.6041

Zero-point correction (Hartree): 0.095670

TS.diMeCOO+O3.b

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -492.58456056

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -493.00294467

E(CCSD/Aug-CC-pVDZ) (Hartree): -492.50784681

T1 diagnostic: 0.034191

E(CCSD/Aug-CC-pVTZ) (Hartree): -492.90100468

T1 diagnostic: 0.033006

E(MP2/Aug-CC-pVDZ) (Hartree): -492.49309609

E(MP2/Aug-CC-pVTZ) (Hartree): -492.90959279

E(PMP2/Aug-CC-pVDZ) (Hartree): -492.49309609

E(PMP2/Aug-CC-pVTZ) (Hartree): -492.90959279

E(PUHF/Aug-CC-pVDZ) (Hartree): -490.98220265

E(PUHF/Aug-CC-pVTZ) (Hartree): -491.09939965

E(ROHF/Aug-CC-pVDZ) (Hartree): -490.98220265

E(ROHF/Aug-CC-pVTZ) (Hartree): -491.09939965

E(UM062X/Aug-CC-pVTZ) (Hartree): -493.64021109

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.097037	-0.085565	-0.139876
O	-0.360601	0.630935	-0.896863
O	0.071314	1.794485	-0.379260
O	2.311428	-0.316307	-0.520904
O	0.788016	-0.922577	0.854578
O	1.717282	-0.080009	0.562766
C	-1.635122	0.481222	1.113330
C	-1.570459	-1.357354	-0.735231
H	-2.283712	1.320466	0.844979
H	-0.831028	0.890737	1.718209
H	-2.196156	-0.271802	1.658414
H	-1.017289	-1.583198	-1.642174
H	-2.636571	-1.276783	-0.958597
H	-1.439054	-2.161449	-0.012702

Rotational constants (GHz): 2.8507300 1.6394700 1.4382700

Vibrational harmonic frequencies (cm-1):

i364.7195	53.0053	120.2268
126.6942	141.8412	184.9199
216.6601	267.3718	341.7630
350.5947	378.1289	448.0011
617.3408	735.3185	810.1068
917.8069	941.2055	992.6000
1029.2863	1101.7947	1121.9541
1219.9331	1325.4992	1396.0786
1414.2256	1438.2771	1455.1041
1471.0600	1488.6000	1521.6189
3058.9943	3066.1589	3134.8444
3142.5589	3183.3187	3191.8128

Zero-point correction (Hartree): 0.096605

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*****
CH2OO + H2O2
*****

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(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

HOOH
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -151.37360293
E(CCSD/Aug-CC-pVTZ) (Hartree): -151.35395883
E(MP2/Aug-CC-pVTZ) (Hartree): -151.34746732
E(MP3/Aug-CC-pVTZ) (Hartree): -151.34969232
E(RHF/Aug-CC-pVTZ) (Hartree): -150.84120796
E(RM062X/Aug-CC-pVTZ) (Hartree): -151.55365122
Point group : C2
Electronic state : 1-A
Cartesian coordinates (Angs):
  H      0.782665      0.903903      0.469995
  O      0.000000      0.711559     -0.058749
  O      0.000000     -0.711559     -0.058749
  H     -0.782665     -0.903903      0.469995
Rotational constants (GHz):  307.5402200  27.3244300  26.4893600
Vibrational harmonic frequencies (cm-1):
  375.1669 ( A)      1042.8577 ( A)      1356.2273 ( B)
  1463.0625 ( A)      3836.9778 ( B)      3838.3242 ( A)
Zero-point correction (Hartree): 0.027139

HO2
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -150.72604227
E(CCSD/Aug-CC-pVTZ) (Hartree): -150.70776156
E(MP2/Aug-CC-pVTZ) (Hartree): -150.69256562
E(MP3/Aug-CC-pVTZ) (Hartree): -150.69875048
E(PMP2/Aug-CC-pVTZ) (Hartree): -150.69558162
E(PMP3/Aug-CC-pVTZ) (Hartree): -150.70048665
E(PUHF/Aug-CC-pVTZ) (Hartree): -150.24520710
E(UHF/Aug-CC-pVTZ) (Hartree): -150.24027983
E(UM062X/Aug-CC-pVTZ) (Hartree): -150.90809490
Point group : CS

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Electronic state : 2-A"
 Cartesian coordinates (Angs):

O	0.055051	0.708170	0.000000
O	0.055051	-0.600032	0.000000
H	-0.880820	-0.865110	0.000000

 Rotational constants (GHz): 628.4125900 34.7009900 32.8850700
 Vibrational harmonic frequencies (cm-1):
 1252.7630 (A') 1459.6208 (A') 3687.0476 (A')
 Zero-point correction (Hartree): 0.014579

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

OH

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -75.64558436
 E(CCSD/Aug-CC-pVTZ) (Hartree): -75.63969620
 E(MP2/Aug-CC-pVTZ) (Hartree): -75.62633190
 E(MP3/Aug-CC-pVTZ) (Hartree): -75.63789728
 E(PMP2/Aug-CC-pVTZ) (Hartree): -75.62832220
 E(PMP3/Aug-CC-pVTZ) (Hartree): -75.63904001
 E(PUHF/Aug-CC-pVTZ) (Hartree): -75.42491597
 E(UHF/Aug-CC-pVTZ) (Hartree): -75.42156344
 E(UM062X/Aug-CC-pVTZ) (Hartree): -75.73381016
 Point group : C*V
 Cartesian coordinates (Angs):

O	0.000000	0.000000	0.107984
H	0.000000	0.000000	-0.863871

 Rotational constants (GHz): 0.0000000 564.3727589 564.3727589
 Vibrational harmonic frequencies (cm-1):
 3770.5842 (SG)
 Zero-point correction (Hartree): 0.008590

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

complex.CH2O2+H2O2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.72130914
E(CCSD/Aug-CC-pVTZ) (Hartree): -340.66828413
E(MP2/Aug-CC-pVTZ) (Hartree): -340.65020774
E(MP3/Aug-CC-pVTZ) (Hartree): -340.65280619
E(RHF/Aug-CC-pVTZ) (Hartree): -339.49383845
E(RM062X/Aug-CC-pVTZ) (Hartree): -341.14872871
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.205269	1.040506	0.009492
O	-1.320261	-0.116830	-0.396363
O	-0.919428	-1.116675	0.462508
H	-0.824740	1.213320	1.008301
H	-1.504005	1.815442	-0.685860
O	1.563092	-0.578151	-0.422774
O	1.504592	0.699825	0.206768
H	0.748485	-0.999893	-0.061905
H	2.187908	0.622733	0.881399

Rotational constants (GHz):	7.8888100 3.2749400 2.5921400
Vibrational harmonic frequencies (cm-1):	
61.2048	102.7476 132.3404
225.6194	232.9889 273.8892
524.1805	687.2245 825.1308
880.8225	1036.2613 1094.9557
1258.3653	1373.4674 1447.3376
1546.9231	1678.6710 3146.5877
3292.7487	3376.1151 3836.7806
Zero-point correction (Hartree):	0.061589

complex.HOOCH2O+OH.a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.72825465
E(CCSD/Aug-CC-pVTZ) (Hartree): -340.68588080
E(MP2/Aug-CC-pVTZ) (Hartree): -340.64867669
E(MP3/Aug-CC-pVTZ) (Hartree): -340.67586473
E(PMP2/Aug-CC-pVTZ) (Hartree): -340.67129580
E(PMP3/Aug-CC-pVTZ) (Hartree): -340.69839189
E(PUHF/Aug-CC-pVTZ) (Hartree): -339.60453131
E(UHF/Aug-CC-pVTZ) (Hartree): -339.58176507
E(UM062X/Aug-CC-pVTZ) (Hartree): -341.16055971
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.283166	-0.350128	0.053047
H	-2.008482	-0.666972	0.816939
H	-1.836788	-0.051910	-0.852582
O	-0.606255	0.738139	0.597228
O	-0.515122	-1.407567	-0.283682
O	0.067866	1.395462	-0.467316
H	0.976851	1.068567	-0.344678
O	2.195248	-0.383424	0.155691
H	1.433523	-0.989798	0.046671

Rotational constants (GHz):	5.5928400 3.8887900 2.5853000
Vibrational harmonic frequencies (cm-1):	
83.3141	150.2932 163.4546
226.4473	330.3932 421.0436

436.2402	615.3342	676.2953
856.4119	966.6001	1049.8119
1130.3255	1239.4888	1346.4323
1373.3732	1476.0513	2966.3688
3020.1279	3625.8963	3680.3365

Zero-point correction (Hartree): 0.058854

complex.HOOCH2O+OH.a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.72825465
 E(CCSD/Aug-CC-pVTZ) (Hartree): -340.68588080
 E(MP2/Aug-CC-pVTZ) (Hartree): -340.64867669
 E(MP3/Aug-CC-pVTZ) (Hartree): -340.67586473
 E(PMP2/Aug-CC-pVTZ) (Hartree): -340.67129580
 E(PMP3/Aug-CC-pVTZ) (Hartree): -340.69839189
 E(PUHF/Aug-CC-pVTZ) (Hartree): -339.60453131
 E(UHF/Aug-CC-pVTZ) (Hartree): -339.58176507
 E(UM062X/Aug-CC-pVTZ) (Hartree): -341.16055971
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.283166	-0.350128	0.053047
H	-2.008482	-0.666972	0.816939
H	-1.836788	-0.051910	-0.852582
O	-0.606255	0.738139	0.597228
O	-0.515122	-1.407567	-0.283682
O	0.067866	1.395462	-0.467316
H	0.976851	1.068567	-0.344678
O	2.195248	-0.383424	0.155691
H	1.433523	-0.989798	0.046671

Rotational constants (GHz): 5.5928400 3.8887900 2.5853000
 Vibrational harmonic frequencies (cm-1):

83.3141	150.2932	163.4546
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226.4473	330.3932	421.0436
436.2402	615.3342	676.2953
856.4119	966.6001	1049.8119
1130.3255	1239.4888	1346.4323
1373.3732	1476.0513	2966.3688
3020.1279	3625.8963	3680.3365

Zero-point correction (Hartree): 0.058854

complex.HOOCH2O+OH.b

E(UM062X/Aug-CC-pVTZ) (Hartree): -341.15555285
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.265013	-0.725614	0.217057
H	0.595539	-1.329866	-0.114891
H	-0.242165	-0.661798	1.317437
O	-0.049124	0.550034	-0.344856
O	-1.415062	-1.305640	-0.135004
O	-1.010816	1.428122	0.213783
H	-1.759147	1.316576	-0.388213
O	2.582256	-0.132377	0.025057
H	2.137821	0.707658	-0.188517

Rotational constants (GHz): 6.2220300 2.9818600 2.1068900
 Vibrational harmonic frequencies (cm-1):

15.8676	90.1322	133.7562
162.2623	278.7105	294.2388
312.6586	400.0202	642.1182
841.0559	951.0708	1081.8300
1115.5435	1232.0857	1336.4083
1375.0887	1421.3981	2955.3454
2993.2172	3738.0600	3801.9210

Zero-point correction (Hartree): 0.057348

H2COOHOOH.pmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22100182

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.016867	0.918575	0.336446
H	-0.004301	2.002419	0.223120
H	-0.073124	0.603804	1.379386
O	-1.135206	0.469246	-0.353336
O	1.193481	0.509634	-0.243304
O	-1.507167	-0.807566	0.146189
H	-0.863980	-1.391091	-0.280410
O	1.319707	-0.894500	-0.037139
H	2.076088	-0.941101	0.559948

Rotational constants (GHz): 9.1487300 4.2241600 3.1389200

Vibrational harmonic frequencies (cm-1):

105.0476	187.4313	204.8011
386.1963	403.4805	483.2731
641.3113	937.9862	967.5458
1096.1746	1134.2981	1183.7785
1331.2599	1389.1149	1416.5526
1448.8447	1459.4008	3080.9386
3155.3534	3794.3010	3828.4681

Zero-point correction (Hartree): 0.065237

H2COOHOOH.pmmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22071520

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.021297	0.931671	0.319317
H	-0.000362	2.011808	0.179492
H	-0.132071	0.646140	1.366186
O	-1.096656	0.449339	-0.417323
O	1.218053	0.511596	-0.176695
O	-1.530385	-0.780902	0.146547
H	-0.831567	-1.388840	-0.134012
O	1.301898	-0.892723	0.101849
H	1.948512	-1.157609	-0.562592

Rotational constants (GHz): 9.1299900 4.2380200 3.1523500

Vibrational harmonic frequencies (cm-1):

75.6077	187.7283	208.1941
384.3107	418.2190	490.1061
634.5944	938.5408	965.3283
1098.1052	1129.2563	1173.7283
1317.2055	1407.5518	1430.6849
1449.8935	1465.3038	3085.6112
3159.4608	3785.6725	3846.9263

Zero-point correction (Hartree): 0.065274

H2COOHOOH.pmmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22071520

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.021284	0.931707	0.319286
H	-0.000319	2.011835	0.179379
H	-0.132093	0.646283	1.366181
O	-1.096618	0.449315	-0.417350
O	1.218083	0.511598	-0.176644
O	-1.530375	-0.780862	0.146569
H	-0.831557	-1.388830	-0.133927

O	1.301827	-0.892784	0.101845	
H	1.948332	-1.157662	-0.562713	
Rotational constants (GHz):			9.1297300	4.2381800 3.1524000
Vibrational harmonic frequencies (cm-1):				
75.7039		187.8056		208.2821
384.2934		418.2674		490.1041
634.6001		938.4990		965.3500
1098.0690		1129.2861		1173.7148
1317.1951		1407.5524		1430.6699
1449.9261		1465.3104		3085.6114
3159.4440		3785.6491		3846.8791
Zero-point correction (Hartree): 0.065275				

H2COOHOOH.pmpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22251479

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.000057	0.878921	0.000071	
H	-0.494165	1.477777	0.764197	
H	0.493838	1.478183	-0.763888	
O	0.928130	0.093846	0.688100	
O	-0.928185	0.093979	-0.688078	
O	1.822097	-0.457599	-0.267949	
H	1.323252	-1.204576	-0.624961	
O	-1.822012	-0.457768	0.267860	
H	-1.322810	-1.204571	0.624764	
Rotational constants (GHz):			11.7708000	3.2151500 3.1310900
Vibrational harmonic frequencies (cm-1):				
113.7867		188.4254		261.5372
310.2867		367.7169		540.0518
680.1811		946.9920		961.9387
1106.2404		1108.6769		1189.2775
1319.8250		1401.2517		1416.8386
1429.2169		1465.1059		3093.1378
3164.5534		3800.1711		3802.4124
Zero-point correction (Hartree): 0.065310				

H2COOHOOH.pmpt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22208990

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.022282	0.885066	0.089445	
H	0.453411	1.568603	-0.614107	
H	-0.477475	1.395970	0.938870	
O	-0.980028	0.212395	-0.660302	
O	0.913654	0.024766	0.670578	
O	-1.776621	-0.541626	0.239444	
H	-1.260779	-1.353903	0.332967	
O	1.697319	-0.527655	-0.385133	
H	2.583938	-0.264109	-0.111099	
Rotational constants (GHz):			11.3494500	3.3034800 3.1651900
Vibrational harmonic frequencies (cm-1):				
102.8856		207.0449		233.8924
285.6786		358.1809		522.8154
676.8783		947.3658		964.4889
1101.8388		1123.8422		1186.8272
1328.0124		1403.1240		1419.4709
1427.1713		1465.2191		3083.0485
3151.9932		3801.6309		3833.8673
Zero-point correction (Hartree): 0.065213				

H2COOHOOH.pmtm

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21697400
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.004132      0.714991      0.260692
  H       0.240142      1.767287      0.101217
  H       0.078500      0.423011      1.307070
  O      -1.286020      0.553802     -0.225284
  O       0.837682     -0.126567     -0.517510
  O      -1.757585     -0.713683      0.207019
  H      -1.358235     -1.310039     -0.441226
  O       2.004237     -0.371169      0.252036
  H       2.677861      0.090737     -0.261299
Rotational constants (GHz):   13.9380300    2.9726600    2.6989100
Vibrational harmonic frequencies (cm-1):
   39.5617          187.0211          253.0980
  300.0303          381.4050          425.3546
   604.4080          966.7701        1032.7773
  1097.4714        1146.6751        1185.2707
  1288.2974        1409.6373        1420.7618
  1431.9684        1506.6431        3071.5613
  3142.1025        3798.7764        3828.8135
Zero-point correction (Hartree): 0.064970

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H2COOHOOH.pmtpr

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21659260
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.013051      0.690339      0.248118
  H      0.304196      1.722844      0.050738
  H      0.070063      0.444276      1.309736
  O     -1.271677
0.559313     -0.239320
  O      0.830471     -0.205678     -0.491155
  O     -1.792783     -0.674295      0.236700
  H     -1.560930     -1.278214     -0.480895
  O      2.106157     -0.178831      0.126305
  H      2.131016     -1.035006      0.571471
Rotational constants (GHz):   14.8624300    2.8832000    2.6385600
Vibrational harmonic frequencies (cm-1):
   72.3744          175.7575          261.8637
  287.6492          367.3750          418.7863
   603.7282          965.6765        1043.5414
  1106.8226        1148.7084        1184.3976
  1283.1172        1410.5944        1414.1962
  1429.9461        1510.5918        3071.0811
  3136.1436        3812.7313        3819.7433
Zero-point correction (Hartree): 0.064984

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H2COOHOOH.pppmp

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22100182
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.016867      0.918575      0.336446
  H      0.004301      2.002419      0.223120
  H      0.073124      0.603804      1.379386
  O     -1.193481      0.509634     -0.243304
  O      1.135206      0.469246     -0.353336
  O     -1.319707     -0.894500     -0.037139
  H     -2.076088     -0.941101      0.559948
  O      1.507167     -0.807566      0.146189
  H      0.863980     -1.391091     -0.280410

```

Rotational constants (GHz): 9.1487300 4.2241600 3.1389200
 Vibrational harmonic frequencies (cm-1):
 105.0475 187.4311 204.8010
 386.1962 403.4805 483.2731
 641.3113 937.9862 967.5458
 1096.1746 1134.2981 1183.7785
 1331.2599 1389.1149 1416.5526
 1448.8447 1459.4008 3080.9386
 3155.3534 3794.3010 3828.4681

Zero-point correction (Hartree): 0.065237

H2COOHOOH.ptmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22071520

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.021284	0.931707	0.319286
H	0.000319	2.011835	0.179379
H	0.132093	0.646283	1.366181
O	-1.218083	0.511598	-0.176644
O	1.096618	0.449315	-0.417350
O	-1.301827	-0.892784	0.101845
H	-1.948332	-1.157662	-0.562713
O	1.530375	-0.780862	0.146569
H	0.831557	-1.388830	-0.133927

Rotational constants (GHz): 9.1297300 4.2381800 3.1524000

Vibrational harmonic frequencies (cm-1):
 75.7037 187.8055 208.2819
 384.2934 418.2674 490.1041
 634.6001 938.4990 965.3500
 1098.0690 1129.2861 1173.7148
 1317.1951 1407.5523 1430.6699
 1449.9261 1465.3104 3085.6114
 3159.4440 3785.6491 3846.8792

Zero-point correction (Hartree): 0.065275

H2COOHOOH.ptmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21621086

Point group : CS

Electronic state : 1-A'

Cartesian coordinates (Angs):

C	0.548562	0.756050	0.000000
H	0.766813	1.824233	0.000000
H	1.447320	0.138727	0.000000
O	-0.179386	0.548982	1.169095
O	-0.179386	0.548982	-1.169095
O	-0.179386	-0.849478	1.449418
H	0.117426	-0.845663	2.367001
O	-0.179386	-0.849478	-1.449418
H	0.117426	-0.845663	-2.367001

Rotational constants (GHz): 9.5849300 3.9234100 3.0018300

Vibrational harmonic frequencies (cm-1):
 75.7632 (A'') 143.2460 (A'') 153.0843 (A')
 164.8923 (A') 418.8206 (A'') 469.2670 (A')
 613.9634 (A') 932.8658 (A') 968.0730 (A'')
 1104.8687 (A') 1127.4251 (A'') 1178.2045 (A')
 1345.2225 (A'') 1410.9855 (A'') 1426.7832 (A')
 1427.3757 (A'') 1447.1897 (A') 3082.1224 (A')
 3152.2079 (A') 3837.9191 (A'') 3838.5837 (A')

Zero-point correction (Hartree): 0.064515

H2COOHOOH.ptpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.22208995
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.022243	0.885094	0.089474
H	-0.477683	1.395743	0.938890
H	0.453552	1.568670	-0.613954
O	0.913486	0.024721	0.670686
O	-0.979934	0.212521	-0.660345
O	1.697190	-0.527819	-0.385103
H	2.583613	-0.263015	-0.111702
O	-1.776407	-0.541666	0.239413
H	-1.260705	-1.354020	0.332718

Rotational constants (GHz): 11.3477700 3.3040400 3.1656700
 Vibrational harmonic frequencies (cm-1):

103.0413	207.0820	233.9758
285.1478	357.9537	522.8126
676.9866	947.2521	964.4700
1101.7889	1123.8857	1186.9180
1328.0578	1403.0692	1419.3419
1427.0654	1465.1688	3083.1643
3152.1566	3802.0350	3834.0598

Zero-point correction (Hartree): 0.065214

H2COOHOOH.ptpt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21812100
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.000115	0.844428	0.000498
H	0.458291	1.447845	-0.784188
H	-0.458612	1.446753	0.785968
O	-0.955797	0.084571	-0.665921
O	0.955566	0.083597	0.665938
O	-1.759533	-0.547114	0.328084
H	-2.640416	-0.279088	0.041120
O	1.759858	-0.546425	-0.328727
H	2.640671	-0.279109	-0.040880

Rotational constants (GHz): 12.1678700 3.1266800 3.0551600
 Vibrational harmonic frequencies (cm-1):

102.5896	190.2494	206.2458
213.8322	337.4374	524.6163
655.2202	945.8433	959.0450
1105.5062	1129.6056	1180.0818
1334.8236	1404.0422	1416.1886
1431.1380	1457.8156	3075.3723
3142.6929	3837.0077	3837.7068

Zero-point correction (Hartree): 0.064898

H2COOHOOH.pttm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21333287
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.030573	0.608269	0.272407
H	0.359359	1.643667	0.154199
H	0.023687	0.301975	1.319422
O	-1.227565	0.553394	-0.291645
O	0.869743	-0.264514	-0.462682
O	-1.823551	-0.681152	0.098512
H	-2.614654	-0.364275	0.551093
O	2.100193	-0.276585	0.248045
H	2.697606	0.119877	-0.396992

Rotational constants (GHz): 16.3041000 2.7565100 2.5734500
 Vibrational harmonic frequencies (cm-1):

81.7446	165.3590	210.6936
230.5780	351.2102	420.9234
592.5949	963.4557	1042.2475
1116.9963	1149.1042	1175.0238
1290.5432	1405.8771	1415.0815
1440.2538	1505.0584	3061.2138
3124.0435	3830.9231	3833.0218

Zero-point correction (Hartree): 0.064714

H2COOHOOH.pttp

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21376065

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.026792	0.623126	0.285370
H	0.328000	1.669093	0.202097
H	0.047181	0.276387	1.320506
O	-1.241330	0.556273	-0.253977
O	0.872614	-0.193028	-0.505209
O	-1.784536	-0.717575	0.088217
H	-2.600951	-0.450822	0.527707
O	2.134645	-0.165186	0.144511
H	2.213869	-1.077289	0.449127

Rotational constants (GHz): 15.8491100 2.7878000 2.5829700

Vibrational harmonic frequencies (cm-1):

69.3790	172.6019	202.8258
249.6975	353.8975	420.4760
594.7546	961.3691	1041.7356
1117.9429	1147.7896	1175.8858
1287.1422	1405.4200	1411.7801
1438.9148	1506.3657	

3062.1562

3125.2173	3825.2082	3830.7865
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Zero-point correction (Hartree): 0.064703

H2COOHOOH.tpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21697400

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.004132	0.714991	0.260692
H	-0.240142	1.767287	0.101217
H	-0.078500	0.423011	1.307070
O	-0.837682	-0.126567	-0.517510
O	1.286020	0.553802	-0.225284
O	-2.004237	-0.371169	0.252036
H	-2.677861	0.090737	-0.261299
O	1.757585	-0.713683	0.207019
H	1.358235	-1.310039	-0.441226

Rotational constants (GHz): 13.9380300 2.9726600 2.6989100

Vibrational harmonic frequencies (cm-1):

39.5617	187.0210	253.0979
300.0303	381.4050	425.3546
604.4080	966.7701	1032.7773
1097.4714	1146.6751	1185.2707
1288.2974	1409.6372	1420.7618
1431.9684	1506.6431	3071.5613
3142.1025	3798.7764	3828.8135

Zero-point correction (Hartree): 0.064970

H2COOHOOH.tpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21333287

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.030573	0.608269	0.272407
H	-0.359359	1.643667	0.154199
H	-0.023687	0.301975	1.319422
O	-0.869743	-0.264514	-0.462682
O	1.227565	0.553394	-0.291645
O	-2.100193	-0.276585	0.248045
H	-2.697606	0.119877	-0.396992
O	1.823551	-0.681152	0.098512
H	2.614654	-0.364275	0.551093

Rotational constants (GHz): 16.3041000 2.7565100 2.5734500

Vibrational harmonic frequencies (cm-1):

81.7445	165.3589	210.6938
230.5781	351.2101	420.9234
592.5949	963.4557	1042.2475
1116.9963	1149.1042	1175.0238
1290.5432	1405.8771	1415.0815
1440.2538	1505.0584	3061.2139
3124.0435	3830.9231	3833.0218

Zero-point correction (Hartree): 0.064714

H2COOHOOH.tppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21659261

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.013064	0.690399	0.248141
H	0.070039	0.444214	1.309750
H	0.304204	1.722934	0.050913
O	0.830475	-0.205557	-0.491250
O	-1.271665	0.559292	-0.239279
O	2.106081	-0.178936	0.126310
H	2.130786	-1.034963	0.571790
O	-1.792719	-0.674344	0.236673
H	-1.560788	-1.278222	-0.480931

Rotational constants (GHz): 14.8610300 2.8833500 2.6386800

Vibrational harmonic frequencies (cm-1):

72.3384	175.7302	261.7890
287.6237	367.3766	418.8157
603.7443	965.6888	1043.5741
1106.8003	1148.7187	1184.4013
1283.1144	1410.5657	1414.2129
1429.9431	1510.6052	3071.0041
3136.0931	3812.7346	3819.5924

Zero-point correction (Hartree): 0.064984

H2COOHOOH.tppt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.21376063

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.026799	0.623008	0.285326
H	0.046816	0.276702	1.320630
H	0.328265	1.668877	0.201744
O	0.872481	-0.193822	-0.504890
O	-1.241131	0.556297	-0.254160
O	2.134803	-0.164841	0.144033
H	2.213770	-1.075974	0.451604
O	-1.784672	-0.717316	0.088413
H	-2.601499	-0.450196	0.526905

Rotational constants (GHz): 15.8552200 2.7877200 2.5829500

Vibrational harmonic frequencies (cm-1):

69.5972	172.6170	202.0997
249.3559	353.7639	420.5620

594.7557	961.4343	1041.8754
1117.7767	1147.9555	1175.9598
1287.1383	1405.4296	1411.7708
1438.9346	1506.3605	3062.0481
3125.1425	3825.3521	3830.9411

Zero-point correction (Hartree): 0.064702

H2COOHOOH.tptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.20664635

Point group : CS

Electronic state : 1-A'

Cartesian coordinates (Angs):

C	0.025389	-0.329153	0.000000
H	0.981368	-0.863477	0.000000
H	-0.813698	-1.027814	0.000000
O	-0.058797	0.547380	1.096143
O	-0.058797	0.547380	-1.096143
O	-0.058797	-0.297930	2.235910
H	0.780753	-0.062494	2.649262
O	-0.058797	-0.297930	-2.235910
H	0.780753	-0.062494	-2.649262

Rotational constants (GHz): 27.2333100 2.3447500 2.2161700

Vibrational harmonic frequencies (cm-1):

58.5938 (A'')	94.7927 (A')	215.6968 (A'')
228.7583 (A')	244.2585 (A')	464.7533 (A')
495.1438 (A'')	1020.6388 (A'')	1081.8325 (A')
1138.0748 (A'')	1168.6801 (A')	1197.9928 (A')
1221.7645 (A'')	1409.2156 (A'')	1421.2226 (A')
1436.4190 (A'')	1556.1950 (A')	3031.7765 (A')
3105.3019 (A')	3827.1782 (A'')	3828.4717 (A')

Zero-point correction (Hartree): 0.064351

H2COOHOOH.tptp

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.20700755

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.000013	-0.329680	0.000450
H	0.015314	-0.949598	-0.900218
H	-0.015277	-0.948727	0.901718
O	1.095911	0.550881	0.027274
O	-1.095891	0.550860	-0.027236
O	2.235982	-0.290042	0.100135
H	2.635720	-0.148456	-0.766905
O	-2.235947	-0.290058	-0.100603
H	-2.636277	-0.148270	0.766134

Rotational constants (GHz): 27.1810900 2.3448500 2.2171400

Vibrational harmonic frequencies (cm-1):

68.4773	94.2808	233.6510
267.7773	268.2903	464.5785
496.1564	1020.5079	1080.8720
1139.0432	1168.2038	1199.9795
1222.0774	1413.2730	1419.1443
1436.1786	1555.9182	3040.5372
3096.8918	3821.4865	3822.7137

Zero-point correction (Hartree): 0.064541

H2COOHOOH.tttt

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.20700755

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.000019	-0.329756	0.000290
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H	0.014741	-0.949527	-0.900488
H	-0.014814	-0.948966	0.901461
O	1.095864	0.550846	0.026714
O	-1.095869	0.550862	-0.026667
O	2.235937	-0.289938	0.100430
H	2.636027	-0.148787	-0.766509
O	-2.235877	-0.289938	-0.100758
H	-2.636278	-0.148847	0.766051
Rotational constants (GHz):	27.1835800	2.3449600	2.2172400
Vibrational harmonic frequencies (cm-1):			
68.2559	94.2909		233.5843
267.6146	268.1064		464.6244
496.1523	1020.6271		1081.0196
1139.0700	1168.2045		1199.9727
1222.0492	1413.3265		1419.2097
1436.1795	1555.9276		3040.5278
3096.8752	3821.6244		3822.8521
Zero-point correction (Hartree):	0.064541		

H2COOHOHO

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.72092614
 E(CCSD/Aug-CC-pVTZ) (Hartree): -340.67016061
 E(MP2/Aug-CC-pVTZ) (Hartree): -340.65179105
 E(MP3/Aug-CC-pVTZ) (Hartree): -340.65925700
 E(PMP2/Aug-CC-pVTZ) (Hartree): -340.65179105
 E(PMP3/Aug-CC-pVTZ) (Hartree): -340.65925700
 E(PUHF/Aug-CC-pVTZ) (Hartree): -339.49873657
 E(UHF/Aug-CC-pVTZ) (Hartree): -339.49873657
 E(UM062X/Aug-CC-pVTZ) (Hartree): -341.15361215
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.163584	1.085633	-0.017976
O	-1.079938	0.214687	-0.523450
O	-1.197941	-0.850123	0.409566
H	-0.485320		
	1.578691	0.902155	
H	0.101731	1.776306	-0.812052
O	1.306491	-0.822025	-0.421472
O	1.073802	0.389187	0.365984
H	-0.412412	-1.367577	0.108395
H	0.958197	0.044972	1.264331
Rotational constants (GHz):	8.1083600	4.8522800	3.7099300
Vibrational harmonic frequencies (cm-1):			
126.5766	221.1799		329.5558
417.8924	653.3284		769.4051
797.4587	878.6257		932.2240
984.6590	1132.0428		1187.7885
1289.3474	1351.1551		1421.0226
1497.5126	1500.8901		3075.7418
3192.9040	3422.7221		3765.9491
Zero-point correction (Hartree):	0.065948		

H2COOHOHO.b

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.14815286
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.032443	0.633523	-0.222616
O	1.214103	0.531686	0.341447
O	1.911149	-0.524101	-0.305878
H	-0.050322	0.433724	-1.287816
H	-0.443733	1.604814	0.039870
O	-0.902584	-0.388577	0.338421

H	1.806453	-1.256518	0.315572	
O	-2.232269	-0.164956	-0.250752	
H	-1.040928	-0.215588	1.282165	
Rotational constants (GHz):	16.2124900	2.6672500	2.5212300	
Vibrational harmonic frequencies (cm-1):				
99.0004	170.6076		212.8810	
307.1969	411.9296		568.1511	
840.6719	912.1253		965.4540	
1004.0984	1101.1231		1160.2488	
1253.3361	1335.5137		1399.9805	
1426.3869	1492.3767		3133.8223	
3221.4560	3756.9469		3814.8449	
Zero-point correction (Hartree): 0.065129				

TS.H-OOH

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.71021483
E(CCSD/Aug-CC-pVTZ) (Hartree): -340.65486136
E(MP2/Aug-CC-pVTZ) (Hartree): -340.64019336
E(MP3/Aug-CC-pVTZ) (Hartree): -340.63940527
E(RHF/Aug-CC-pVTZ) (Hartree): -339.47243365
E(RM062X/Aug-CC-pVTZ) (Hartree): -341.13834215
Electronic state : 1-A
Cartesian coordinates (Angs):

O	-1.010150	-1.086095	0.355735
O	-1.083564	-0.012316	-0.573749
C	-0.783713	1.061764	-0.004402
H	-0.979666	1.181734	1.054537
H	-0.583654	1.906616	-0.654455
O	1.050008	0.333770	0.646108
H	0.420669	-0.401883	0.934980
O	1.651697	-0.255528	-0.493059
H	0.980998	-0.895695	-0.788934

Rotational constants (GHz):	8.1562900	3.9708700	3.4275200
Vibrational harmonic frequencies (cm-1):			
i323.0885	133.9901		208.9683
218.6757	366.8065		451.5491
560.2060	821.8556		887.0653
958.8274	1060.3422		1162.5078
1234.4253	1428.8647		1493.8619
1599.2096	1619.2981		2987.2819
3135.2131	3266.2243		3704.6661
Zero-point correction (Hartree): 0.062194			

TS.H-OHO

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.70991430
E(CCSD/Aug-CC-pVTZ) (Hartree): -340.65506201
E(MP2/Aug-CC-pVTZ) (Hartree): -340.64255925
E(MP3/Aug-CC-pVTZ) (Hartree): -340.64161410
E(RHF/Aug-CC-pVTZ) (Hartree): -339.47263980
E(UM062X/Aug-CC-pVTZ) (Hartree): -341.14021288
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.557936	1.094764	0.062874
O	-1.124418	0.109636	-0.489531
O	-1.046305	-1.016853	0.411330
H	-0.638626	1.191061	1.141181
H	-0.452035	1.973569	-0.563714
O	1.276552	-0.791014	-0.315693
O	1.223425	0.560590	0.138023
H	0.314236	-1.127401	0.025863
H	1.490014	0.495315	1.066389

Rotational constants (GHz):	7.8804700	4.7823600	3.4285200
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Vibrational harmonic frequencies (cm-1):

i284.2013	118.6203	341.0534
428.7592	467.1653	559.7197
686.0540	885.8512	962.1900
1003.1531	1210.1781	1224.6924
1264.8400	1319.2962	1404.8823
1557.1777	1674.2223	2015.7847
3122.0521	3241.6453	3775.8980

Zero-point correction (Hartree): 0.062110

TS.H2COOHOOH.OH2COOHOOH

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -340.70197796

E(CCSD/Aug-CC-pVTZ) (Hartree): -340.64803717

T1 diagnostic: 0.020748

E(MP2/Aug-CC-pVTZ) (Hartree): -340.63291734

E(MP3/Aug-CC-pVTZ) (Hartree): -340.63406905

E(PMP2/Aug-CC-pVTZ) (Hartree): -340.63291734

E(PMP3/Aug-CC-pVTZ) (Hartree): -340.63406905

E(PUHF/Aug-CC-pVTZ) (Hartree): -339.46479970

E(UHF/Aug-CC-pVTZ) (Hartree): -339.46479970

E(UM062X/Aug-CC-pVTZ) (Hartree): -341.13208829

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.113378	1.081672	-0.001231
O	-1.033258	0.232521	-0.556877
O	-1.331587	-0.768565	0.404253
H	-0.475142	1.561236	0.909968
H	0.142541	1.791292	-0.784391
O	1.355820	-0.872431	-0.381113
O	1.107188	0.429597	0.405681
H	-0.767854	-1.484222	0.065288
H	0.995417	-0.527321	0.840969

Rotational constants (GHz): 8.1074300 4.5479000 3.5071600

Vibrational harmonic frequencies (cm-1):

i1391.4587	74.9419	210.0662
311.9637	411.9773	516.8174
666.0666	785.2517	888.6114
978.4394	991.4996	1172.6506
1180.8304	1308.6375	1416.8080
1444.7424	1493.9646	2904.3281
3082.4273	3171.8611	3722.2754

Zero-point correction (Hartree): 0.060905

TS.H2COOHOOH.OCH2OOH+OH

E(RM062X/Aug-CC-pVTZ) (Hartree): -341.11721798

E(UM062X/Aug-CC-pVTZ) (Hartree): -341.15865082

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.177159	0.832717	0.333050
H	0.795386	1.691454	0.018617
H	-0.386797	1.087663	1.235195
O	-0.640114	0.603166	-0.720639
O	0.986582	-0.245513	0.694922
O	-2.205416	-0.642085	0.195427
H	-2.771005	-0.325272	-0.528057
O	1.855619	-0.507769	-0.393904
H	1.326097	-1.112542	-0.930498

Rotational constants (GHz): 9.2944100 2.6872700 2.5572200

Vibrational harmonic frequencies (cm-1):

i97.0648	68.8143	134.1968
152.4296	216.7127	305.5282
412.0149	545.0392	650.5892

923.3553	966.6009	1081.6551
1121.1549	1253.2265	1365.7670
1392.6800	1419.2823	2958.1209
3081.3226	3779.2197	3806.1523

Zero-point correction (Hartree): 0.058398

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*****
CH2OO + CH3OOH
*****

CH3OOH
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -190.60509732
E(CCSD/Aug-CC-pVTZ) (Hartree): -190.57759767
  T1 diagnostic: 0.012209
E(MP2/Aug-CC-pVTZ) (Hartree): -190.55983559
E(PMP2/Aug-CC-pVTZ) (Hartree): -190.55983559
E(PUHF/Aug-CC-pVTZ) (Hartree): -189.88179069
E(ROHF/Aug-CC-pVTZ) (Hartree): -189.88179069
E(RM062X/Aug-CC-pVTZ) (Hartree): -190.85222021
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      1.118067      -0.221969      0.020348
  O     -0.025341       0.601946     -0.016639
  H      1.962438       0.465207      0.031912
  H      1.128293      -0.840714      0.919796
  H      1.164964      -0.854673     -0.866365
  O     -1.149052      -0.265945     -0.103479
  H     -1.568954      -0.126011      0.753521
Rotational constants (GHz):  44.0845100  10.6699600  9.3268600
Vibrational harmonic frequencies (cm-1):
  223.4492      256.1011      468.1683
  955.4601      1114.9648      1183.0861
  1228.3160      1402.0750      1460.1005
  1478.5862      1518.1430      3048.5979
  3120.1282      3153.7049      3830.0239
Zero-point correction (Hartree): 0.055680

CH3
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -39.76363018
E(CCSD/Aug-CC-pVTZ) (Hartree): -39.75858056
  T1 diagnostic: 0.014219
E(MP2/Aug-CC-pVTZ) (Hartree): -39.73878121
E(PMP2/Aug-CC-pVTZ) (Hartree): -39.73878121
E(PUHF/Aug-CC-pVTZ) (Hartree): -39.57351373
E(ROHF/Aug-CC-pVTZ) (Hartree): -39.57351373
E(UM062X/Aug-CC-pVTZ) (Hartree): -39.82535515
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      0.000000      0.000000     -0.000071
  H     -0.758704     -0.763627      0.000142
  H     -0.281979      1.038859      0.000142
  H      1.040685     -0.275232      0.000142
Rotational constants (GHz):  288.5064700  288.4961000  144.2506500
Vibrational harmonic frequencies (cm-1):
  440.4314      1413.9478      1414.3486
  3143.8053      3320.2583      3320.4627
Zero-point correction (Hartree): 0.029738

CH3O
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.88502793
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.87126248
  T1 diagnostic: 0.021220
E(MP2/Aug-CC-pVTZ) (Hartree): -114.84430086
E(PMP2/Aug-CC-pVTZ) (Hartree): -114.84430086
E(PUHF/Aug-CC-pVTZ) (Hartree): -114.46258260
E(ROHF/Aug-CC-pVTZ) (Hartree): -114.46258260
E(UM062X/Aug-CC-pVTZ) (Hartree): -115.04237439

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Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.576858	0.000306	-0.012193
O	0.790695	0.000086	-0.007172
H	-0.870190	-0.011507	1.050439
H	-0.997410	0.910106	-0.450982
H	-0.996814	-0.901119	-0.468924

 Rotational constants (GHz): 158.2284300 28.0121400 27.8384300
 Vibrational harmonic frequencies (cm-1):

407.4781	969.0953	1136.6721
1385.0947	1386.5134	1518.4740
2964.9617	3038.6648	3080.0413

 Zero-point correction (Hartree): 0.036193

CH3OO

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.96049279
 E(CCSD/Aug-CC-pVTZ) (Hartree): -189.93389628
 T1 diagnostic: 0.031645
 E(MP2/Aug-CC-pVTZ) (Hartree): -189.90724621
 E(PMP2/Aug-CC-pVTZ) (Hartree): -189.90724621
 E(PUHF/Aug-CC-pVTZ) (Hartree): -189.27411839
 E(ROHF/Aug-CC-pVTZ) (Hartree): -189.27411839
 E(UM062X/Aug-CC-pVTZ) (Hartree): -190.20981264
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-1.083207	-0.179756	-0.000003
O	0.159265	0.538048	-0.000002
H	-1.863610	0.575519	-0.000167
H	-1.132802	-0.795845	-0.894456
H	-1.132956	-0.795559	0.894640
O	1.169311	-0.276245	0.000002

 Rotational constants (GHz): 53.6438000 11.5597600 10.1250100
 Vibrational harmonic frequencies (cm-1):

131.8022	513.0995	980.9130
1145.6008	1201.8262	1294.1489
1458.6130	1484.5533	1495.2332
3083.3553	3174.3469	3189.4926

 Zero-point correction (Hartree): 0.043634

complex

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -379.95321157
 E(CCSD/Aug-CC-pVTZ) (Hartree): -379.89196829
 T1 diagnostic: 0.026183
 E(MP2/Aug-CC-pVTZ) (Hartree): -379.86302619
 E(PMP2/Aug-CC-pVTZ) (Hartree): -379.86302619
 E(PUHF/Aug-CC-pVTZ) (Hartree): -378.53272523
 E(ROHF/Aug-CC-pVTZ) (Hartree): -378.53272523
 E(RM062X/Aug-CC-pVTZ) (Hartree): -380.44769742
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.431140	1.092151	-0.227752
O	-1.743163	-0.098535	-0.191638
O	-1.237575	-0.832243	0.861880
H	-0.837521	1.507468	0.576956
H	-1.799871	1.653249	-1.077770
O	0.953809	-1.042800	-0.733756
O	1.115989	0.347607	-0.495922
H	0.214956	-1.253192	-0.119172
C	1.962373	0.487155	0.625509
H	2.918918	-0.001352	0.440732
H	1.490957	0.066169	1.516615
H	2.112683	1.559596	0.751593

Rotational constants (GHz): 5.5359100 2.1744900 1.9859000
 Vibrational harmonic frequencies (cm-1):
 63.8702 71.1640 110.0586
 159.4915 212.0584 242.8878
 297.0551 472.4894 524.8860
 685.2174 786.0708 878.2732
 955.1379 1091.5034 1119.9762
 1182.7862 1231.4259 1254.6689
 1445.9460 1456.8611 1478.0271
 1509.0168 1528.5535 1681.1616
 3043.4020 3120.2072 3139.5849
 3144.6882 3288.7375 3439.3720
 Zero-point correction (Hartree): 0.090249

H2O

E(RM062X/Aug-CC-pVTZ) (Hartree): -76.43010672
 Point group : C2V
 Electronic state : 1-A1
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.116436
 H 0.000000 0.762487 -0.465742
 H 0.000000 -0.762487 -0.465742
 Rotational constants (GHz): 832.9836600 431.2582400 284.1474200
 Vibrational harmonic frequencies (cm-1):
 1620.1208 3867.7526 3970.5372
 Zero-point correction (Hartree): 0.021548

H2OO

E(RM062X/Aug-CC-pVTZ) (Hartree): -151.48060900
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 O 0.633110 -0.000002 -0.114394
 H 0.898371 0.783716 0.387691
 H 0.901971 -0.782097 0.388461
 O -0.858153 -0.000200 0.017375
 Rotational constants (GHz): 295.9154200 24.9814400 24.0733600
 Vibrational harmonic frequencies (cm-1):
 767.9970 935.3775 942.6055
 1595.0057 3747.5539 3842.5581
 Zero-point correction (Hartree): 0.026953

H2COOHOOCH3.pmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.52007241
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.644047 -0.902130 0.402151
 H 0.927944 -1.951674 0.474434
 H 0.411695 -0.463839 1.374556
 O 1.733551 -0.248251 -0.161073
 O -0.488159 -0.908443 -0.423868
 O 1.647616 1.137479 0.140055
 H 0.956082 1.437155 -0.467176
 O -1.029001 0.410502 -0.429792
 C -2.239557 0.359349 0.297063
 H -2.060095 0.082294 1.337426
 H -2.929445 -0.345566 -0.165903
 H -2.645182 1.368023 0.248812
 Rotational constants (GHz): 7.1537000 2.3751500 1.9727400
 Vibrational harmonic frequencies (cm-1):
 47.7661 97.2495 171.6694
 236.0859 345.4644 377.5238

424.8436	521.7482	655.6469
898.6299	961.1112	1061.6668
1112.8425	1131.7950	1176.7878
1190.0713	1235.3330	1332.3284
1408.9203	1449.8252	1457.3088
1465.8006	1481.4902	1516.3716
3053.2843	3076.2869	3128.2366
3152.6718	3160.1671	3784.3639

Zero-point correction (Hartree): 0.093663

H2COOHOOCH3.pmmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.52033645

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.816982	0.956506	0.299442
H	-1.121314	1.985202	0.110749
H	-0.863669	0.689617	1.355902
O	-1.685459	0.153335	-0.432184
O	0.502467	0.902359	-0.160600
O	-1.680826	-1.154533	0.123845
H	-0.823802	-1.497238	
	-0.168361		
O	1.018407	-0.375500	0.239130
C	2.383427	-0.342965	-0.113208
H	2.897641	0.451859	0.427340
H	2.499263	-0.203029	-1.188175
H	2.776495	-1.312947	0.183612

Rotational constants (GHz): 7.5171400 2.2790600 1.8682900

Vibrational harmonic frequencies (cm-1):

45.4493	116.6661	161.9813
239.4517	308.4565	399.1919
432.2206	490.0531	659.1379
897.5299	961.8340	1087.5271
1125.0929	1131.9936	1167.2877
1188.1357	1255.5195	1337.2796
1407.6866	1449.9359	1458.6246
1463.8078	1475.3862	1522.9215
3058.9765	3086.3182	3132.4513
3159.4548	3162.6923	3777.7679

Zero-point correction (Hartree): 0.093771

H2COOHOOCH3.pmpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.52151401

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.702162	-1.021742	-0.107650
H	0.436066	-1.671543	-0.940532
H	1.418896	-1.478032	0.575248
O	1.239189	0.122910	-0.697892
O	-0.415817	-0.741946	0.681476
O	1.826219	0.902797	0.332305
H	1.057495	1.323308	0.742588
O	-1.497854	-0.454687	-0.199274
C	-1.783922	0.922624	-0.078347
H	-0.964549	1.528823	-0.470223
H	-1.996543	1.180001	0.959885
H	-2.674710	1.079557	-0.683900

Rotational constants (GHz): 6.2809600 2.5542700 2.1417600

Vibrational harmonic frequencies (cm-1):

84.3651	116.6301	190.9608
226.4501	298.2029	343.0277
467.3112	524.1710	682.0841

900.4622	956.4941	1071.3168
1110.5489	1124.4461	1173.9231
1187.4951	1237.9137	1326.0719
1405.6243	1420.8349	1457.4785
1467.7353	1485.2046	1517.8540
3047.8894	3090.0151	3120.9383
3154.9564	3159.2615	3782.1673

Zero-point correction (Hartree): 0.093705

H2COOHOOCH3.pmpp

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.52083736

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.529358	0.869371	0.132459
H	-0.023793	1.571282	-0.532520
H	-1.006718	1.361479	0.980815
O	-1.472722	0.237171	-0.670985
O	0.376642	-0.022700	0.711501
O	-2.302166	-0.541434	0.176422
H	-1.786658	-1.353835	0.271618
O	1.206406	-0.529515	-0.331527
C	2.503344	-0.031449	-0.081018
H	2.861890	-0.363478	0.893326
H	2.521974	1.059022	-0.134393
H	3.124110	-0.450177	-0.870781

Rotational constants (GHz): 10.6323600 1.8529600 1.8127300

Vibrational harmonic frequencies (cm-1):

53.9609	86.1489	178.3053
228.6122	295.7201	338.7356
464.4233	520.3908	692.5545
902.0393	963.1762	1069.8323
1114.6522	1121.4710	1176.9258
1191.4472	1236.3073	1328.0587
1411.1576	1424.0963	1459.3051
1466.4026	1479.4955	1517.1308
3048.9413	3078.4687	3121.5868
3145.0866	3157.3045	3799.9976

Zero-point correction (Hartree): 0.093568

H2COOHOOCH3.pmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51525145

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.518835	0.664023	0.333476
H	-0.188618	1.697994	0.212623
H	-0.569829	0.366762	1.380724
O	-1.752199	0.591110	-0.284381
O	0.340496	-0.229294	-0.359861
O	-2.351598	-0.641420	0.087514
H	-1.927715	-1.264118	-0.518871
O	1.467058	-0.432059	0.481707
C	2.587416	0.062178	-0.222240
H	2.488780	1.131511	-0.415727
H	2.720114	-0.475864	-1.160791
H	3.435726	-0.120196	0.434789

Rotational constants (GHz): 12.4701100 1.6862400 1.6073400

Vibrational harmonic frequencies (cm-1):

39.4018	45.2871	162.5178
217.5043	307.4251	360.5169
406.1707	481.1062	598.8156
965.8098	982.3026	1077.8753
1121.6367	1147.6973	1179.8608

1189.4880	1239.2286	1288.1647
1419.2415	1430.5063	1461.0957
1478.8508	1509.0187	1518.6108
3053.5230	3070.5709	3126.1139
3137.9918	3157.2932	3797.0580

Zero-point correction (Hartree): 0.093338

H2COOHOOCH3.pmtmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51651260

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.663819	-0.903710	0.355300
H	0.992309	-1.943630	0.377744
H	0.316953	-0.561311	1.329931
O	1.783710	-0.201861	-0.071392
O	-0.378835	-0.738370	-0.586405
O	1.509605	1.183323	0.068659
H	1.141248	1.398768	-0.798692
O	-1.597137	-0.525720	0.110407
C	-1.856797	0.862756	0.086361
H	-1.926477	1.219421	-0.942128
H	-1.087095	1.415463	0.628798
H	-2.817813	0.978024	0.584233

Rotational constants (GHz): 6.5911500 2.4739500 1.9600000

Vibrational harmonic frequencies (cm-1):

48.8075	93.8741	185.7833
239.1192	296.8881	390.1990
436.6258	484.4573	599.8845
938.4452	966.9604	1066.0563
1102.8643	1135.4246	1182.2538
1191.6957	1230.7809	1301.3035
1412.7955	1421.0549	1456.8274
1479.6404	1497.5198	1523.6538
3048.5176	3080.6336	3121.2930
3145.8667	3155.9073	3802.7315

Zero-point correction (Hartree): 0.093491

H2COOHOOCH3.pptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51169657

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.494749	0.521436	0.411949
H	-0.089131	1.536144	0.431201
H	-0.650050	0.129847	1.418635
O	-1.679665	0.610566	-0.292590
O	0.372100	-0.340550	-0.300081
O	-2.393491	-0.607282	-0.095190
H	-3.204320	-0.277912	0.311043
O	1.545959	-0.409279	0.500086
C	2.591569	0.119209	-0.287526
H	2.401511	1.163530	-0.542009
H	2.719950	-0.467041	-1.197343
H	3.481888	0.043916	0.334137

Rotational constants (GHz): 13.3469000 1.6255600 1.5755700

Vibrational harmonic frequencies (cm-1):

46.4849	69.6814	149.4027
192.9294	217.6838	348.7398
401.4701	477.9864	585.9519
962.2474	980.7935	1094.8757
1131.9491	1148.3095	1174.7260
1187.9107	1238.8947	1294.5349
1413.8161	1438.4665	1461.2064

1478.2175	1505.2544	1518.5429
3051.5657	3060.7923	3121.3727
3124.1400	3156.1199	3830.9564

Zero-point correction (Hartree): 0.093097

H2COOHOOCH3.ptmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51837799

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.776239	-1.031353	0.140557
H	1.218964	-1.944088	-0.258228
H			
0.898846	-0.941810	1.219864	
O	1.460442	0.007850	-0.503427
O	-0.569403	-1.118306	-0.191568
O	1.292438	1.200777	0.259637
H	2.211236	1.435993	0.434960
O	-1.277958	-0.156196	0.585030
C	-1.759109	0.822918	-0.314700
H	-2.418370	0.368601	-1.054694
H	-0.935059	1.342890	-0.802048
H	-2.322549	1.516021	0.307626

Rotational constants (GHz): 5.5485500 2.9289100 2.1834300

Vibrational harmonic frequencies (cm-1):

81.1304	129.9338	149.1582
197.6275	228.2388	387.6291
434.6665	500.8010	624.6769
893.4295	950.7375	1078.3668
1098.2655	1133.7932	1172.7802
1192.8021	1238.3005	1344.0589
1408.5342	1418.9980	1452.4544
1461.8984	1479.4866	1515.3076
3059.7913	3086.3173	3137.8585
3155.0569	3157.1198	3835.0308

Zero-point correction (Hartree): 0.093415

H2COOHOOCH3.ptpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.52030165

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.664872	-1.042803	-0.084645
H	0.443263	-1.692736	-0.932330
H	1.356810	-1.498690	0.624576
O	1.222870	0.095670	-0.672734
O	-0.479156	-0.782674	0.657511
O	1.709314	0.923806	0.381468
H	2.636680	1.011117	0.130841
O	-1.498236	-0.401053	-0.260243
C	-1.757055	0.971278	-0.032029
H	-0.873664	1.572990	-0.242945
H	-2.087403	1.130316	0.994636
H	-2.560923	1.220151	-0.722750

Rotational constants (GHz): 6.1580600 2.6003400 2.1470800

Vibrational harmonic frequencies (cm-1):

90.1627	118.1043	186.9098
209.8450	231.4334	318.5992
463.9136	513.3192	674.9006
905.0848	948.6564	1078.2965
1102.7769	1131.8780	1173.6907
1192.0731	1240.2264	1334.6350
1399.5392	1422.2261	1462.0520
1467.0146	1478.5598	1518.6625

3060.8214	3079.9065	3138.5960
3146.0391	3157.8438	3832.2821

Zero-point correction (Hartree): 0.093583

H2COOHOOCH3.ptpp

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51671120

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.519291	0.833254	0.036463
H	-0.043422	1.459540	-0.720607
H	-0.992591	1.416969	0.827175
O	-1.466904	0.100941	-0.673765
O	0.420345	0.047931	0.695193
O	-2.294620	-0.555687	0.283563
H	-3.167195	-0.262598	-0.004147
O	1.256563	-0.538063	-0.298607
C	2.554757	-0.043054	-0.055918
H	2.887457	-0.309661	0.947506
H	2.593929	1.040857	-0.185572
H	3.185958	-0.527285	-0.798693

Rotational constants (GHz): 11.4090100 1.7724100 1.7527200

Vibrational harmonic frequencies (cm-1):

35.2519	87.3229	162.6591
195.6053	233.0150	321.5616
454.8786	522.2251	673.5471
903.3919	953.1115	1080.3236
1111.7079	1130.0680	1172.4445
1188.6116	1238.5707	1336.1602
1406.4383	1424.3929	1455.1273
1461.2443	1479.0747	1517.6704
3046.3872	3070.8770	3117.9647
3136.8504	3155.6879	3836.0641

Zero-point correction (Hartree): 0.093196

H2COOHOOCH3.tpmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51236559

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.523079	0.505887	0.402560
H	-0.917537	1.463137	0.751660
H	-0.341620	-0.179785	1.233056
O	-1.426721	-0.095957	-0.508088
O	0.635084	0.801095	-0.286070
O	-2.541684	-0.484351	0.282953
H	-3.237857	0.076253	-0.079184
O	1.352594	-0.416448	-0.471574
C	2.510070	-0.315484	0.329170
H	2.250492	-0.238938	1.387399
H	3.113270	0.541352	0.028622
H	3.057126	-1.239148	0.150300

Rotational constants (GHz): 11.8445300 1.6642300 1.6224100

Vibrational harmonic frequencies (cm-1):

47.2422	83.6280	143.0125
234.4325	244.4379	322.0555
383.1129	483.3472	616.6429
907.3251	1041.1990	1089.0405
1114.8863	1145.6147	1173.1595
1188.0122	1236.1256	1291.9546
1403.3206	1430.1825	1459.4708
1479.0959	1505.2927	1516.9044
3046.5786	3056.5175	3115.7256
3119.2108	3157.0845	3832.6545

Zero-point correction (Hartree): 0.093102

H2COOHOOCH3.tpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51497912

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.612639	0.865726	0.044373
H	-1.147374	1.650667	-0.495289
H	-0.714342	0.974338	1.124147
O	-1.093069	-0.416762	-0.338818
O	0.701542	0.957430	-0.360480
O	-2.359067	-0.555935	0.289009
H	-2.955917	-0.537515	-0.468580
O	1.489229	0.214756	0.566768
C	2.016605	-0.893723	-0.135821
H	2.618832	-0.558964	-0.980566
H	1.217542	-1.553265	-0.472540
H	2.648389	-1.403198	0.589684

Rotational constants (GHz): 7.9012200 2.0618400 1.7965800

Vibrational harmonic frequencies (cm-1):

76.5529	95.3649	157.8438
226.2440	261.7782	323.2466
399.5410	487.3708	598.4339
901.4281	1038.5785	1087.7133
1101.5701	1149.1434	1177.6865
1191.0568	1232.6298	1297.2829
1406.6969	1427.5550	1459.9001
1476.5567	1509.5711	1518.6184
3059.5802	3068.4770	3134.2571
3137.6387	3157.6261	3827.5319

Zero-point correction (Hartree): 0.093376

H2COOHOOCH3.tppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.51507512

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.622492	0.867619	0.046452
H	0.746848	0.975087	1.125711
H	1.150063	1.650196	-0.500593
O	1.090092	-0.412381	-0.358378
O	-0.700779	0.966745	-0.324825
O	2.426640	-0.498329	0.109267
H	2.340583	-1.116490	0.845474
O	-1.459968	0.181696	0.592584
C	-2.038981	-0.868981	-0.156107
H	-1.267758	-1.512937	-0.578162
H	-2.675092	-0.469854	-0.946141
H	-2.643593	-1.419673	0.562461

Rotational constants (GHz): 8.0109600 2.0473100 1.7874700

Vibrational harmonic frequencies (cm-1):

76.6396	92.6739	158.7026
231.6766	253.4584	323.2498
396.2541	487.2504	599.6843
901.8583	1040.4728	1088.5313
1106.0201	1149.1896	1178.1811
1191.4080	1232.0662	1296.5700
1405.2801	1426.3664	1460.3741
1477.6854	1511.2114	1519.7482
3059.7230	3067.8852	3132.4598
3137.2128	3157.1050	3820.7595

Zero-point correction (Hartree): 0.093359

H2COOHOOCH3.tppp

E(RM062X/Aug-CC-pVTZ)

(Hartree): -380.51268755

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.532867	0.551317	0.385259
H	0.375353	-0.101485	1.247753
H	0.914644	1.528521	0.686371
O	1.435449	-0.064699	-0.517155
O	-0.642277	0.792303	-0.295098
O	2.596339	-0.347074	0.250572
H	2.589035	-1.311752	0.261614
O	-1.326238	-0.452543	-0.425826
C	-2.518609	-0.320085	0.317212
H	-3.122403	0.501977	-0.067286
H	-2.305535	-0.164624	1.377037
H	-3.042819	-1.263925	0.179736

Rotational constants (GHz): 11.8526000 1.6648500 1.6133000

Vibrational harmonic frequencies (cm-1):

45.3815	74.0328	145.6244
238.6318	252.1308	325.0876
383.8270	476.0583	621.8799
906.2516	1041.0378	1090.0156
1116.6473	1144.1884	1174.5034
1188.9773	1238.0537	1289.5757
1404.9652	1428.5110	1460.6093
1479.7072	1505.5588	1517.8777
3047.5073	3054.2162	3118.5609
3120.9870	3157.2951	3827.3346

Zero-point correction (Hartree): 0.093120

H2COOHOOCH3.tptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.50557663

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.504682	-0.178404	-0.344779
H	0.273231	0.698910	-0.958380
H	0.752678	-1.037968	-0.970847
O	1.558395	0.090828	0.547869
O	-0.565101	-0.468142	0.518608
O	2.722723	0.146545	-0.262572
H	2.975748	1.072886	-0.169732
O	-1.710129	-0.517289	-0.319591
C	-2.493791	0.610717	0.010241
H	-1.953053	1.536802	-0.195051
H	-2.790690	0.576458	1.058078
H	-3.370354	0.543496	-0.631346

Rotational constants (GHz): 14.2802000 1.5028700 1.4939300

Vibrational harmonic frequencies (cm-1):

34.5407	60.5104	117.7604
198.5707	233.0924	280.5297
400.5183	486.7791	514.4960
964.8193	1053.5565	1105.7656
1132.8618	1170.0665	1179.7206
1198.5999	1223.9636	1245.2621
1414.2659	1434.7352	1459.6581
1478.4689	1515.2398	1553.9150
3030.7487	3050.1782	3099.7891
3124.5353	3157.9110	3828.9552

Zero-point correction (Hartree): 0.092835

HOOCH2OCH2

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.31027526
E(CCSD/Aug-CC-pVTZ) (Hartree): -304.26563531
  T1 diagnostic: 0.017410
E(MP2/Aug-CC-pVTZ) (Hartree): -304.24036065
E(PMP2/Aug-CC-pVTZ) (Hartree): -304.24036065
E(PUHF/Aug-CC-pVTZ) (Hartree): -303.18205347
E(ROHF/Aug-CC-pVTZ) (Hartree): -303.18205347
E(UM062X/Aug-CC-pVTZ) (Hartree): -304.72046354
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      0.022343      0.914708     -0.082055
  O      0.957299      0.182332      0.647389
  O      1.706792     -0.597230     -0.271768
  H      0.493814      1.407616     -0.928514
  H     -0.388955      1.624067      0.639639
  O     -0.990857      0.100184     -0.612502
  H      1.146431     -1.376485     -0.387930
  C     -1.799303     -0.481932      0.309704
  H     -1.425647     -0.604842      1.315809
  H     -2.549753     -1.129295     -0.109840
Rotational constants (GHz):  11.0759200      3.5005300      3.2907000
Vibrational harmonic frequencies (cm-1):
  91.8012      184.7667      257.6864
  269.6713      358.7436      492.6373
  520.9593      652.3548      958.1846
  1002.1512     1112.9063     1133.2246
  1236.4648     1269.5703     1331.5314
  1420.0412     1426.6425     1479.2179
  1506.7840     3076.5459     3162.7134
  3169.6654     3311.6434     3799.6226
Zero-point correction (Hartree): 0.075693

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HOOCH2OCH3

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.97602227
E(CCSD/Aug-CC-pVTZ) (Hartree): -304.93063258
  T1 diagnostic: 0.012772
E(MP2/Aug-CC-pVTZ) (Hartree): -304.90506369
E(PMP2/Aug-CC-pVTZ) (Hartree): -304.90506369
E(PUHF/Aug-CC-pVTZ) (Hartree): -303.81493494
E(ROHF/Aug-CC-pVTZ) (Hartree): -303.81493495
E(RM062X/Aug-CC-pVTZ) (Hartree): -305.38423802
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.068636      0.899371     -0.116017
  O      0.994813      0.196052      0.665735
  O      1.790248     -0.582954     -0.214965
  H      0.576087      1.393416     -0.942445
  H     -0.372627      1.617994      0.582285
  O     -0.893131      0.062643     -0.669597
  H      1.180238     -1.284651     -0.481728
  C     -1.800108     -0.457511      0.286134
  H     -1.281859     -1.043181      1.047635
  H     -2.499000     -1.093732     -0.249134
  H     -2.349437      0.353069      0.773304
Rotational constants (GHz):  10.9313100      3.2967300      3.1377000
Vibrational harmonic frequencies (cm-1):
  100.9163      145.5251      219.0594
  288.6088      363.7184      501.3367
  654.8891      954.4935      979.5363
  1102.1272     1127.1338     1187.4354
  1209.8734     1248.3483     1335.5577
  1419.4748     1428.4043     1477.0509

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1498.3790	1502.7246	1519.5499
3038.6924	3054.4381	3102.7651
3143.6464	3165.1546	3791.6303

Zero-point correction (Hartree): 0.090125

HOOCH2OCH3O

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -379.96716295
 E(CCSD/Aug-CC-pVTZ) (Hartree): -379.90769627
 T1 diagnostic: 0.016145
 E(MP2/Aug-CC-pVTZ) (Hartree): -379.88109694
 E(PMP2/Aug-CC-pVTZ) (Hartree): -379.88109694
 E(PUHF/Aug-CC-pVTZ) (Hartree): -378.54800722
 E(ROHF/Aug-CC-pVTZ) (Hartree): -378.54800722
 E(UM062X/Aug-CC-pVTZ) (Hartree): -380.46514724

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.280952	-0.756441	0.737047
O	1.102781	-0.774948	-0.340159
O	1.852058	0.441346	-0.370277
H	0.723902	-0.286056	1.610576
H	-0.087776	-1.766802	0.905973
O	-0.479666	1.421537	0.206382
O	-0.912309	0.063774	0.481098
H	1.098307	1.093140	-0.301758
C	-1.707699	-0.382341	-0.636436
H	-1.093106	-0.358158	-1.531593
H	-2.526491	0.323203	-0.699324
H	-2.057265	-1.386313	-0.403896

Rotational constants (GHz): 5.8597300 3.0222200 2.5107400

Vibrational harmonic frequencies (cm-1):

101.6101	222.1436	262.1155
309.4662	374.7880	414.9731
513.9152	655.9254	774.9631
802.4926	903.8435	958.3308
997.9354	1174.5504	1199.5809
1213.5726	1236.6870	1324.8525
1403.7609	1461.6676	1475.9510
1479.4337	1504.5802	1607.6100
3090.9125	3111.8941	3167.7586
3187.3287	3194.9799	3222.8913

Zero-point correction (Hartree): 0.094203

OH2COOCH3

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.28815238
 E(CCSD/Aug-CC-pVTZ) (Hartree): -304.24448136
 T1 diagnostic: 0.020552
 E(MP2/Aug-CC-pVTZ) (Hartree): -304.20837640
 E(PMP2/Aug-CC-pVTZ) (Hartree): -304.20837640
 E(PUHF/Aug-CC-pVTZ) (Hartree): -303.17615661
 E(ROHF/Aug-CC-pVTZ) (Hartree): -303.17615661
 E(UM062X/Aug-CC-pVTZ) (Hartree): -304.69732134

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-1.322325	-0.329224	0.140507
H	-1.341804	-0.631808	1.189095
H	-2.133882	-0.778859	-0.436528
O	-1.318572	1.056800	0.001734
O	-0.145418	-0.787444	-0.470127
O	0.930701	-0.547882	0.422054
C	1.675467	0.535748	-0.099404
H	1.073031	1.446060	-0.107326
H	2.032995	0.307249	-1.102937

H 2.517113 0.646422 0.581796
 Rotational constants (GHz): 10.0401100 4.0372200 3.2455400
 Vibrational
 harmonic frequencies (cm-1):
 123.0090 158.0565 235.6130
 364.7207 480.7789 544.4963
 898.7102 999.9459 1086.4231
 1122.0733 1175.9790 1190.5208
 1235.2256 1364.9934 1384.9027
 1457.8178 1477.3154 1513.5094
 1519.5965 3051.6923 3053.7765
 3119.1593 3129.8459 3158.4817
 Zero-point correction (Hartree): 0.077108

OOCH2OCH3

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.32599146
 E(CCSD/Aug-CC-pVTZ) (Hartree): -304.28181074
 T1 diagnostic: 0.025187
 E(MP2/Aug-CC-pVTZ) (Hartree): -304.24737832
 E(PMP2/Aug-CC-pVTZ) (Hartree): -304.24737832
 E(PUHF/Aug-CC-pVTZ) (Hartree): -303.20477422
 E(ROHF/Aug-CC-pVTZ) (Hartree): -303.20477422
 E(UM062X/Aug-CC-pVTZ) (Hartree): -304.73601634
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 C 0.098089 0.878171 0.104712
 O 1.055353 -0.094458 0.591444
 O 1.799101 -0.538841 -0.379801
 H 0.631021 1.562524 -0.549038
 H -0.257179 1.356625 1.022229
 O -0.907244 0.288895 -0.609550
 C -1.761694 -0.533712 0.168521
 H -1.224430 -1.399849 0.555949
 H -2.560681 -0.865028 -0.487247
 H -2.184781 0.034199 1.001969
 Rotational constants (GHz): 11.8041600 3.3581300 3.1786600
 Vibrational harmonic frequencies (cm-1):
 75.6651 139.3531 210.7685
 341.4170 483.6276 631.2282
 919.5438 988.8978 1133.0127
 1186.7004 1212.8295 1241.1952
 1276.3758 1336.7189 1423.6700
 1478.7247 1500.8324 1505.9391
 1517.2481 3042.1947 3058.0911
 3113.9341 3171.1335 3174.4252
 Zero-point correction (Hartree): 0.077830

TS.H-OOCH3

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -379.94375085
 E(CCSD/Aug-CC-pVTZ) (Hartree): -379.88012553
 T1 diagnostic: 0.024416
 E(MP2/Aug-CC-pVTZ) (Hartree): -379.85613276
 E(PMP2/Aug-CC-pVTZ) (Hartree): -379.85613276
 E(PUHF/Aug-CC-pVTZ) (Hartree): -378.51149843
 E(ROHF/Aug-CC-pVTZ) (Hartree): -378.51149843
 E(RM062X/Aug-CC-pVTZ) (Hartree): -380.43805221
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 O 1.153713 1.252358 0.324584
 O 1.460295 0.257235 -0.639516
 C 1.491697 -0.855918 -0.062972
 H 1.803387 -0.917363 0.972313

H	1.459286	-1.726276	-0.709517
O	-0.385854	-0.614998	0.770164
H	0.072165	0.343319	0.782524
O	-1.211390	-0.554563	-0.381671
C	-2.185772	0.442566	-0.150838
H	-1.710920	1.417238	-0.017663
H	-2.795471	0.190089	0.717094
H	-2.798109	0.452851	-1.050382
Rotational constants (GHz):	6.4763100	2.3633500	2.0731200
Vibrational harmonic frequencies (cm-1):			
i410.5111	59.4504		136.3108
154.6527	265.3196		337.2555
465.5160	490.1893		575.9274
824.7689	903.9141		961.5754
1111.8035	1155.6840		1183.6667
1230.6096	1235.7407		1329.7461
1434.0861	1459.1379		1480.7419
1513.9501	1588.6653		1616.0266
2195.7075	3047.2021		3121.4173
3137.8658	3158.2361		3268.4417
Zero-point correction (Hartree):	0.089859		

TS.H-OOCH3.b

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.43265668

Electronic state : 1-A

Cartesian coordinates (Angs):

O	1.404469	-0.469867	-1.035577
O	1.369984	-0.586666	0.385117
C	1.136365	0.550371	0.870998
H	1.529750	1.434702	0.381936
H	0.838889	0.570654	1.914386
O	-0.414787	1.016281	-0.303451
H	0.180463	0.422351	-0.935785
O	-1.694436	0.409418	-0.295810
C	-1.627587	-0.858734	0.327543
H	-1.344249	-0.763656	1.378382
H	-0.936943	-1.521894	-0.194641
H	-2.642414	-1.245304	0.262246
Rotational constants (GHz):	5.8325200	2.4026300	2.3172600
Vibrational harmonic frequencies (cm-1):			
i381.4259	83.5124		161.4990
180.3466	304.1109		361.4393
406.6529	516.3238		569.6709
842.7443	898.8038		942.1095
1091.2781	1175.8600		1190.6972
1222.8710	1233.6814		1237.0064
1415.0104	1465.5830		1485.3009
1512.0791	1527.3673		1606.0766
2396.7402	3044.9494		3121.3409
3126.8435	3161.4037		3252.7044
Zero-point correction (Hartree):	0.090065		

TS.H-OCH3O

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -379.94752233

E(CCSD/Aug-CC-pVTZ) (Hartree): -379.88450329

T1 diagnostic: 0.021205

E(MP2/Aug-CC-pVTZ) (Hartree): -379.86097822

E(PMP2/Aug-CC-pVTZ) (Hartree): -379.86097822

E(PUHF/Aug-CC-pVTZ) (Hartree): -378.51761916

E(ROHF/Aug-CC-pVTZ) (Hartree): -378.51761916

E(RM062X/Aug-CC-pVTZ) (Hartree): -380.44331149

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.714656	1.135168	-0.186882
O	-1.570407	0.222656	-0.282539
O	-1.398695	-0.697494	0.812415
H	-0.370489	1.417915	0.803139
H	-0.675943	1.828314	-1.020406
O	0.580773	-1.178250	-0.634406
O	0.937106	0.188082	-0.501063
H	-0.218186	-1.226879	0.031786
C	1.834000	0.307981	0.598264
H	2.713958	-0.294530	0.390144
H	1.342629	-0.025879	1.512759
H	2.101748	1.362220	0.659036

Rotational constants (GHz): 5.7396200 2.7721700 2.4334100

Vibrational harmonic frequencies (cm-1):

i190.6074	83.1954	235.8061
251.1854	339.5369	403.8716
433.3469	470.8139	537.5320
872.2149	923.8516	935.3094
1104.8337	1116.8946	1188.5117
1207.0748	1231.5167	1257.1653
1417.8834	1458.6494	1482.2689
1510.3267	1596.2563	1683.6890
2416.4664	3063.0902	3121.5813
3150.0003	3173.4122	3246.4490

Zero-point correction (Hartree): 0.090928

TS.HOOCH2OCH3O.OOCH2OCH3+OH

E(UM062X/Aug-CC-pVTZ) (Hartree): -380.44605734

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.804661	-0.775374	0.805377
O	1.336272	-0.586078	-0.313817
O	1.466309	0.809864	-0.599385
H	0.876901	-0.006958	1.566850
H	0.604276	-1.811961	1.055964
O	-0.815640	1.265497	0.432473
O	-1.029652	-0.141623	0.509903
H	0.101679	1.278763	-0.043999
C	-1.522110	-0.582677	-0.751777
H	-0.778922	-0.398689	-1.527649
H	-2.442428	-0.045467	-0.964710
H	-1.715116	-1.648655	-0.641444

Rotational constants (GHz): 5.2193200 2.9186200 2.5501600

Vibrational harmonic frequencies (cm-1):

i197.0250	105.1246	210.2413
232.6908	325.2484	363.4222
435.7865	479.5457	558.4510
866.5833	910.9670	926.9747
1001.7510	1088.0390	1191.6191
1209.4882	1231.0265	1248.6946
1426.0456	1458.6144	1478.4779
1511.0838	1600.9490	1729.1279
2543.5053	3068.0808	3131.5375
3155.4493	3173.2337	3257.9294

Zero-point correction (Hartree): 0.090944

complex.HOOCH2OCH3O+H2O

E(RM062X/Aug-CC-pVTZ) (Hartree): -456.91064733

E(UM062X/Aug-CC-pVTZ)

(Hartree): -456.91064733

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.354528	-0.264820	-0.985460
O	1.397646	-0.930049	-0.429716
O	0.910670	-1.796608	0.594025
H	-0.565237	-0.840198	-1.050529
H	0.686031	0.167348	-1.927695
O	-0.456786	0.408339	1.147833
O	-0.031204	0.892764	-0.148607
H	0.426000	-1.142084	1.152353
C	1.022345	1.854316	0.062815
H	1.849548	1.360046	0.563883
H	0.584120	2.625174	0.684029
H	1.304356	2.237711	-0.915291
O	-2.689074	-0.239919	-0.340580
H	-3.484073	-0.617869	0.037454
H	-2.112004	-0.003313	0.408025

Rotational constants (GHz): 2.6556300 1.9922000 1.4826800

Vibrational harmonic frequencies (cm-1):

46.2661	99.2051	107.6241
138.2746	199.3333	216.8433
250.6412	303.6497	368.1753
429.1636	466.6425	519.3899
614.6261	648.5974	704.9734
778.4266	902.8090	960.3839
1005.7060	1174.4752	1197.7538
1211.1187	1235.3515	1324.3547
1409.9263	1462.4006	1477.5321
1488.1835	1505.5698	1569.6799
1651.9001	3093.5563	3115.1441
3189.5428	3202.7347	3222.6954
3383.5796	3603.2530	3940.0846

Zero-point correction (Hartree): 0.118965

complex.HOOCH2OCH3O+SO2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -927.97328105

E(CCSD/Aug-CC-pVTZ) (Hartree): -927.87661600

T1 diagnostic: 0.017924

E(MP2/Aug-CC-pVTZ) (Hartree): -927.86196555

E(PMP2/Aug-CC-pVTZ) (Hartree): -927.86196555

E(PUHF/Aug-CC-pVTZ) (Hartree): -925.84632393

E(ROHF/Aug-CC-pVTZ) (Hartree): -925.84632393

E(UM062X/Aug-CC-pVTZ) (Hartree): -929.10358593

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.960615	0.602368	-0.714197
O	2.799391	0.030983	0.185059
O	2.744805	-1.385389	0.053604
H	1.873724	0.044153	-1.641462
H	2.244649	1.645433	-0.837966
O	0.135285	-0.699006	0.011555
O	0.580313	0.645966	-0.204226
H	1.801561	-1.552874	0.257888
C	0.404349	1.400210	1.025701
H	1.005930	0.933291	1.799868
H	-0.655566	1.347896	1.243594
H	0.718566	2.417956	0.808343
S	-2.160077	-0.500863	-0.319662
O	-2.527479	-0.509671	1.077985
O	-2.059494	0.812427	-0.922064

Rotational constants (GHz): 2.9074500 0.7255500 0.6810200

Vibrational harmonic frequencies (cm-1):

32.6544	62.8340	81.6989
115.6673	134.1331	193.3416

199.8390	247.9770	290.5568
320.5826	384.3667	426.6344
518.6529	553.2178	585.1073
658.5918	790.0654	927.0018
961.9372	985.8959	1174.1432
1195.8958	1210.0398	1212.1941
1242.9482	1327.7793	1358.2959
1402.8498	1468.2328	1472.0858
1482.7132	1497.8253	1529.5266
3096.1851	3120.4948	3196.6092
3206.8211	3228.2988	3569.2629

Zero-point correction (Hartree): 0.103572

TS.HOOCH2OCH3O+SO2.HOOCH2OCH3+SO3

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -927.96058045

E(CCSD/Aug-CC-pVTZ) (Hartree): -927.85767062

T1 diagnostic: 0.025173

E(MP2/Aug-CC-pVTZ) (Hartree): -927.84456083

E(PMP2/Aug-CC-pVTZ) (Hartree): -927.84456083

E(PUHF/Aug-CC-pVTZ) (Hartree): -925.81552671

E(ROHF/Aug-CC-pVTZ) (Hartree): -925.81552671

E(RM062X/Aug-CC-pVTZ) (Hartree): -929.08478284

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.949132	0.119415	0.898661
O	-2.653580	-0.219986	-0.219018
O	-2.300388	-1.533258	-0.628251
H	-1.683734	-0.739351	1.507774
H	-2.516242	0.882145	1.433372
O	0.165108	-0.292834	-0.326657
O	-0.679832	0.752242	0.572152
H	-1.405975	-1.404383	-0.987685
C	-0.768804	1.962967	-0.215571
H	-1.307461	1.751886	-1.134786
H	0.257178	2.255452	-0.408745
H	-1.290932	2.695674	0.397869
S	1.913676	-0.432003	-0.262744
O	2.403879	0.917696	-0.508018
O	2.269309	-1.001818	1.021989

Rotational constants (GHz): 2.4824000 0.8173600 0.7084200

Vibrational harmonic frequencies (cm-1):

i710.3637	25.6616	60.4200
75.2708	90.0679	160.8509
195.9730	234.1657	270.9288
309.9092	442.8230	461.0161
493.8151	507.4414	576.2042
589.0632	674.7612	833.5292
963.1036	991.0067	1157.6644
1169.7426	1190.5933	1196.1226
1236.1854	1315.7729	1324.2576
1403.7227	1462.9454	1472.7658
1480.1053	1485.8591	1507.0655
3083.1658	3100.4956	3181.1255
3193.7494	3213.7072	3712.6065

Zero-point correction (Hartree): 0.102161

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*****
(CH3)2COO + CH3OOH
*****

complex
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -458.47162135
E(CCSD/Aug-CC-pVTZ) (Hartree): -458.39469086
  T1 diagnostic: 0.021968
E(MP2/Aug-CC-pVTZ) (Hartree): -458.34791864
E(PMP2/Aug-CC-pVTZ) (Hartree): -458.34791864
E(PUHF/Aug-CC-pVTZ) (Hartree): -456.66236174
E(ROHF/Aug-CC-pVTZ) (Hartree): -456.66236174
E(RM062X/Aug-CC-pVTZ) (Hartree): -459.09791613
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      1.432628      -0.140386      0.014149
  O      1.042814      1.025118     -0.200804
  O      0.269492      1.613280      0.793915
  C      1.149367     -0.799875      1.299228
  C      2.177020     -0.792494     -1.088064
  H      0.066452     -0.845300      1.419694
  H      1.511359     -0.157069      2.103506
  H      1.596810     -1.787979      1.339899
  H      2.322179     -0.107643     -1.917541
  H      1.595704     -1.655247     -1.420169
  H      3.134660     -1.161942     -0.720593
  O     -1.781116      0.880568     -0.761348
  O     -1.440329     -0.483075     -0.545701
  H     -1.150698      1.329647     -0.142648
  C     -2.404868     -1.006524      0.336739
  H     -3.404959     -0.910278     -0.087045
  H     -2.367260     -0.494644      1.302310
  H     -2.156022     -2.061004      0.461776
Rotational constants (GHz):    2.6085200    1.2881900    1.1681600
Vibrational harmonic frequencies (cm-1):
  40.1961      63.4464      81.8951
 114.8956     159.3917     168.0876
 200.7675     217.9056     292.5307
 324.1346     339.3310     373.6232
 472.4396     494.5758     601.8037
 822.2409     860.0857     911.1293
 947.6423     958.3979     992.6361
1089.2881    1105.5561    1125.2447
1181.9859    1230.6007    1315.1857
1383.4860    1407.9212    1445.7819
1456.7100    1462.7052    1473.4751
1474.5119    1489.5476    1518.4977
1553.3657    1673.7313    3035.1068
3066.2647    3075.1481    3107.8772
3128.6395    3133.3357    3137.8490
3187.9960    3189.3472    3276.8320
Zero-point correction (Hartree): 0.146174

TS.H-OOCH3
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -458.45604524
E(CCSD/Aug-CC-pVTZ) (Hartree): -458.37590540
  T1 diagnostic: 0.020635
E(MP2/Aug-CC-pVTZ) (Hartree): -458.33536475

E(PMP2/Aug-CC-pVTZ) (Hartree): -458.33536475
E(PUHF/Aug-CC-pVTZ) (Hartree): -456.62955182
E(ROHF/Aug-CC-pVTZ) (Hartree): -456.62955182

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E(RM062X/Aug-CC-pVTZ) (Hartree): -459.08166108
 Electronic state : 1-A
 Cartesian coordinates (Angs):

O	-0.108363	-1.742264	-0.501099
O	-0.702622	-0.579922	-1.060995
C	-1.165482	0.170986	-0.130624
C	-1.896626	-0.359702	1.051584
C	-1.347258	1.589335	-0.527060
O	0.641241	0.041952	0.898565
H	0.492308	-0.959274	0.358901
O	1.507508	0.758900	0.033329
C	2.747820	0.087328	0.022682
H	2.636043	-0.923935	-0.374838
H	3.174861	0.054109	1.026081
H	3.387717	0.671579	-0.636481
H	-1.812106	0.344572	1.874667
H	-1.540579	-1.339967	1.341935
H	-2.948300	-0.427420	0.758151
H	-2.374721	1.905433	-0.353392
H	-1.059033	1.736262	-1.563396
H	-0.689027	2.181627	0.110475

Rotational constants (GHz): 2.9225300 1.5071200 1.3113000
 Vibrational harmonic frequencies (cm-1):

i775.1718	59.1211	90.2705
111.1931	151.1624	178.6865
234.2912	265.8225	273.8884
334.6618	379.1419	419.9439
503.3089	538.1656	593.4246
799.9622	874.9668	952.7168
959.5646	981.2269	985.4593
1080.6145	1115.2175	1144.8850
1185.4581	1233.1775	1313.8681
1399.9128	1420.0530	1443.2759
1457.5604	1459.1225	1471.5546
1479.9596	1492.4492	1515.1764
1583.4027	1596.1792	1774.3320
3044.2310	3062.9771	3077.3353
3114.4477	3146.1593	3149.4589
3155.3324	3188.3265	3218.4714

Zero-point correction (Hartree): 0.143547

TS.H-OCH3O

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -458.45498076
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -458.37478859
 T1 diagnostic: 0.018602
 E(MP2/Aug-CC-pVTZ) (Hartree): -458.33520777
 E(PMP2/Aug-CC-pVTZ) (Hartree): -458.33520777
 E(PUHF/Aug-CC-pVTZ) (Hartree): -456.62715590
 E(ROHF/Aug-CC-pVTZ) (Hartree): -456.62715590
 E(RM062X/Aug-CC-pVTZ) (Hartree): -459.08162178
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.647268	0.595938	0.048559
O	-1.407228	-0.190169	-0.628540
O	-1.483394	-1.500598	-0.057374
C	-0.509705	0.432538	1.525468
C	-0.541769	1.951658	-0.565581
O	0.919814	-1.549116	-0.139613
O	1.030673	-0.161092	-0.494018
H	-0.269575	-1.683457	-0.115441
C	2.242820	0.293207	0.076552
H	3.053428	-0.306524	-0.332118
H	2.216432	0.183409	1.161327

H	2.363726	1.336144	-0.213104	
H	-0.036184	-0.512457	1.774246	
H	-1.520001	0.416569	1.936742	
H	0.046259	1.267479	1.944437	
H	-1.405655	2.532828	-0.238809	
H	-0.547764	1.875149	-1.648854	
H	0.355947	2.458601	-0.222064	
Rotational constants (GHz):	2.4231800	2.0091400	1.4638900	
Vibrational harmonic frequencies (cm-1):				
i787.4010	80.9859		169.5976	
182.1209	220.4528		236.2060	
247.7243	292.7444		307.9681	
380.3450	394.0737		420.2850	
454.8491	515.2567		579.8966	
720.0742	821.7748		923.8549	
944.6268	960.7157		1012.5098	
1085.5092	1091.1366		1136.8827	
1185.5127	1191.9225		1223.4833	
1315.8726	1406.2288		1415.4777	
1447.4567	1461.0728		1467.7364	
1473.7997	1483.6122		1498.7916	
1515.4669	1552.6562		1922.7976	
3061.5504	3079.2278		3082.2217	
3143.2929	3154.2058		3156.6502	
3159.6002	3186.3466		3192.2159	
Zero-point correction (Hartree):	0.143426			

diMeCOOHOOCH3.pmpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -459.15011373

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.709195	-0.311615	0.002396
C	0.845676	-1.545424	-0.866083
C	1.896789	-0.093100	0.918503
O	0.522124	0.747748	-0.918529
O	-0.403219	-0.373118	0.881891
O	0.540423	1.988128	-0.232512
H	-0.306448	1.981964	0.236323
O	-1.550024	-0.834465	0.178555
C	-2.419038	0.265104	0.013412
H	-2.010234	0.989084	-0.695007
H	-2.630055	0.734256	0.975786
H	-3.336774	-0.157274	-0.392190
H	0.057619	-1.577859	-1.612310
H	0.777481	-2.429914	-0.236358
H	1.813330	-1.526876	-1.362637
H	2.109651	-1.013639	1.457309
H	1.697457	0.701628	1.631265
H	2.757810	0.182498	0.313210
Rotational constants (GHz):	2.6511800	1.8204700	1.4275700
Vibrational harmonic frequencies (cm-1):			
95.4364	112.3583		167.6625
188.2306	215.6646		231.4402
270.9834	289.9448		338.0342
347.7539	390.4398		412.4163
500.2804	595.8403		626.6080
817.5465	881.8759		949.2342
957.8841	993.0082		1026.5608
1054.8927	1113.4705		1179.4467
1202.8596	1235.0349		1250.4031
1314.0231	1413.2144		1417.5851
1423.5457	1454.2759		1478.6081
1484.6534	1488.9503		1494.0801

1506.8428	1523.0032	3043.9030
3089.7502	3092.4890	3115.6511
3150.8898	3167.0871	3171.8814
3182.1044	3184.3568	3777.1516

Zero-point correction (Hartree): 0.149036

HOOCdiMeOCH3O

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -458.46519597
 E(CCSD/Aug-CC-pVTZ) (Hartree): -458.38823894
 T1 diagnostic: 0.015296
 E(MP2/Aug-CC-pVTZ) (Hartree): -458.34507558
 E(PMP2/Aug-CC-pVTZ) (Hartree): -458.34507558
 E(PUHF/Aug-CC-pVTZ) (Hartree): -456.64734939
 E(ROHF/Aug-CC-pVTZ) (Hartree): -456.64734939
 E(UM062X/Aug-CC-pVTZ) (Hartree): -459.09205019
 Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.208504	0.600518	0.022772
O	-1.351518	0.262822	-0.643786
O	-2.007998	-0.842960	-0.033442
C	-0.290144	0.532037	1.528514
C	0.224036	1.930423	-0.550756
O	0.368763	-1.771807	-0.155897
O	0.821277	-0.432898	-0.461928
H	-1.262878	-1.506334	-0.106338
C	2.154172	-0.330083	0.058903
H	2.713292	-1.110709	-0.443532
H	2.134165	-0.509890	1.130793
H	2.543744	0.653022	-0.189994
H	-0.294222	-0.500741	1.864011
H	-1.222915	1.003015	1.830853
H	0.541986	1.070229	1.978188
H	-0.561062	2.650923	-0.331222
H	0.338666	1.849817	-1.629416
H	1.147670	2.282030	-0.099518

Rotational constants (GHz): 2.5428700 2.0611400 1.5334000

Vibrational harmonic frequencies (cm-1):

80.4032	176.9854	209.5200
235.1898	252.3000	278.9500
318.7184	334.8910	362.8815
396.3364	427.5268	483.8023
520.6414	599.6344	631.2384
811.3961	833.7845	880.3081
953.1882	967.4600	1019.6488
1067.1284	1090.5988	1152.7308

1198.5290	1217.6292	1299.6274
1320.5376	1408.7933	1418.3358
1456.3385	1472.8893	1478.7011
1483.7918	1502.6645	1505.6096
1511.9459	1586.9613	3089.1460
3090.4921	3097.4099	3150.5396
3164.8170	3170.7569	3179.4651
3188.4291	3191.5734	3208.3027

Zero-point correction (Hartree): 0.149171

H2COO + CO : M06-2X/aug-cc-pVTZ geometry

CH2O2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -189.16882447
E(CCSD/Aug-CC-pVDZ) (Hartree): -189.14423973
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(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-pVQZ) (Hartree): -189.37915905
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.34290813
E(MP2/Aug-CC-pVQZ) (Hartree): -189.33750951
E(MP3/Aug-CC-pVQZ) (Hartree): -189.33168557
E(PMP2/Aug-CC-pVQZ) (Hartree): -189.33750951
E(PMP3/Aug-CC-pVQZ) (Hartree): -189.33168557
E(PUHF/Aug-CC-pVQZ) (Hartree): -188.64753905
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(UHF/Aug-CC-pVQZ) (Hartree): -188.64753905
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

CH2O

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -114.24389342
E(CCSD/Aug-CC-pVDZ) (Hartree): -114.23209840
E(MP2/Aug-CC-pVDZ) (Hartree): -114.21758993
E(MP3/Aug-CC-pVDZ) (Hartree): -114.22538752
E(RHF/Aug-CC-pVDZ) (Hartree): -113.88577091
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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -114.37217858
E(CCSD/Aug-CC-pVQZ) (Hartree): -114.35371877
E(MP2/Aug-CC-pVQZ) (Hartree): -114.34839120

E(MP3/Aug-CC-pVQZ) (Hartree): -114.34960898
 E(RHF/Aug-CC-pVQZ) (Hartree): -113.92207192
 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

CO2

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -188.18410034
 E(CCSD/Aug-CC-pVDZ) (Hartree): -188.16343511
 E(MP2/Aug-CC-pVDZ) (Hartree): -188.16725957
 E(MP3/Aug-CC-pVDZ) (Hartree): -188.15424654
 E(RHF/Aug-CC-pVDZ) (Hartree): -187.66351659
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -188.34004352
 E(CCSD/Aug-CC-pVTZ) (Hartree): -188.31061741
 E(MP2/Aug-CC-pVTZ) (Hartree): -188.32075380
 E(MP3/Aug-CC-pVTZ) (Hartree): -188.30348611
 E(RHF/Aug-CC-pVTZ) (Hartree): -187.71044324
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -188.38934575
 E(CCSD/Aug-CC-pVQZ) (Hartree): -188.35793327
 E(MP2/Aug-CC-pVQZ) (Hartree): -188.37330559
 E(MP3/Aug-CC-pVQZ) (Hartree): -188.35211986
 E(RHF/Aug-CC-pVQZ) (Hartree): -187.72322281
 E(RM062X/Aug-CC-pVTZ) (Hartree): -188.59420665
 Point group : D*H
 Electronic state : 1-SGG
 Cartesian coordinates (Angs):

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.155211
O	0.000000	0.000000	-1.155211

 Rotational constants (GHz): 0.0000000 11.8381197 11.8381197
 Vibrational harmonic frequencies (cm-1):

694.1973 (PIU)	694.1973 (PIU)	1410.8752 (SGG)
2443.4879 (SGU)		

 Zero-point correction (Hartree): 0.011944

CO

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -113.07259050
 E(CCSD/Aug-CC-pVDZ) (Hartree): -113.06047737
 E(MP2/Aug-CC-pVDZ) (Hartree): -113.05320194
 E(MP3/Aug-CC-pVDZ) (Hartree): -113.05266381
 E(RHF/Aug-CC-pVDZ) (Hartree): -112.75518774
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16172564
 E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14439442
 E(MP2/Aug-CC-pVTZ) (Hartree): -113.14174739
 E(MP3/Aug-CC-pVTZ) (Hartree): -113.13823014
 E(RHF/Aug-CC-pVTZ) (Hartree): -112.78216153
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -113.19013043
 E(CCSD/Aug-CC-pVQZ) (Hartree): -113.17161585
 E(MP2/Aug-CC-pVQZ) (Hartree): -113.17251416
 E(MP3/Aug-CC-pVQZ) (Hartree): -113.16630089
 E(RHF/Aug-CC-pVQZ) (Hartree): -112.78983403
 E(RM062X/Aug-CC-pVTZ) (Hartree): -113.32024079

Point group : C*V
 Electronic state : 1-SG
 Cartesian coordinates (Angs):
 C 0.000000 0.000000 -0.640796
 O 0.000000 0.000000 0.480597
 Rotational constants (GHz): 0.0000000 58.6161395 58.6161395
 Vibrational harmonic frequencies (cm-1):
 2272.1194 (SG)
 Zero-point correction (Hartree): 0.005176

complex

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.24677644
 E(CCSD/Aug-CC-pVDZ) (Hartree): -302.20938166
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.18241322
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.18530763
 E(RHF/Aug-CC-pVDZ) (Hartree): -301.34482508
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49725650
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.44518229
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.43164145
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.42643724
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.41829855
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.57385012
 E(CCSD/Aug-CC-pVQZ) (Hartree): -302.51843479
 E(MP2/Aug-CC-pVQZ) (Hartree): -302.51498054
 E(MP3/Aug-CC-pVQZ) (Hartree): -302.50231217
 E(RHF/Aug-CC-pVQZ) (Hartree): -301.43785785
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.90141597
 E(UM062X/Aug-CC-pVTZ) (Hartree): -302.90141597
 Electronic state : 1-A

Cartesian coordinates (Angs):
 C -1.529267 -0.874975 0.170818
 O -1.381874 0.220442 -0.388152
 O -0.625484 1.150256 0.228700
 H -1.073513 -1.035866 1.139818
 H -2.128596 -1.598548 -0.365144
 C 1.483161 -0.551738 -0.025496
 O 2.442202 0.028638 -0.046373
 Rotational constants (GHz): 11.6729600 2.5595000 2.1913500
 Vibrational harmonic frequencies (cm-1):
 60.7078 94.4003 125.4856
 187.0966 197.7678 539.9184
 694.2125 930.0956 1030.7501
 1259.9429 1437.5029 1637.2139
 2273.8591 3147.4681 3294.8688
 Zero-point correction (Hartree): 0.038527

complex2

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.24625098
 E(CCSD/Aug-CC-pVDZ) (Hartree): -302.20863930
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.18051849
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.18406415
 E(RHF/Aug-CC-pVDZ) (Hartree): -301.34483409
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49650028
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.44424900
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.42952878
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.42503232
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.41817863
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.57308690
 E(CCSD/Aug-CC-pVQZ) (Hartree): -302.51751337
 E(MP2/Aug-CC-pVQZ) (Hartree): -302.51286537
 E(MP3/Aug-CC-pVQZ) (Hartree): -302.50094224
 E(RHF/Aug-CC-pVQZ) (Hartree): -301.43771785

E(RM062X/Aug-CC-pVTZ) (Hartree): -302.90067743
 E(UM062X/Aug-CC-pVTZ) (Hartree): -302.90067743
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.165511	-0.966457	0.210347
O	1.209291	0.107709	-0.405217
O	0.721945	1.208305	0.199571
H	0.761900	-0.977973	1.215902
H	1.551850	-1.827519	-0.317792
C	-1.934320	0.484013	-0.009608
O	-1.643848	-0.603494	-0.057172

 Rotational constants (GHz): 9.5548500 3.4937400 2.7067500
 Vibrational harmonic frequencies (cm-1):

76.6653	112.1001	136.8227
168.8397	191.5138	541.7292
699.2591	930.9904	1039.4100
1261.9474	1437.0229	1635.7654
2225.7897	3144.4975	3292.9087

 Zero-point correction (Hartree): 0.038490

complex3

 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.89833414
 E(UM062X/Aug-CC-pVTZ) (Hartree): -302.89833414
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.415528	-0.240581	0.000399
O	-1.178704	-0.291982	-0.000458
O	-0.487606	0.862757	-0.000239
H	-2.897182	0.730839	0.001285
H	-2.925967	-1.193924	0.000185
C	1.979449	-0.671093	-0.000029
O	2.721263	0.170866	0.000236

 Rotational constants (GHz): 23.1827500 1.8169100 1.6848600
 Vibrational harmonic frequencies (cm-1):

19.9077	37.1816	45.4557
84.9036	151.6417	540.2449
697.8406	925.4125	1031.5767
1260.7128	1435.5300	1636.1170
2265.7034	3140.1588	3290.9552

 Zero-point correction (Hartree): 0.037734

complex4

 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.89832852
 E(UM062X/Aug-CC-pVTZ) (Hartree): -302.89832852
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	2.159975	-0.458199	0.000158
O	0.946436	-0.213100	-0.000256
O	0.549363	1.072494	-0.000041
H	2.859157	0.370504	0.000679
H	2.428398	-1.505737	-0.000044
C	-2.313976	0.409079	0.000087
O	-2.041242	-0.680649	0.000034

 Rotational constants (GHz): 15.1172100 2.2983500 1.9950300
 Vibrational harmonic frequencies (cm-1):

30.0728	45.5093	47.9503
99.1971	132.0165	541.4805
700.6698	925.4950	1032.6602
1261.6245	1436.4296	1636.3485
2255.2642	3140.4743	3291.3010

 Zero-point correction (Hartree): 0.037764

cycadduct

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.30635881
E(CCSD/Aug-CC-pVDZ) (Hartree): -302.27120355
E(MP2/Aug-CC-pVDZ) (Hartree): -302.25465339
E(MP3/Aug-CC-pVDZ) (Hartree): -302.25760581
E(RHF/Aug-CC-pVDZ) (Hartree): -301.40350665
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.56338266
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.51363449
E(MP2/Aug-CC-pVTZ) (Hartree): -302.50956712
E(MP3/Aug-CC-pVTZ) (Hartree): -302.50483217
E(RHF/Aug-CC-pVTZ) (Hartree): -301.47713432
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.64060981
E(CCSD/Aug-CC-pVQZ) (Hartree): -302.58743216
E(MP2/Aug-CC-pVQZ) (Hartree): -302.59311892
E(MP3/Aug-CC-pVQZ) (Hartree): -302.58105220
E(RHF/Aug-CC-pVQZ) (Hartree): -301.49592889
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.97324675
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.595701 0.972101 0.000115
O 1.399685 -0.217141 -0.000286
O 0.205947 -1.045287 0.000182
C -0.604620 0.060966 0.000129
H 0.725968 1.564950 0.902872
H 0.725652 1.565542 -0.902254
O -1.780396 0.096316 -0.000156
Rotational constants (GHz): 13.9910600 5.3690400 3.9804300
Vibrational harmonic frequencies (cm-1):
233.7957 496.6635 506.8130
766.2451 944.6427 994.9479
1020.5686 1061.3723 1154.6463
1178.6450 1317.7486 1483.5131
2001.5359 3107.6475 3172.7747
Zero-point correction (Hartree): 0.044291

TS1

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.22819800
E(CCSD/Aug-CC-pVDZ) (Hartree): -302.18635705
T1 diagnostic: 0.035647
E(MP2/Aug-CC-pVDZ) (Hartree): -302.16771519
E(MP3/Aug-CC-pVDZ) (Hartree): -302.16339550
E(RHF/Aug-CC-pVDZ) (Hartree): -301.30740911
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47989761
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42314635
E(MP2/Aug-CC-pVTZ) (Hartree): -302.41827826
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40560570
E(RHF/Aug-CC-pVTZ) (Hartree): -301.38023608
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.55639032
E(CCSD/Aug-CC-pVQZ) (Hartree): -302.49618754
E(MP2/Aug-CC-pVQZ) (Hartree): -302.50150489
E(MP3/Aug-CC-pVQZ) (Hartree): -302.48131839
E(RHF/Aug-CC-pVQZ) (Hartree): -301.39937506
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.88496137
Electronic state : 1-A
Cartesian coordinates (Angs):
C 1.072898 0.919130 0.160624
O 1.333181 -0.245997 -0.280892
O 0.382667 -1.108089 0.194637
C -0.974194 0.289981 -0.177670
H 0.723382 1.042936 1.177305
H 1.563116 1.731808 -0.363654

O	-2.075688	0.100410	-0.002666	
Rotational constants (GHz):	12.6739800	3.8284400	3.0862300	
Vibrational harmonic frequencies (cm-1):				
i403.4856	145.4057		171.6204	
473.8103	514.1450		623.6806	
817.8737	1007.2722		1098.9254	
1227.8143	1397.6826		1562.3837	
2177.1617	3140.7354		3265.4246	
Zero-point correction (Hartree): 0.040150				

TS3

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-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.22466403
E(CCSD/Aug-CC-pVDZ) (Hartree): -302.18267508
  T1 diagnostic: 0.035125
E(MP2/Aug-CC-pVDZ) (Hartree): -302.16079371
E(MP3/Aug-CC-pVDZ) (Hartree): -302.15919422
E(RHF/Aug-CC-pVDZ) (Hartree): -301.30541568
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47552806
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41880546
E(MP2/Aug-CC-pVTZ) (Hartree): -302.41061461
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40089284
E(RHF/Aug-CC-pVTZ) (Hartree): -301.37749567
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.55171997
E(CCSD/Aug-CC-pVQZ) (Hartree): -302.49157795
E(MP2/Aug-CC-pVQZ) (Hartree): -302.49352925
E(MP3/Aug-CC-pVQZ) (Hartree): -302.47639016
E(RHF/Aug-CC-pVQZ) (Hartree): -301.39643229
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.88138315
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.911008      -0.864178      0.216329
  O      1.057791      0.257328     -0.349909
  O      0.185738      1.182368      0.188378
  H      0.653061     -0.907681      1.265541
  H      1.330051     -1.707086     -0.318365
  C     -1.383313      0.389595     -0.008123
  O     -1.137190     -0.756913     -0.113021
Rotational constants (GHz):   9.7692000   6.3562800   4.1673300
Vibrational harmonic frequencies (cm-1):
  i449.1696      273.6428      342.0431
  454.7687      576.4015      695.8792
  779.3183      982.3963     1100.0234
  1242.6860     1414.2119     1575.2684
  1835.1529     3155.4267     3290.9502
Zero-point correction (Hartree): 0.040365

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TS2

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-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.22554685
E(CCSD/Aug-CC-pVDZ) (Hartree): -302.18696706
  T1 diagnostic: 0.029128
E(MP2/Aug-CC-pVDZ) (Hartree): -302.15691914
E(MP3/Aug-CC-pVDZ) (Hartree): -302.16170210
E(RHF/Aug-CC-pVDZ) (Hartree): -301.32561525
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47421567
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42139280
E(MP2/Aug-CC-pVTZ) (Hartree): -302.40461627
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40178615
E(RHF/Aug-CC-pVTZ) (Hartree): -301.39817008
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.55032644
E(CCSD/Aug-CC-pVQZ) (Hartree): -302.49417843
E(MP2/Aug-CC-pVQZ) (Hartree): -302.48733594
E(MP3/Aug-CC-pVQZ) (Hartree): -302.47715408

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E(RHF/Aug-CC-pVQZ) (Hartree): -301.41733763
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.87640190
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.381716	0.242198	0.000188
O	-1.478746	-0.564794	-0.000003
O	-0.056960	0.161961	0.000014
H	-2.148263	1.307843	0.000337
H	-3.408407	-0.128560	0.000203
C	1.792988	0.446061	-0.000046
O	2.671835	-0.260771	-0.000184

 Rotational constants (GHz): 44.3302800 1.8591600 1.7843300
 Vibrational harmonic frequencies (cm-1):

i714.2823	21.6816	99.4980
246.4734	307.6852	501.9706
513.6730	573.6912	1187.6009
1241.0190	1465.0323	1781.1551
2200.9732	3063.7538	3186.7381

 Zero-point correction (Hartree): 0.037341

TS4

 E(UM062X/Aug-CC-pVTZ) (Hartree):
 -302.83871314
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.153073	0.431660	0.001385
O	-1.521738	-0.591104	-0.001431
O	0.314639	-0.046746	-0.001447
H	-1.646685	1.404193	0.003654
H	-3.250622	0.398829	0.001705
C	1.859352	-0.609484	0.003146
O	2.039553	0.545841	-0.001191

 Rotational constants (GHz): 26.4346800 2.3461700 2.1549200
 Vibrational harmonic frequencies (cm-1):

i593.6268	12.4315	132.1140
218.6436	223.1878	374.6704
384.9825	548.2264	1218.0308
1259.2284	1505.2720	1834.8640
1881.7898	3005.3283	3105.5278

 Zero-point correction (Hartree): 0.035777

TS5

 E(UM062X/Aug-CC-pVTZ) (Hartree): -302.83729130
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.494820	-0.757776	0.156727
O	-1.301247	0.443294	-0.171762
O	0.009629	0.885345	0.148632
H	-2.488072	-1.056936	-0.190545
H	-0.258910	-1.194861	0.158933
C	0.924528	-0.397193	-0.097532
O	2.062710	-0.180937	-0.017315

 Rotational constants (GHz): 17.6062300 3.6150600 3.0462200
 Vibrational harmonic frequencies (cm-1):

i1471.6054	219.0709	307.2003
330.7085	484.1211	665.1050
759.4919	792.3484	924.0189
1318.9380	1333.9825	1482.1131
1849.0118	2004.9870	3096.1332

 Zero-point correction (Hartree): 0.035465

TS.CH2O2+CO.DIO+CO.a

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.46513538
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41202830
  T1 diagnostic: 0.039443
E(MP2/Aug-CC-pVTZ) (Hartree): -302.39497524
E(MP3/Aug-CC-pVTZ) (Hartree): -302.39030890
E(RHF/Aug-CC-pVTZ) (Hartree): -301.38724391
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86530405
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -1.363001      0.805514      0.257817
  O      -1.514779     -0.133149     -0.565676
  O      -0.731486     -1.024361      0.292033
  H      -1.100237      1.791385     -0.127168
  H      -1.580710      0.649844      1.308792
  C      1.564175      0.548046     -0.038909
  O      2.430502     -0.162814     -0.038241
Rotational constants (GHz): 12.1982200 2.4758300 2.2210000
Vibrational harmonic frequencies (cm-1):
  i831.0831      50.4358      86.2317
    92.6751      134.2026      186.8474
   790.4808      820.8481     1103.9318
  1228.6605      1453.0286     1615.1048
  2279.3848      3087.8902     3228.3178
Zero-point correction (Hartree): 0.036811

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TS.CH2O2+CO.DIO+CO.b

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.46415663
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41121113
  T1 diagnostic: 0.040697
E(MP2/Aug-CC-pVTZ) (Hartree): -302.39307582
E(MP3/Aug-CC-pVTZ) (Hartree): -302.38893679
E(RHF/Aug-CC-pVTZ) (Hartree): -301.38782104
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.86262544
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      1.244348      0.948748     -0.013555
  O      0.924586     -0.204067      0.367844
  O      2.128407     -0.776566     -0.238548
  H      0.463664      1.575987     -0.447631
  H      2.248058      1.318900      0.161925
  C     -2.012270      0.386257     -0.123070
  O     -2.816016     -0.382482      0.008886
Rotational constants (GHz): 15.3983200 1.7494000 1.6056400
Vibrational harmonic frequencies (cm-1):
  i833.8722      i10.5293      42.8461
    71.1871      110.0077      137.5493
   787.0238      804.2291     1106.5496
  1233.7763      1451.1224     1610.8812
  2284.7601      3085.1262     3232.2395
Zero-point correction (Hartree): 0.036353

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TS.CH2O2+CO.13Hshift

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.44140013
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.38955971
  T1 diagnostic: 0.025853
E(MP2/Aug-CC-pVTZ) (Hartree): -302.37882243
E(MP3/Aug-CC-pVTZ) (Hartree): -302.37319480
E(RHF/Aug-CC-pVTZ) (Hartree): -301.35794625
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.84440793
Electronic state : 1-A
Cartesian coordinates (Angs):

```

C	-2.409085	0.481198	0.000038
O	-1.763176	-0.581818	-0.000016
O	-0.412414	-0.083496	-0.000037
H	-1.185071	1.024636	0.000023
H	-3.495248	0.341684	0.000063
C	2.278771	0.625105	-0.000038
O	2.858365	-0.335204	0.000042
Rotational constants (GHz): 31.7400500 1.5382500 1.4671400			
Vibrational harmonic frequencies (cm-1):			
i1782.4416	20.2378	28.0585	
63.9561	70.2613	116.9795	
757.7251	768.9806	939.2074	
1194.1162	1294.3572	1614.3325	
2141.7942	2269.2044	3091.6389	
Zero-point correction (Hartree): 0.032739			

H2COO + CO : CCSD/aug-cc-pVDZ geometry

CH2O2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33147697
E(CCSD/Aug-CC-pVDZ) (Hartree): -189.15545224
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29636880
T1 diagnostic: 0.044900
E(MP2/Aug-CC-pVDZ) (Hartree): -189.13438383
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28360198
E(MP3/Aug-CC-pVDZ) (Hartree): -189.13747360
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28208686
E(PMP2/Aug-CC-pVDZ) (Hartree): -189.13438383
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.28360198
E(PMP3/Aug-CC-pVDZ) (Hartree): -189.13747360
E(PMP3/Aug-CC-pVTZ) (Hartree): -189.28208686
E(PUHF/Aug-CC-pVDZ) (Hartree): -188.59607603
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.63335164
E(QCI,CC/Aug-CC-pVDZ) (Hartree): -189.14561050
E(UHF/Aug-CC-pVDZ) (Hartree): -188.59607603
E(UHF/Aug-CC-pVTZ) (Hartree): -188.63335164
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
C 1.069459 -0.188054 0.000000
O 0.000000 0.479397 0.000000
O -1.177102 -0.228277 0.000000
H 1.010168 -1.281230 0.000000
H 1.989891 0.400602 0.000000
Rotational constants (GHz): 75.7402299 12.3942904 10.6512908

CO

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16214974
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14421444
T1 diagnostic: 0.018919
E(MP2/Aug-CC-pVDZ) (Hartree): -113.05477963
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14240606
E(MP3/Aug-CC-pVDZ) (Hartree): -113.05286655
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13742420
E(QCI,CC/Aug-CC-pVDZ) (Hartree): -113.06131286
E(RHF/Aug-CC-pVDZ) (Hartree): -112.75326947
E(RHF/Aug-CC-pVTZ) (Hartree): -112.77962050
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
C 0.000000 0.000000 -0.651726
O 0.000000 0.000000 0.488794
Rotational constants (GHz): 0.0000000 56.6666521 56.6666521

complex

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49845497
E(CCSD/Aug-CC-pVDZ) (Hartree): -302.21177709
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.44505089
T1 diagnostic: 0.037043
E(MP2/Aug-CC-pVDZ) (Hartree): -302.18425750
E(MP2/Aug-CC-pVTZ) (Hartree): -302.43121612
E(MP3/Aug-CC-pVDZ) (Hartree): -302.18566010
E(MP3/Aug-CC-pVTZ) (Hartree): -302.42437425
E(PMP2/Aug-CC-pVDZ) (Hartree): -302.18425750
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.43121612

E(PMP3/Aug-CC-pVDZ) (Hartree): -302.18566010
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.42437425
 E(PUHF/Aug-CC-pVDZ) (Hartree): -301.34274658
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.41496905
 E(UHF/Aug-CC-pVDZ) (Hartree): -301.34274658
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.41496905
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.549334	-0.908255	0.184039
O	-1.434979	0.192489	-0.416423
O	-0.729406	1.180727	0.235319
H	-1.111376	-1.019125	1.180101
H	-2.102722	-1.681182	-0.355243
C	1.583888	-0.556387	-0.015344
O	2.540232	0.062803	-0.048525

 Rotational constants (GHz): 11.0199296 2.3519135 2.0254719

complex2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49774256
 E(CCSD/Aug-CC-pVDZ) (Hartree): -302.22642712
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.44423533
 T1 diagnostic: 0.037684
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.19793903
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.42922286
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.19995763
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.42317563
 E(PMP2/Aug-CC-pVDZ) (Hartree): -302.19793903
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.42922286
 E(PMP3/Aug-CC-pVDZ) (Hartree): -302.19995763
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.42317563
 E(PUHF/Aug-CC-pVDZ) (Hartree): -301.35878367
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.41515822
 E(QCI,CC/Aug-CC-pVDZ) (Hartree): -302.21099223
 E(UHF/Aug-CC-pVDZ) (Hartree): -301.35878367
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.41515822
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.201422	-0.989937	0.213232
O	1.273037	0.093134	-0.425995
O	0.812084	1.221687	0.214098
H	0.801723	-0.980008	1.231718
H	1.563443	-1.873453	-0.318287
C	-2.069232	0.500811	-0.029307
O	-1.729909	-0.591295	-0.040227

 Rotational constants (GHz): 9.2773464 3.1189679 2.4669883

TS.cycadduct.CO

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.48085465
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42237137
 T1 diagnostic: 0.035156
 E(CCSD/CC-pVDZ) (Hartree): -302.12148519
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.16981503
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.41833030
 E(MP2/CC-pVDZ) (Hartree): -302.09898464
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.16352012
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40350460
 E(MP3/CC-pVDZ) (Hartree): -302.09555090
 E(PMP2/Aug-CC-pVDZ) (Hartree): -302.16981503
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.41833030
 E(PMP2/CC-pVDZ) (Hartree): -302.09898464
 E(PMP3/Aug-CC-pVDZ) (Hartree): -302.16352012
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.40350460

E(PMP3/CC-pVDZ) (Hartree): -302.09555090
 E(PUHF/Aug-CC-pVDZ) (Hartree): -301.30344443
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.37490448
 E(PUHF/CC-pVDZ) (Hartree): -301.28050848
 E(QCI,CC/Aug-CC-pVDZ) (Hartree): -302.18789176
 E(UHF/Aug-CC-pVDZ) (Hartree): -301.30344443
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.37490448
 E(UHF/CC-pVDZ) (Hartree): -301.28050848
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.993573	0.950552	0.169978
O	1.362840	-0.200713	-0.300609
O	0.443330	-1.134984	0.199228
C	-0.964953	0.256330	-0.151578
H	0.702057	1.032082	1.221451
H	1.402750	1.817612	-0.362514
O	-2.090736	0.074323	-0.019787

 Rotational constants (GHz): 12.1846349 3.8097835 3.0539023

TS.CH2O2+CO.CH2O+CO2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47640781
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41812564
 T1 diagnostic: 0.033925
 E(CCSD/CC-pVDZ) (Hartree): -302.11692991
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.16244065
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.41033279
 E(MP2/CC-pVDZ) (Hartree): -302.09080770
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.15962899
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.39924326
 E(MP3/CC-pVDZ) (Hartree): -302.09074019
 E(PMP2/Aug-CC-pVDZ) (Hartree): -302.16244065
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.41033279
 E(PMP2/CC-pVDZ) (Hartree): -302.09080770
 E(PMP3/Aug-CC-pVDZ) (Hartree): -302.15962899
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.39924326
 E(PMP3/CC-pVDZ) (Hartree): -302.09074019
 E(PUHF/Aug-CC-pVDZ) (Hartree): -301.30160040
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.37251541
 E(PUHF/CC-pVDZ) (Hartree): -301.27888738
 E(QCI,CC/Aug-CC-pVDZ) (Hartree): -302.18418326
 E(UHF/Aug-CC-pVDZ) (Hartree): -301.30160039
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.37251541
 E(UHF/CC-pVDZ) (Hartree): -301.27888738
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.881832	-0.876511	0.225820
O	1.081235	0.251403	-0.357290
O	0.178198	1.197198	0.193741
H	0.640272	-0.900063	1.291058
H	1.280219	-1.745008	-0.307823
C	-1.374705	0.406017	-0.015992
O	-1.129840	-0.765097	-0.116727

 Rotational constants (GHz): 9.4980567 6.3816360 4.1440475

TS.CH2O2+CO.CH2O+CO2.b

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47473824
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42135562
 T1 diagnostic: 0.028167
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.15794818
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40281268
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.16292413

E(MP3/Aug-CC-pVTZ) (Hartree): -302.40010674
 E(PMP2/Aug-CC-pVDZ) (Hartree): -302.15794818
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.40281268
 E(PMP3/Aug-CC-pVDZ) (Hartree): -302.16292413
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.40010674
 E(PUHF/Aug-CC-pVDZ) (Hartree): -301.32728228
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.39810593
 E(QCI,CC/Aug-CC-pVDZ) (Hartree): -302.18990509
 E(UHF/Aug-CC-pVDZ) (Hartree): -301.32728228
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.39810593
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-2.436626	0.322722	0.000192
O	-1.608793	-0.586581	0.000006
O	-0.081128	0.053256	0.000006
H	-2.099065	1.371111	0.000326
H	-3.506231	0.055584	0.000218
C	1.839054	0.381598	-0.000055
O	2.838762	-0.173251	-0.000183

 Rotational constants (GHz): 46.5253140 1.6920487 1.6326712

H2COO + CO : CCSD(T)/cc-pVDZ geometry

CH2O2

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33141982
E(CCSD(T)/CC-pVDZ) (Hartree): -189.12070178
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29442918
  T1 diagnostic: 0.046668
E(CCSD/CC-pVDZ) (Hartree): -189.09679677
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28473513
E(MP2/CC-pVDZ) (Hartree): -189.07405177
E(MP3/Aug-CC-pVTZ) (Hartree): -189.27976108
E(MP3/CC-pVDZ) (Hartree): -189.07673926
E(RHF/Aug-CC-pVTZ) (Hartree): -188.62534250
E(RHF/CC-pVDZ) (Hartree): -188.55949956
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -1.084122      0.204478      -0.000011
  O       0.018976     -0.472625     -0.000009
  O      1.172072      0.206902      0.000008
  H      -1.029103      1.299632     -0.000003
  H     -1.994555     -0.400716      0.000074
Rotational constants (GHz):  76.6189086  12.3339247  10.6237409

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CO

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16203397
E(CCSD(T)/CC-pVDZ) (Hartree): -113.05497596
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14396338
  T1 diagnostic: 0.019156
E(CCSD/CC-pVDZ) (Hartree): -113.04388038
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14234392
E(MP2/CC-pVDZ) (Hartree): -113.03679403
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13702997
E(MP3/CC-pVDZ) (Hartree): -113.03468155
E(RHF/Aug-CC-pVTZ) (Hartree): -112.77885093
E(RHF/CC-pVDZ) (Hartree): -112.74712015
Point group : C*v
Electronic state : 1-SG
Cartesian coordinates (Angs):
  C      0.000000      0.000000     -0.654117
  O      0.000000      0.000000      0.490588
Rotational constants (GHz):  0.0000000  56.2530561  56.2530561

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TS.cycadduct.CO

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.48074836
E(CCSD(T)/CC-pVDZ) (Hartree): -302.15917590
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42101283
  T1 diagnostic: 0.035829
E(CCSD/CC-pVDZ) (Hartree): -302.12108970
E(MP2/Aug-CC-pVTZ) (Hartree): -302.41923257
E(MP2/CC-pVDZ) (Hartree): -302.10054713
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40200318
E(MP3/CC-pVDZ) (Hartree): -302.09496344
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.41923257
E(PMP2/CC-pVDZ) (Hartree): -302.10054713
E(PMP3/Aug-CC-pVTZ) (Hartree): -302.40200318
E(PMP3/CC-pVDZ) (Hartree): -302.09496344
E(PUHF/Aug-CC-pVTZ) (Hartree): -301.36916111
E(PUHF/CC-pVDZ) (Hartree): -301.27502028
E(UHF/Aug-CC-pVTZ) (Hartree): -301.36916111

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E(UHF/CC-pVDZ) (Hartree): -301.27502027
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.979104	0.970433	0.158268
O	1.371789	-0.207431	-0.268194
O	0.443209	-1.132773	0.193451
C	-0.963065	0.210788	-0.210366
O	-2.090132	0.091885	0.008736
H	0.650504	1.082436	1.199896
H	1.454341	1.816784	-0.359251

 Rotational constants (GHz): 12.1474503 3.8136914 3.0473431

TS.CH2O2+CO.CH2O+CO2.b

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47484984
 E(CCSD(T)/CC-pVDZ) (Hartree): -302.15487233
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42093348
 T1 diagnostic: 0.028596
 E(CCSD/CC-pVDZ) (Hartree): -302.12267546
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40404273
 E(MP2/CC-pVDZ) (Hartree): -302.08996938
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.39964004
 E(MP3/CC-pVDZ) (Hartree): -302.09565511
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.39498225
 E(RHF/CC-pVDZ) (Hartree): -301.30490895
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

C	-2.030881	1.360420	0.000000
O	-1.622531	0.192329	0.000000
O	0.000000	0.157315	0.000000
H	-1.306215	2.193404	0.000000
H	-3.123139	1.531455	0.000000
C	1.832823	-0.455141	0.000000
O	2.324744	-1.494211	0.000000

 Rotational constants (GHz): 43.2538856 1.7646922 1.6955176

H2COO + CO : CCSD(T)/cc-pVTZ geometry

CH2O2

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33192074
E(CCSD(T)/CC-pVTZ) (Hartree): -189.31371537
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29580625
  T1 diagnostic: 0.045421
E(CCSD/CC-pVTZ) (Hartree): -189.27920564
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28551465
E(MP2/CC-pVTZ) (Hartree): -189.26658440
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28166406
E(MP3/CC-pVTZ) (Hartree): -189.26420066
E(RHF/Aug-CC-pVTZ) (Hartree): -188.62913631
E(RHF/CC-pVTZ) (Hartree): -188.62428411
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -1.075338      0.204936      -0.000043
  O       0.011540     -0.469692      0.000031
  O       1.169058      0.203674     -0.000016
  H      -1.014727      1.285246      0.000148
  H      -1.978031     -0.386717     -0.000008
Rotational constants (GHz):  77.9403672  12.4665241  10.7474713

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CO

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16219351
E(CCSD(T)/CC-pVTZ) (Hartree): -113.15557861
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14441054
  T1 diagnostic: 0.018652
E(CCSD/CC-pVTZ) (Hartree): -113.13843768
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14238990
E(MP2/CC-pVTZ) (Hartree): -113.13563613
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13778019
E(MP3/CC-pVTZ) (Hartree): -113.13139527
E(RHF/Aug-CC-pVTZ) (Hartree): -112.78040481
E(RHF/CC-pVTZ) (Hartree): -112.77932153
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
  C      0.000000      0.000000     -0.649009
  O      0.000000      0.000000      0.486757
Rotational constants (GHz):  0.0000000  57.1420587  57.1420587

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TS.cycadduct.CO

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.48117854
E(CCSD(T)/CC-pVTZ) (Hartree): -302.45513171
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42244380
  T1 diagnostic: 0.035467
E(CCSD/CC-pVTZ) (Hartree): -302.39903564
E(MP2/Aug-CC-pVTZ) (Hartree): -302.41955601
E(MP2/CC-pVTZ) (Hartree): -302.39357531
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40388924
E(MP3/CC-pVTZ) (Hartree): -302.37945024
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.41955601
E(PMP2/CC-pVTZ) (Hartree): -302.39357531
E(PMP3/Aug-CC-pVTZ) (Hartree): -302.40388924
E(PMP3/CC-pVTZ) (Hartree): -302.37945024
E(PUHF/Aug-CC-pVTZ) (Hartree): -301.37368165
E(PUHF/CC-pVTZ) (Hartree): -301.36863546
E(UHF/Aug-CC-pVTZ) (Hartree): -301.37368165

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E(UHF/CC-pVTZ) (Hartree): -301.36863546
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.012767	0.954742	0.160206
O	1.360901	-0.223243	-0.264886
O	0.415551	-1.123152	0.192178
C	-0.967282	0.234138	-0.221462
O	-2.080118	0.099024	0.015413
H	0.653251	1.068434	1.175157
H	1.503161	1.777248	-0.349258

 Rotational constants (GHz): 12.3432148 3.8283668 3.0676772

TS.CH2O2+CO.CH2O+CO2.b

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47538478
 E(CCSD(T)/CC-pVTZ) (Hartree): -302.44776642
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42178907
 T1 diagnostic: 0.028193
 E(CCSD/CC-pVTZ) (Hartree): -302.39749272
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40540221
 E(MP2/CC-pVTZ) (Hartree): -302.37915072
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40118526
 E(MP3/CC-pVTZ) (Hartree): -302.37655876
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.39626004
 E(RHF/CC-pVTZ) (Hartree): -301.39162113
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

C	-2.026748	1.317994	0.000000
O	-1.607780	0.162365	0.000000
O	0.000000	0.151975	0.000000
H	-1.315898	2.143559	0.000000
H	-3.106661	1.472665	0.000000
C	1.810412	-0.419914	0.000000
O	2.322851	-1.439927	0.000000

 Rotational constants (GHz): 44.1144899 1.8075861 1.7364359

H2COO + CO : CCSD(T)/aug-cc-pVTZ geometry

CH2O2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -189.17129107
E(CCSD/Aug-CC-pVDZ) (Hartree): -189.14509680
T1 diagnostic: 0.047719
E(MP2/Aug-CC-pVDZ) (Hartree): -189.12505837
E(MP3/Aug-CC-pVDZ) (Hartree): -189.12714619
E(RHF/Aug-CC-pVDZ) (Hartree): -188.58395976
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -189.38009561
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.34205539
T1 diagnostic: 0.044434
E(MP2/Aug-CC-pVQZ) (Hartree): -189.33755183
E(MP3/Aug-CC-pVQZ) (Hartree): -189.32956866
E(RHF/Aug-CC-pVQZ) (Hartree): -188.64231985
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33199173
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29611748
T1 diagnostic: 0.045563
E(MP2/Aug-CC-pVTZ) (Hartree):
-189.28503503
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28183830
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63042120
Electronic state : 1-A
Cartesian coordinates (Angs):
C 1.073568 0.207856 0.000101
O -0.004617 -0.472307 -0.000264
O -1.174016 0.202658 0.000176
H 1.006933 1.289309 -0.000821
H 1.980722 -0.379249 0.000917
Rotational constants (GHz): 77.3283027 12.4254041 10.7052462

CO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -113.07378573
E(CCSD/Aug-CC-pVDZ) (Hartree): -113.06126817
T1 diagnostic: 0.019434
E(MP2/Aug-CC-pVDZ) (Hartree): -113.05455671
E(MP3/Aug-CC-pVDZ) (Hartree): -113.05297492
E(RHF/Aug-CC-pVDZ) (Hartree): -112.75387261
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -113.19033247
E(CCSD/Aug-CC-pVQZ) (Hartree): -113.17134951
T1 diagnostic: 0.018281
E(MP2/Aug-CC-pVQZ) (Hartree): -113.17292092
E(MP3/Aug-CC-pVQZ) (Hartree): -113.16556714
E(RHF/Aug-CC-pVQZ) (Hartree): -112.78789386
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16219357
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14440254
T1 diagnostic: 0.018666
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14239311
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13776379
E(RHF/Aug-CC-pVTZ) (Hartree): -112.78036562
Point group : C*v
Electronic state : 1-SG
Cartesian coordinates (Angs):
C 0.000000 0.000000 -0.649153
O 0.000000 0.000000 0.486865
Rotational constants (GHz): 0.0000000 57.1166665 57.1166665

TS.cycadduct.CO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -302.23118309

E(CCSD/Aug-CC-pVDZ) (Hartree): -302.18753587
 T1 diagnostic: 0.037456
 E(MP2/Aug-CC-pVDZ) (Hartree): -302.17008179
 E(MP3/Aug-CC-pVDZ) (Hartree): -302.16323417
 E(RHF/Aug-CC-pVDZ) (Hartree): -301.30225752
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -302.55706719
 E(CCSD/Aug-CC-pVQZ) (Hartree): -302.49486986
 T1 diagnostic: 0.034992
 E(MP2/Aug-CC-pVQZ) (Hartree): -302.50175619
 E(MP3/Aug-CC-pVQZ) (Hartree): -302.47876804
 E(RHF/Aug-CC-pVQZ) (Hartree): -301.39293933
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.48122505
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42249762
 T1 diagnostic: 0.035780
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.41909697
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40368790
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.41909697
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.40368790
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.37409567
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.37409567
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.998730	0.959004	0.164073
O	1.366591	-0.209357	-0.270317
O	0.433930	-1.130678	0.191690
C	-0.971604	0.233143	-0.214577
O	-2.084896	0.089242	0.011994
H	0.646925	1.058651	1.184423
H	1.465314	1.794813	-0.348335

 Rotational constants (GHz): 12.2456217 3.8140031 3.0539861

TS.CH2O2+CO.CH2O+CO2.b

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47542296
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42188422
 T1 diagnostic: 0.028196
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40513260
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40118402
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.39675591
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

C	-1.877621	1.537476	0.000000
O	-1.601810	0.338640	0.000000
O	0.000000	0.134414	0.000000
H	-1.071939	2.272322	0.000000
H	-2.932468	1.817621	0.000000
C	1.754741	-0.619689	0.000000
O	2.194521	-1.672637	0.000000

 Rotational constants (GHz): 44.9560641 1.7804244 1.7125992

H2COO + CO : BLYP/aug-cc-pVTZ geometry

CH2O2

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -189.64498430
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33152999
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29547188
T1 diagnostic: 0.046225
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28344650
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28059891
E(RHF/Aug-CC-pVTZ) (Hartree): -188.62996036
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
C 1.087947 -0.203412 0.000000
O 0.000000 0.466854 0.000000
O -1.196008 -0.202672 0.000000
H 1.048056 -1.291229 0.000000
H 1.992327 0.398250 0.000000
Rotational constants (GHz): 78.3725400 12.0305200 10.4295400
Vibrational harmonic frequencies (cm-1):
513.3341 (A') 640.1053 (A'') 856.9476 (A'')
892.2496 (A') 1196.8308 (A') 1324.5425 (A')
1456.0247 (A') 3044.9763 (A') 3194.0738 (A')
Zero-point correction (Hartree): 0.029887

CO

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E(RB-LYP/Aug-CC-pVTZ) (Hartree): -113.34573425
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.16218794
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.14434671
T1 diagnostic: 0.018754
E(MP2/Aug-CC-pVTZ) (Hartree): -113.14240719
E(MP3/Aug-CC-pVTZ) (Hartree): -113.13765538
E(RHF/Aug-CC-pVTZ) (Hartree): -112.78011548
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
C 0.000000 0.000000 -0.650051
O 0.000000 0.000000 0.487538
Rotational constants (GHz): 0.0000000 56.9590376 56.9590376
Vibrational harmonic frequencies (cm-1):
2109.9405 (SG)
Zero-point correction (Hartree): 0.004807

TS1

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -302.98109282
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.51300904
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.46858013
T1 diagnostic: 0.032909
E(MP2/Aug-CC-pVTZ) (Hartree): -302.43580787
E(MP3/Aug-CC-pVTZ) (Hartree): -302.45478005
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.46157172
E(PMP3/Aug-CC-pVTZ) (Hartree): -302.48036263
E(PUHF/Aug-CC-pVTZ) (Hartree): -301.52427166
E(UHF/Aug-CC-pVTZ) (Hartree): -301.49831257
Electronic state : 1-A
Cartesian coordinates (Angs):
C 1.064825 0.955201 0.157928
O 1.383066 -0.242988 -0.251060
O 0.383294 -1.137274 0.187438

C	-0.993084	0.252426	-0.244680	
H	0.671054	1.104169	1.159953	
H	1.598542	1.755667	-0.355628	
O	-2.103866	0.117063	0.028145	
Rotational constants (GHz):	12.1108000	3.7066600	2.9736700	
Vibrational harmonic frequencies (cm-1):				
i332.6790	123.7555		184.5250	
446.2290	478.8528		585.7822	
749.1668	882.6519		975.7127	
1156.2026	1263.5465		1462.6474	
1991.6354	3035.4933		3155.8292	
Zero-point correction (Hartree):	0.037572			

TS2

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -302.97936291
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47596624
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42224327
 T1 diagnostic: 0.030207
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40602814
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40125106
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.39552263
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	2.465710	0.192032	0.000287
O	1.452560	-0.537350	-0.000189
O	0.092054	0.222108	-0.000326
H	2.358988	1.280420	0.000533
H	3.436775	-0.312656	0.000444
C	-1.867852	0.468079	-0.000147
O	-2.717478	-0.300811	0.000288

Rotational constants (GHz): 43.3793800 1.7801000 1.7099300
 Vibrational harmonic frequencies (cm-1):

i552.7148	8.0193	93.9265
226.6574	238.5395	477.1219
505.5622	573.3334	1009.3695
1178.2809	1381.2044	1528.7977
2030.0220	2982.9307	3109.5449

Zero-point correction (Hartree): 0.034955

TS3

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -302.95338304
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47409360
 E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41540456
 T1 diagnostic: 0.039442
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40396862
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.39382143
 E(PMP2/Aug-CC-pVTZ) (Hartree): -302.40396862
 E(PMP3/Aug-CC-pVTZ) (Hartree): -302.39382143
 E(PUHF/Aug-CC-pVTZ) (Hartree): -301.37282628
 E(UHF/Aug-CC-pVTZ) (Hartree): -301.37282628
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.639290	0.708025	0.090825
O	1.311252	-0.522849	-0.210288
O	-0.163746	-0.784819	0.253650
H	2.689571	0.937177	-0.077156
H	0.935439	1.387485	0.557614
C	-0.941244	0.272493	-0.223208
O	-2.124167	0.281697	-0.004132

Rotational constants (GHz): 18.1903000 3.2854300 2.8689400
 Vibrational harmonic frequencies (cm-1):

i1137.6557	85.1511	244.8571
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300.8226	419.1743	488.8423
555.3426	591.6991	695.2320
1091.5142	1147.3416	1401.3364
1694.6576	3062.2743	3196.0893

Zero-point correction (Hartree): 0.034114

TS5

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -302.97848656

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.189260	-0.816396	0.218336
O	1.118679	0.329088	-0.354804
O	0.071886	1.180931	0.185391
H	0.833294	-0.956443	1.234527
H	1.741112	-1.569720	-0.341043
C	-1.469879	0.327348	0.028241
O	-1.301902	-0.827462	-0.127205

Rotational constants (GHz): 9.6514100 5.1004000 3.5745200

Vibrational harmonic frequencies (cm-1):

i500.4457	136.6534	269.4465
349.5985	459.7693	579.7615
623.4061	774.6471	893.5262
1175.1934	1311.8319	1464.0531
1802.0060	3053.0960	3191.3636

Zero-point correction (Hartree): 0.036643

TS6

E(UB-LYP/Aug-CC-pVTZ) (Hartree): -303.02720842

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.51300904

E(CCSD/Aug-CC-pVTZ) (Hartree): -302.46858013

T1 diagnostic: 0.032909

E(MP2/Aug-CC-pVTZ) (Hartree): -302.43580787

E(MP3/Aug-CC-pVTZ) (Hartree): -302.45478005

E(PMP2/Aug-CC-pVTZ) (Hartree): -302.46157172

E(PMP3/Aug-CC-pVTZ) (Hartree): -302.48036263

E(PUHF/Aug-CC-pVTZ) (Hartree): -301.52427166

E(UHF/Aug-CC-pVTZ) (Hartree): -301.49831257

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.774794	-0.834132	0.104914
O	-1.622796	0.197578	-0.146052
O	0.267397	1.251972	0.078750
C	0.582879	-0.002190	0.009338
H	-0.788868	-1.177729	1.158379
H	-0.856296	-1.677247	-0.597404
O	1.704981	-0.465436	-0.088509

Rotational constants (GHz): 11.5003200 4.8190600 3.5092500

Vibrational harmonic frequencies (cm-1):

i224.9305	190.7534	408.3136
456.7599	554.1462	597.4790
908.4638	1037.0152	1104.0603
1139.9723	1187.6887	1413.5068
1616.9538	2860.1005	2960.9031

Zero-point correction (Hartree): 0.037444

syn-(CH3)CHOO + CO : M06-2X/aug-cc-pVTZ geometry

acetaldehyde

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -153.59813072
E(CCSD/Aug-CC-pVTZ) (Hartree): -153.57311884
  T1 diagnostic: 0.014211
E(MP2/Aug-CC-pVTZ) (Hartree): -153.55397918
E(MP3/Aug-CC-pVTZ) (Hartree): -153.56815916
E(RHF/Aug-CC-pVTZ) (Hartree): -152.97761192
E(RM062X/Aug-CC-pVTZ) (Hartree): -153.82079216
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.233166      0.397901      -0.000065
  C     -1.162576     -0.147806     -0.000051
  H      0.314150      1.502135      0.000064
  H     -1.696388      0.225942     -0.875547
  H     -1.147971     -1.233967     -0.002113
  H     -1.694426      0.222324      0.878216
  O      1.225137     -0.277125      0.000009
Rotational constants (GHz):   57.3542800   10.2552900   9.1901100
Vibrational harmonic frequencies (cm-1):
  158.0587      513.5312      776.0791
  901.0798      1138.4769      1145.9905
  1380.5265      1430.3358      1464.9250
  1474.8121      1866.0660      2943.3840
  3063.0340      3125.2985      3180.1712
Zero-point correction (Hartree): 0.055956

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CH3CHO2s

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.59065163
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.54908137
  T1 diagnostic: 0.035105
E(MP2/Aug-CC-pVTZ) (Hartree): -228.52797754
E(MP3/Aug-CC-pVTZ) (Hartree): -228.53654107
E(RHF/Aug-CC-pVTZ) (Hartree): -227.70288046
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.90272701
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.471417      0.702258      0.000009
  O     -0.770016      0.584690      0.000003
  O     -1.269067     -0.677676      0.000002
  C      1.348246     -0.472175     -0.000015
  H      0.807438      1.732755      0.000032
  H      1.095834     -1.089417     -0.866318
  H      1.095907     -1.089400      0.866323
  H      2.395505     -0.190547     -0.000045
Rotational constants (GHz):   17.8489200   7.2532700   5.3217500
Vibrational harmonic frequencies (cm-1):
  216.1377      321.0560      471.8577
  683.1234      781.1765      928.5602
  998.9468      1068.7093      1112.1445
  1361.4043      1410.3805      1440.5155
  1464.6823      1647.0242      3053.7590
  3098.7604      3190.5974      3206.8169
Zero-point correction (Hartree): 0.060270

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complex.s

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.75687884
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.69731891

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T1 diagnostic: 0.030831
E(MP2/Aug-CC-pVTZ) (Hartree): -341.67451039
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67892475
E(RHF/Aug-CC-pVTZ) (Hartree): -340.48517946
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.22785766
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.392062	0.136616	0.660063
O	-0.733537	-0.910919	0.506205
O	-0.234636	-1.145981	-0.737466
C	1.781386	0.643604	0.231691
O	2.768604	0.178156	-0.024105
C	-1.652063	1.052719	-0.453661
H	-1.750473	0.272948	1.674157
H	-2.117679	0.482994	-1.262263
H	-0.691396	1.385771	-0.852967
H	-2.267470	1.890609	-0.144553

Rotational constants (GHz): 5.9454600 1.9038900 1.6961400
Vibrational harmonic frequencies (cm-1):

42.3170	74.7489	93.3883
122.5346	169.6676	203.1082
323.9852	468.6427	681.4055
784.1955	926.7680	999.0795
1073.5177	1112.4471	1360.3914
1409.6460	1442.0671	1464.4178
1650.3588	2274.8253	3057.0037
3106.9516	3189.1033	3205.3672

Zero-point correction (Hartree): 0.066604

complex2.s

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.75637391
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.69669362
T1 diagnostic: 0.031239
E(MP2/Aug-CC-pVTZ) (Hartree): -341.67306751
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67799797
E(RHF/Aug-CC-pVTZ) (Hartree): -340.48511642
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.22747212
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.160601	-0.277889	0.645372
O	-0.633097	0.851688	0.618969
O	-0.265890	1.331031	-0.599021
C	2.303973	0.063670	-0.333541
O	1.823700	-0.718569	0.317808
C	-1.411535	-1.038951	-0.582249
H	-1.417901	-0.608301	1.645305
H	-0.462090	-1.184595	-1.102000
H	-2.010943	-0.416214	-1.251877
H	-1.897793	-1.985070	-0.370963

Rotational constants (GHz): 5.2085600 2.4783800 2.0880400
Vibrational harmonic frequencies (cm-1):

55.2120	85.5224	112.5029
124.7396	167.4686	206.3842
323.6338	474.6944	682.2609
780.6659	929.7492	998.6832
1072.5025	1113.2319	1363.4265
1412.2295	1443.8772	1465.1158
1649.8865	2235.7408	3058.8307
3109.2127	3190.2107	3205.1720

Zero-point correction (Hartree): 0.066661

TS1

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73109078
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66640622
 T1 diagnostic: 0.031097
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.65169091
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.64884675
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.43730728
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20201990
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.020173	0.141580	-0.582667
O	0.832438	-1.092644	-0.281144
O	-0.163689	-1.173797	0.665804
C	-1.127549	0.185478	-0.355220
O	-2.169926	0.507570	-0.047521
C	1.215827	1.227754	0.419783
H	1.492192	0.252190	-1.556763
H	0.704703	1.000021	1.348388
H	0.870335	2.178362	0.019274
H	2.291484	1.311521	0.600613

 Rotational constants (GHz): 5.5224600 3.1194900 2.3817600
 Vibrational harmonic frequencies (cm-1):

i430.7917	99.6704	162.1903
211.2633	326.7388	371.3768
514.0661	546.1853	680.5180
880.5570	930.1537	1005.2088
1093.1493	1166.7532	1347.3218
1398.1310	1458.5267	1487.2532
1553.1970	2158.8255	3056.1139
3138.9605	3157.4155	3202.6238

 Zero-point correction (Hartree): 0.068222

TS2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73488744
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67275594
 T1 diagnostic: 0.026220
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.64816237
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.65289583
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.45918940
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20310311
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.948134	-0.464005	-0.000902
O	0.879696	-1.056914	0.000318
O	-0.367013	-0.054475	0.002399
H	2.836289	-1.103631	-0.001963
C	2.075040	1.007066	-0.000806
C	-2.105361	0.514913	0.001782
O	-3.079488	-0.057274	-0.002320
H	1.540321	1.394834	0.867783
H	1.535444	1.395528	-0.866027
H	3.115504	1.314726	-0.003412

 Rotational constants (GHz): 11.4578300 1.4864800 1.3262400
 Vibrational harmonic frequencies (cm-1):

i738.1047	8.3428	91.1112
142.6595	187.3392	239.0073
428.5666	464.0819	525.0138
643.7831	758.3001	991.4700
1097.8903	1135.6069	1364.2357
1414.4945	1448.3716	1459.9781
1751.6858	2183.0719	3070.8063
3087.7892	3127.4781	3192.7811

 Zero-point correction (Hartree): 0.065643

TS3

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73004014
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66536899
T1 diagnostic: 0.030913
E(MP2/Aug-CC-pVTZ) (Hartree): -341.64740278
E(MP3/Aug-CC-pVTZ) (Hartree): -341.64751898
E(RHF/Aug-CC-pVTZ) (Hartree): -340.43776181
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20194172
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.902719 0.163103 0.569366
O -0.079908 1.126965 0.458010
O 0.804705 0.946319 -0.602309
C 1.524537 -0.568701 -0.292153
O 0.815081 -1.132202 0.463782
C -1.574019 -0.523180 -0.555763
H -1.324193 0.111581 1.569348
H -1.676519 -1.581740 -0.328848
H -1.026863 -0.387470 -1.481578
H -2.578245 -0.098363 -0.643484
Rotational constants (GHz): 5.5308900 3.9781900 3.0494000
Vibrational harmonic frequencies (cm-1):
i487.6286 196.7055 209.6287
243.0676 281.3047 409.5622
499.5786 643.3528 733.7425
833.5577 924.1333 962.2732
1076.1726 1175.1246 1361.8858
1403.2474 1452.0928 1476.9341
1581.9222 1823.9778 3058.6288
3145.6909 3181.6163 3209.0227
Zero-point correction (Hartree): 0.068079

TS.CI+CO.vinylperformate.s

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.69421354
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.62948041
T1 diagnostic: 0.022193
E(MP2/Aug-CC-pVTZ) (Hartree): -341.61934305
E(MP3/Aug-CC-pVTZ) (Hartree): -341.61650507
E(RHF/Aug-CC-pVTZ) (Hartree): -340.39657120
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.17066898
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.551636 -0.041868 -0.320482
O -0.794892 -1.070539 -0.245931
O 0.307488 -0.884919 0.649775
C -1.292267 1.171271 0.296144
H -2.335272 -0.179858 -1.061028
H -0.830268 1.131361 1.275383
H -1.975380 1.979580 0.087116
H -0.062164 1.112886 -0.315203
C 1.226082 0.411894 -0.311724
O 2.351156 0.293990 -0.150082
Rotational constants (GHz): 7.0865100 2.6406500 2.1598700
Vibrational harmonic frequencies (cm-1):
i1457.1768 117.4440 214.7502
278.4612 361.5890 464.2967
492.3690 577.6796 675.7510
758.8783 870.0344 920.5153
1020.2879 1059.9793 1242.1443
1262.4395 1357.7982 1452.5226
1519.5239 1648.3624 2106.6749
3161.9700 3175.1331 3272.7530

Zero-point correction (Hartree): 0.063815

TS.CI+CO.VHP+CO.s.a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.72623640

E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66429468

T1 diagnostic: 0.025658

E(MP2/Aug-CC-pVTZ) (Hartree): -341.65070965

E(MP3/Aug-CC-pVTZ) (Hartree): -341.64909586

E(RHF/Aug-CC-pVTZ) (Hartree): -340.43847698

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.19873237

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.405171	0.214832	0.692256
O	-0.710497	-0.857235	0.560207
O	-0.340667	-1.007549	-0.768497
C	-1.647122	0.962327	-0.465309
H	-1.867575	0.304409	1.668619
H	-0.757621	1.377280	-0.938262
H	-2.493914	1.632370	-0.441289
H	-1.359994	-0.135680	-1.135188
C	1.840045	0.672716	0.196940
O	2.770238	0.080080	-0.003860

Rotational constants (GHz): 6.4725600 1.8727700 1.7355400

Vibrational harmonic frequencies (cm-1):

i1608.2907	38.0053	73.3327
83.8850	105.8248	168.0615
500.0166	540.5203	713.0225
755.6129	870.2325	969.1126
992.2740	1056.3454	1218.4965
1318.8716	1352.0013	1493.1300
1591.9282	1876.9683	2274.5263
3114.9972	3203.9988	3238.1726

Zero-point correction (Hartree): 0.062762

TS.CI+CO.VHP+CO.s.b

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.72590895

E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66402750

T1 diagnostic: 0.025644

E(MP2/Aug-CC-pVTZ) (Hartree): -341.65038542

E(MP3/Aug-CC-pVTZ) (Hartree): -341.64881633

E(RHF/Aug-CC-pVTZ) (Hartree): -340.43847355

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.19831760

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.398617	-0.316392	0.673942
O	-0.732537	0.780816	0.662718
O	-0.410669	1.113635	-0.645133
C	-1.658618	-0.915780	-0.563225
H	-1.524243	-0.728815	1.668362
H	-2.266547	-0.326563	-1.248912
H	-1.891586	-1.970215	-0.551696
H	-0.649651	-0.205965	-1.022726
C	1.882191	-0.627093	0.208214
O	2.815993	-0.096058	-0.112412

Rotational constants (GHz): 6.3656200 1.8194800 1.6933200

Vibrational harmonic frequencies (cm-1):

i1618.0376	30.6892	59.2351
73.5363	114.7110	144.2608
498.7612	537.7361	709.1485
755.0966	868.7378	968.3281
990.2773	1054.2005	1219.3508

1321.6920	1354.4470	1491.7562
1594.2030	1878.4469	2275.0724
3113.9727	3205.7714	3241.4837

Zero-point correction (Hartree): 0.062652

cycadduct

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.81476931
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.75697384
 T1 diagnostic: 0.016337
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.74353328
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.74780511
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.53365343
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.28896474
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.654982	-0.035408	0.490460
O	0.430982	1.328833	0.067159
O	-0.936627	1.010234	-0.304932
C	-0.771550	-0.295624	0.073896
O	-1.554806	-1.173334	0.009998
C	1.731956	-0.746396	-0.285921
H	0.799278	-0.082024	1.569915
H	2.705623	-0.319304	-0.054252
H	1.548680	-0.659959	-1.354989
H	1.737697	-1.800008	-0.009080

Rotational constants (GHz): 5.7964500 3.9656300 2.5916400
 Vibrational harmonic frequencies (cm-1):

172.2797	198.0938	217.1654
405.3602	506.6196	693.4193
758.6322	855.4274	919.5095
996.1907	1070.2421	1098.1534
1148.6194	1184.3268	1303.4587
1366.0546	1411.2842	1487.5829
1500.0507	1992.5707	3077.9634
3109.0550	3156.5771	3165.0207

Zero-point correction (Hartree): 0.072431

vinylperformate.cpc

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.79530476
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.73757019
 T1 diagnostic: 0.016426
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.72208617
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.72814984
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.51934642
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.27459485
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.747787	0.870687	0.306108
C	1.438865	-0.194934	-0.406082
H	2.034574	-0.582091	-1.221693
O	0.349320	-1.013297	-0.277312
O	-0.481514	-0.581195	0.774579
C	-1.472577	0.226946	0.312424
O	-1.618064	0.603990	-0.798932
H	2.652878	1.403357	0.063506
H	1.136328	1.228133	1.118795
H	-2.106164	0.458424	1.178018

Rotational constants (GHz): 7.1080400 2.7928000 2.5997100
 Vibrational harmonic frequencies (cm-1):

64.6082	171.9031	240.1102
350.0053	401.2520	641.9158

713.2294	830.1985	888.4798
932.7436	987.6739	990.5347
1040.3646	1124.7274	1179.2811
1328.7597	1388.1932	1432.7115
1737.4644	1898.4355	3079.1963
3207.6753	3227.9760	3301.0059
Zero-point correction (Hartree): 0.070984		

anti-(CH3)CHOO + CO : M06-2X/aug-cc-pVTZ geometry

CH3CHO2a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.58475566
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.54410234
T1 diagnostic: 0.034770
E(MP2/Aug-CC-pVTZ) (Hartree): -228.52150932
E(MP3/Aug-CC-pVTZ) (Hartree): -228.53160723
E(RHF/Aug-CC-pVTZ) (Hartree): -227.70219095
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.89710572
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.370039 0.399961 -0.000016
O 0.566461 -0.412338 -0.000016
O 1.839494 0.076289 0.000014
H -0.096126 1.452422 -0.000002
C -1.762517 -0.093270 0.000005
H -2.286708 0.287505 0.878116
H -1.782679 -1.179231 0.000001
H -2.286786 0.287547 -0.878036
Rotational constants (GHz): 50.1860100 4.4801100 4.2196900
Vibrational harmonic frequencies (cm-1):
167.6530 268.3336 329.1509
566.4967 883.5010 901.6039
986.5165 1094.5197 1168.6110
1362.4820 1421.7142 1467.7291
1469.4722 1672.6658 3064.4357
3120.6224 3166.0899 3183.3546
Zero-point correction (Hartree): 0.059904

complex.a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.75215619
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.69338286
T1 diagnostic: 0.030255
E(MP2/Aug-CC-pVTZ) (Hartree): -341.66930856
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67515979
E(RHF/Aug-CC-pVTZ) (Hartree): -340.48507872
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.22355143
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.191949 -0.090839 0.371214
O -0.743945 0.816347 -0.345841
O 0.328706 1.521372 0.125446
C 1.735245 -0.797330 0.028102
O 2.822586 -0.547032 -0.084120
H -0.713441 -0.230394 1.336120
C -2.328392 -0.902509 -0.108726
H -2.642155 -0.577326 -1.096305
H -3.160014 -0.821352 0.592901
H -2.032601 -1.952355 -0.140125
Rotational constants (GHz): 6.1751200 1.7730600 1.4359400
Vibrational harmonic frequencies (cm-1):
59.3411 75.6299 113.1795
136.3976 188.7722 215.5747
290.4236 335.6697 568.6965
886.1763 905.3877 991.6786
1097.0238 1171.5511 1362.9053
1420.5632 1467.4570 1469.6080

1674.8721	2271.9509	3066.4779
3124.2159	3178.0520	3189.6646

Zero-point correction (Hartree): 0.066662

complex2.a

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.75164223
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.69267979
  T1 diagnostic: 0.030804
E(MP2/Aug-CC-pVTZ) (Hartree): -341.66761820
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67405459
E(RHF/Aug-CC-pVTZ) (Hartree): -340.48489784
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.22318446
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.988422      0.027051      0.387440
  O      0.512562      0.894183     -0.361079
  O     -0.534900      1.632341      0.113626
  C     -2.326764     -0.436546     -0.075734
  O     -1.495076     -1.194972     -0.010619
  H      0.552086     -0.049897      1.379814
  C      2.088800     -0.829633     -0.096173
  H      2.947999     -0.738707      0.569763
  H      2.370755     -0.557052     -1.108937
  H      1.765725     -1.871990     -0.069262
Rotational constants (GHz):   5.0367800   2.5388000   1.7802200
Vibrational harmonic frequencies (cm-1):
  76.0102      77.9597      122.1824
 129.3305      192.3175      209.0676
 292.1113      334.1020      568.8504
 883.5563      905.3820      991.6113
1096.4357      1171.7715     1362.3858
1419.8483      1466.6446     1468.7697
1674.3698      2217.8443     3064.9431
3123.1796      3171.9125     3184.5291
Zero-point correction (Hartree): 0.066534

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TS1

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73454805
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67050005
  T1 diagnostic: 0.029962
E(MP2/Aug-CC-pVTZ) (Hartree): -341.65539075
E(MP3/Aug-CC-pVTZ) (Hartree): -341.65332295
E(RHF/Aug-CC-pVTZ) (Hartree): -340.44403797
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20618974
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.906792     -0.064660      0.362305
  O     -0.592291      1.025002     -0.231152
  O      0.719500      1.317469      0.075384
  C      1.154920     -0.553776     -0.125072
  O      2.235441     -0.887337     -0.029352
  H     -0.537580     -0.211158      1.371148
  C     -2.105889     -0.794231     -0.111512
  H     -1.924837     -1.865112     -0.034594
  H     -2.335485     -0.531896     -1.139992
  H     -2.956732     -0.556901      0.530070
Rotational constants (GHz):   6.4411600   2.5612200   1.9210600
Vibrational harmonic frequencies (cm-1):
  i381.3126      127.0442      130.4338
 169.4695      309.9567      341.7115
 503.9413      551.1095      629.7838

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906.6803	976.6422	1051.0006
1102.0109	1179.0906	1343.5720
1408.9773	1455.2730	1476.5892
1561.6473	2149.9602	3069.0473
3138.4358	3176.5061	3189.2905

Zero-point correction (Hartree): 0.068227

TS2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73260164
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67185047
 T1 diagnostic: 0.024793
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.64611551
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.65263160
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.46346336
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20096959
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.681946	0.318210	0.000007
O	0.784041	-0.503922	-0.000013
O	-0.646072	0.212192	-0.000017
C	3.107749	-0.086427	0.000008
H	1.394896	1.373289	0.000024
C	-2.494028	0.435099	-0.000007
O	-3.333909	-0.319910	0.000018
H	3.208231	-1.167155	-0.000012
H	3.595204	0.342861	-0.876988
H	3.595194	0.342827	0.877027

Rotational constants (GHz): 33.5888500 1.1054600 1.0773100
 Vibrational harmonic frequencies (cm-1):

i685.9363	23.2725	81.7746
155.7279	171.0296	200.5014
372.2963	388.0874	495.3961
635.5462	846.5316	936.4102
1147.6610	1162.8406	1369.9421
1409.0737	1463.3833	1471.4368
1775.9777	2187.2869	3066.1396
3108.7385	3127.1422	3190.3920

Zero-point correction (Hartree): 0.065581

TS3

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73272952
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66895383
 T1 diagnostic: 0.029220
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.65075566
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.65167285
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.44417283
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20500312
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.763692	-0.155547	0.392475
O	-0.104286	-1.002604	-0.287038
O	1.232455	-0.998451	0.095785
C	1.703684	0.663196	-0.078139
O	0.697096	1.279884	-0.062596
H	-0.455176	0.015423	1.417059
C	-2.088291	0.262998	-0.105493
H	-2.205451	0.002625	-1.153181
H	-2.182028	1.340520	0.024513
H	-2.869658	-0.213078	0.489346

Rotational constants (GHz): 6.8692000 3.3423600 2.4018300
 Vibrational harmonic frequencies (cm-1):

i434.5624	139.6240	182.8040
261.5076	341.4017	400.7846
479.1016	565.7595	730.0943
896.6434	956.3519	1027.0140
1097.7811	1179.2241	1356.7276
1412.5509	1454.1145	1472.6799
1585.4364	1820.7990	3071.3952
3138.0942	3183.2590	3201.8638
Zero-point correction (Hartree): 0.068243		

 (CH3)2COO + CO : M06-2X/aug-cc-pVTZ geometry

acetone

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -192.85153613
 E(CCSD/Aug-CC-pVTZ) (Hartree): -192.81857618
 E(MP2/Aug-CC-pVTZ) (Hartree): -192.78982195
 E(MP3/Aug-CC-pVTZ) (Hartree): -192.81362366
 E(RHF/Aug-CC-pVTZ) (Hartree): -192.03701526
 E(RM062X/Aug-CC-pVTZ) (Hartree): -193.13991726
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.000000	0.186099	-0.000021
C	-1.282076	-0.610551	0.000091
C	1.282076	-0.610551	-0.000085
H	-1.312804	-1.262084	0.874754
H	-2.137213	0.058342	0.004163
H	-1.316285	-1.255050	-0.879697
H	1.316259	-1.255045	0.879708
H	1.312831	-1.262088	-0.874744
H	2.137213	0.058342	-0.004135
O	0.000000	1.390949	0.000006

 Rotational constants (GHz): 10.2316100 8.6059200 4.9588800
 Vibrational harmonic frequencies (cm-1):

95.1339	170.9459	382.9875
492.7777	542.5314	807.9496
888.6039	903.2776	1089.2539
1126.2399	1251.8822	1388.9976
1399.9050	1464.3461	1473.4335
1475.5148	1497.0976	1846.9652
3059.5221	3064.9262	3123.8815
3130.7454	3173.4062	3174.3610

 Zero-point correction (Hartree): 0.084348

diMeCO2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.84500760
 E(CCSD/Aug-CC-pVTZ) (Hartree): -267.79627238
 E(MP2/Aug-CC-pVTZ) (Hartree): -267.76526815
 E(MP3/Aug-CC-pVTZ) (Hartree): -267.78404314
 E(PMP2/Aug-CC-pVTZ) (Hartree): -267.76526815
 E(PMP3/Aug-CC-pVTZ) (Hartree): -267.78404314
 E(PUHF/Aug-CC-pVTZ) (Hartree): -266.76658097
 E(RHF/Aug-CC-pVTZ) (Hartree): -266.76658097
 E(UHF/Aug-CC-pVTZ) (Hartree): -266.76658097
 E(UM062X/Aug-CC-pVTZ) (Hartree): -268.22346276
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.371023	0.018452	-0.000027
O	0.558598	-0.817600	-0.000024
O	1.839016	-0.328582	0.000021
C	-0.054287	1.456041	-0.000027
C	-1.752455	-0.524533	0.000001
H	0.577833	1.668419	-0.865255
H	0.577302	1.668413	0.865633
H	-0.955030	2.062056	-0.000193
H	-1.739071	-1.610392	-0.000038
H	-2.287778	-0.159336	-0.877977
H	-2.287572	-0.159472	0.878172

 Rotational constants (GHz): 8.9511500 4.3735300 3.0465400
 Vibrational harmonic frequencies (cm-1):

161.9172	207.9974	291.0495
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329.8759	366.4004	493.5235
609.7892	827.3699	925.0897
952.8532	989.4152	1085.5994
1102.0385	1316.0865	1393.9572
1411.7332	1442.1692	1466.9932
1474.3193	1486.7857	1653.9848
3059.3253	3065.3016	3110.0182
3121.6808	3182.2182	3183.6520

Zero-point correction (Hartree): 0.088190

complex

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.01187029
 E(CCSD/Aug-CC-pVTZ) (Hartree): -380.94504876
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.91252799
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.92700124
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.54891318
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.54906019

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.149231	-0.053940	-0.013746
O	-0.407776	0.368941	-0.927489
O	0.396818	1.441569	-0.631298
C	1.966528	-0.702477	0.435366
O	3.012365	-0.518733	0.075882
C	-1.163057	0.625708	1.291550
C	-1.987480	-1.235039	-0.335935
H	-1.375940	1.683815	1.123875
H	-0.151384	0.598956	1.700568
H	-1.879694	0.169968	1.967827
H	-1.824233	-1.556357	-1.360257
H	-3.039684	-0.990056	-0.183533
H	-1.740875	-2.046062	0.351357

Rotational constants (GHz): 3.7961900 1.4450400 1.3410800

Vibrational harmonic frequencies (cm-1):

38.6579	59.7353	97.4089
111.8654	159.9681	172.1511
208.3930	305.7455	332.7381
367.6709	490.0304	608.7787
827.5229	921.1482	953.2652
989.9776	1086.5708	1101.2127
1315.9596	1389.3096	1410.2373
1443.6252	1466.1657	1473.3438
1488.4770	1654.4295	2274.7605
3063.5955	3066.9137	3120.0173
3123.9174	3182.5553	3183.6060

Zero-point correction (Hartree): 0.094521

complex2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.01152836
 E(CCSD/Aug-CC-pVTZ) (Hartree): -380.94455129
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.91134901
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.92622055
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.54867740
 E(RM062X/Aug-CC-pVTZ) (Hartree):
 -381.54890628

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.980670	0.006986	-0.013618
O	0.293496	0.596365	-0.876352
O	-0.522073	1.609335	-0.439715
C	-2.552700	-0.357220	0.045732
O	-1.751688	-1.134512	0.194929

C	0.929356	0.447829	1.390551
C	1.821545	-1.117003	-0.493251
H	-0.102257	0.380653	1.739908
H	1.171635	1.512505	1.422512
H	1.599069	-0.137473	2.012980
H	1.721060	-1.242735	-1.567109
H	1.514594	-2.032129	0.016577
H	2.864792	-0.933886	-0.232245
Rotational constants (GHz):	3.3926800	1.9059600	1.6427200
Vibrational harmonic frequencies (cm-1):			
59.1243	61.3661		92.3757
117.8186	167.7235		171.5232
199.7005	307.9952		331.6783
368.5286	494.6232		609.6287
827.5766	924.3951		956.8021
990.9894	1087.5606		1102.4418
1316.7144	1392.8529		1411.5036
1444.1485	1466.4611		1474.2328
1487.5516	1654.6154		2230.7637
3063.7432	3066.9981		3120.6826
3123.5662	3182.7306		3184.7428
Zero-point correction (Hartree): 0.094528			

TS3

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98671091
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.91452997
E(MP2/Aug-CC-pVTZ) (Hartree): -380.88715097
E(MP3/Aug-CC-pVTZ) (Hartree): -380.89703142
E(RHF/Aug-CC-pVTZ) (Hartree): -379.50130738
E(RM062X/Aug-CC-pVTZ) (Hartree): -381.52425547
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.738737      -0.119485      0.125442
O       0.037154     -1.134892      0.109974
O      1.336797     -0.834757      0.539905
C      1.847775      0.423762     -0.439668
O      0.881783      0.899513     -0.928890
C     -0.720375      0.894968      1.211285
C     -1.918619     -0.226565     -0.769772
H      0.215453      0.873870      1.756667
H     -1.552596      0.665875      1.882981
H     -0.888999      1.883517      0.791002
H     -1.821734     -1.076715     -1.437667
H     -1.990223      0.692701     -1.351055
H     -2.828030     -0.314241     -0.173556
Rotational constants (GHz):    4.1848300    2.3904200    2.2636800
Vibrational harmonic frequencies (cm-1):
i474.6043      119.3306      141.2789
204.8394      229.5648      268.8083
345.3016      373.2497      419.3519
517.3860      587.6461      758.5133
820.2477      932.5113      948.3288
979.9733     1079.8150     1096.2327
1320.9659     1405.2823     1424.5843
1447.9167     1459.6098     1467.0424
1490.0664     1572.9056     1812.8448
3060.0730     3072.9367     3136.0217
3147.3347     3187.4062     3211.8331
Zero-point correction (Hartree): 0.095772

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TS1

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-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98589879

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E(CCSD/Aug-CC-pVTZ) (Hartree): -380.91345062
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.88940187
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.89607559
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.49833562
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.52246557
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.834285	-0.011363	0.015652
O	-0.411606	1.200982	-0.131475
O	0.879667	1.293936	0.353052
C	1.253592	-0.401325	-0.446217
O	2.313542	-0.809817	-0.406266
C	-0.718040	-0.733729	1.321765
C	-1.941709	-0.393857	-0.904750
H	0.112596	-0.355268	1.906086
H	-0.608373	-1.803258	1.156586
H	-1.654692	-0.571522	1.863897
H	-1.808441	-1.431266	-1.208161
H	-1.955022	0.247248	-1.780745
H	-2.896238	-0.325087	-0.378851

 Rotational constants (GHz): 3.9645600 2.0316600 1.8443700
 Vibrational harmonic frequencies (cm-1):

i406.4489	99.1091	126.0294
131.4155	215.6138	310.7653
334.5987	374.5019	403.4066
521.1084	564.6074	643.1536
824.6352	941.5663	967.0248
1018.9488	1087.9019	1106.6917
1308.4142	1404.5169	1416.4673
1437.3825	1463.1274	1473.3945
1497.4947	1544.1879	2136.0367
3052.1722	3068.0891	3135.5022
3141.0091	3184.4628	3203.5087

 Zero-point correction (Hartree): 0.095995

cycadduct

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.06650528
 E(CCSD/Aug-CC-pVTZ) (Hartree): -381.00036218
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.97833114
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.99082093
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.58858607
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.60472083
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.556762	-0.005715	0.000000
O	0.156527	1.395298	-0.000003
O	-1.245472	1.016324	-0.000001
C	-0.922557	-0.312568	0.000000
O	-1.654155	-1.237817	0.000000
C	1.280233	-0.383366	-1.271315
C	1.280229	-0.383361	1.271319
H	2.268784	0.074325	-1.279875
H	0.724741	-0.048647	-2.144869
H	1.394881	-1.465872	-1.315118
H	0.724739	-0.048629	2.144869
H	2.268783	0.074320	1.279876
H	1.394866	-1.465868	1.315132

 Rotational constants (GHz): 3.7243300 2.6322700 2.3183700
 Vibrational harmonic frequencies (cm-1):

155.9987	166.0264	195.7561
214.0823	291.2145	342.7893
429.9035	553.3390	689.1080
744.9574	789.2040	898.4221

955.3506	997.9882	1009.3775
1019.0454	1126.6926	1243.5569
1249.2388	1326.3992	1403.6163
1417.9484	1475.1178	1483.7487
1500.8154	1509.4540	1985.7814
3071.8944	3074.4241	3148.2999
3153.0751	3160.6814	3161.7405

Zero-point correction (Hartree): 0.100114

TS2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.99175271
 E(CCSD/Aug-CC-pVTZ) (Hartree): -380.92147336
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.88822525
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.90187656
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.52129467
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.52542561
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.483561	-0.059222	0.000000
O	-0.484977	-0.774946	-0.000019
O	0.881643	0.058391	-0.000032
C	-2.819304	-0.725346	0.000015
C	-1.383398	1.421935	0.000009
C	2.674385	0.356204	-0.000014
O	3.540893	-0.370847	0.000032
H	-2.716300	-1.805569	0.000008
H	-3.378097	-0.396158	0.877447
H	-3.378119	-0.396150	-0.877400
H	-0.795560	1.725272	-0.866566
H	-0.795538	1.725260	0.866574
H	-2.365595	1.885140	0.000025

Rotational constants (GHz): 8.3981500 1.0398600 0.9357900
 Vibrational harmonic frequencies (cm-1):

i720.6046	17.0740	79.9015
128.5233	152.3577	188.2859
193.7402	365.9557	398.5666
421.5027	510.8324	519.6736
679.3218	829.2520	894.6145
979.4739	1076.4151	1114.6782
1284.6715	1384.1879	1398.1710
1451.8227	1462.3115	1476.4967
1477.2151	1731.6484	2170.9688
3068.1143	3076.6646	3130.3577
3138.7896	3184.1106	
3190.8773		

Zero-point correction (Hartree): 0.093807

TS.CI+CO.VPF

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.95029779
 E(CCSD/Aug-CC-pVTZ) (Hartree): -380.87766974
 T1 diagnostic: 0.020370
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.85842943
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.86496815
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.45768970
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.49192088
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.153918	0.059998	0.107052
O	-0.419079	-0.997809	0.141816
O	0.866167	-0.790361	0.736639
C	-0.680447	1.305587	0.514640

C	-2.460875	-0.160813	-0.570661
H	-0.035935	1.313369	1.385266
H	-1.349012	2.142581	0.379109
H	0.380980	1.114925	-0.321036
C	1.603641	0.303163	-0.465059
O	2.744328	0.163002	-0.477963
H	-2.445808	-1.075946	-1.155276
H	-3.234825	-0.233752	0.194765
H	-2.697132	0.692556	-1.202596
Rotational constants (GHz):	5.9581800	1.6163700	1.4729400
Vibrational harmonic frequencies (cm-1):			
i1456.2351	62.1322		89.1082
181.3649	276.0556		294.3731
362.6131	403.3755		488.8866
555.5781	621.2217		680.0192
747.6381	876.6673		911.8717
966.5024	1015.1752		1054.0221
1087.7277	1275.9697		1361.1504
1416.0250	1448.5634		1475.8318
1500.2831	1557.0564		1614.1807
2061.2952	3077.6477		3147.9679
3159.8595	3185.9990		3262.7633
Zero-point correction (Hartree):	0.091625		

TS.CI+CO.DIO+CO.a

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -380.97702360
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -380.90957292
T1 diagnostic: 0.030086
E(MP2/Aug-CC-pVTZ) (Hartree): -380.87332321
E(MP3/Aug-CC-pVTZ) (Hartree): -380.88985190
E(RHF/Aug-CC-pVTZ) (Hartree): -379.51723198
E(RM062X/Aug-CC-pVTZ) (Hartree): -381.51107530
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.141518	0.162326	0.165208
O	0.332891	-0.383026	0.981793
O	-0.147158	-1.341222	-0.035274
C	2.215986	-0.577878	-0.544355
C	1.050635	1.634790	0.031978
C	-2.229140	0.568431	-0.342277
O	-3.118610	-0.086302	-0.148704
H	2.211629	-1.623196	-0.261344
H	3.167241	-0.089649	-0.314181
H	2.064077	-0.497786	-1.621561
H	0.720890	2.071396	0.973379
H	0.252225	1.816080	-0.694821
H	1.972965	2.081550	-0.327322
Rotational constants (GHz):	4.5278900	1.4303600	1.2197100
Vibrational harmonic frequencies (cm-1):			
i514.2959	28.2571		72.8332
85.8278	95.4682		155.8402
171.7669	237.1059		352.7255
397.4628	413.4243		492.7540
796.1138	838.2402		898.8272
975.8699	1061.6626		1082.9886
1276.0117	1379.0957		1402.1368
1440.5507	1447.9867		1465.7275
1480.3280	1602.6035		2273.5364
3052.6477	3058.2070		3117.4190
3129.7470	3185.2528		3212.1011
Zero-point correction (Hartree):	0.092677		

TS.CI+CO.DIO+CO.b

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.97599026

E(CCSD/Aug-CC-pVTZ) (Hartree): -380.90868806

T1 diagnostic: 0.030720

E(MP2/Aug-CC-pVTZ) (Hartree): -380.87227708

E(MP3/Aug-CC-pVTZ) (Hartree): -380.88865791

E(RHF/Aug-CC-pVTZ) (Hartree): -379.51678686

E(RM062X/Aug-CC-pVTZ) (Hartree): -381.50911516

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.785971	0.294145	-0.000839
O	0.636580	-0.717200	-0.755815
O	1.875283	-1.355286	-0.268396
C	0.906651	0.211289	1.476857
C	0.733272	1.619609	-0.662093
C	-2.316511	0.168384	0.122910
O	-3.232263	-0.452897	-0.049498
H	0.815968	-0.816204	1.808157
H	0.138618	0.857435	1.910630
H	1.877094	0.600225	1.787883
H	0.085203	1.571922	-1.534860
H	1.749555	1.814747	-1.021030
H	0.440462	2.414383	0.017871

Rotational constants (GHz): 3.5424500 1.3278300 1.2241200

Vibrational harmonic frequencies (cm-1):

i520.7112	25.4431	37.8886
65.0009	80.2520	115.2332
159.6798	242.8049	344.3765
395.8226	411.0499	492.9626
795.7536	834.1940	901.0347
975.4922	1063.3577	1082.0650
1276.9203	1381.6697	1401.5095
1441.6518	1449.7870	1464.1665
1481.8563	1604.8243	2283.9048
3051.7744	3055.6105	3117.6231
3131.9840	3186.1843	3206.1748

Zero-point correction (Hartree): 0.092398

TS.CI+CO.VHP+CO.a

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98194628

E(CCSD/Aug-CC-pVTZ) (Hartree): -380.91247572

T1 diagnostic: 0.023271

E(MP2/Aug-CC-pVTZ) (Hartree): -380.88922363

E(MP3/Aug-CC-pVTZ) (Hartree): -380.89730500

E(RHF/Aug-CC-pVTZ) (Hartree): -379.50176229

E(RM062X/Aug-CC-pVTZ) (Hartree): -381.52009970

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.161622	-0.098116	0.063692
O	-0.388045	0.184726	-0.930349
O	0.320405	1.354258	-0.667224
C	-1.116199	0.800166	1.144878
C	-2.111108	-1.212312	-0.174552
H	-0.158742	0.841208	1.661933
H	-1.974790	0.800022	1.801614
H	-0.589146	1.673090	0.303639
C	2.051138	-0.671096	0.530609
O	3.042998	-0.508537	0.034064
H	-3.110296	-0.899752	0.126885
H	-1.831988	-2.063434	0.446987
H	-2.111148	-1.506563	-1.220748

Rotational constants (GHz): 4.0610900 1.4187200 1.3116800

Vibrational harmonic frequencies (cm-1):		
i1581.2132	21.0728	52.1711
82.7875	100.0709	117.4917
169.4225	294.9564	366.7118
524.1426	550.8295	670.4609
746.5688	854.1472	949.0466
989.2712	1001.9271	1056.7349
1096.1973	1332.1237	1378.6182
1420.1722	1464.1385	1474.4897
1531.5441	1569.4682	1885.6678
2274.5782	3074.9393	3119.1175
3140.5764	3176.2493	3227.6472

Zero-point correction (Hartree): 0.090474

TS.CI+CO.VHP+CO.b

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98203157

E(CCSD/Aug-CC-pVTZ) (Hartree): -380.91257180

T1 diagnostic: 0.023325

E(MP2/Aug-CC-pVTZ) (Hartree): -380.88933905

E(MP3/Aug-CC-pVTZ) (Hartree): -380.89733927

E(RHF/Aug-CC-pVTZ) (Hartree): -379.50175303

E(RM062X/Aug-CC-pVTZ) (Hartree): -381.52010422

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.167124	0.111599	0.008347
O	-0.504726	-0.452739	-0.943679
O	0.108562	-1.614486	-0.480416
C	-1.157538	-0.565890	1.241499
C	-1.649640	1.482272	-0.286159
H	-1.628062	-1.547801	1.232638
H	-1.386885	0.029316	2.114130
H	-0.075433	-1.183194	0.808270
C	1.939200	0.775824	0.260351
O	2.972613	0.367387	0.114585
H	-1.279615	2.151474	0.491046
H	-2.738451	1.510041	-0.257444
H	-1.292539	1.816035	-1.256788

Rotational constants (GHz): 3.4768100 1.5916700 1.3667100

Vibrational harmonic frequencies (cm-1):

i1585.2981	28.2907	44.4002
65.5666	105.7843	117.7542
139.9863	295.0866	367.0538
522.1379	545.7870	674.4897
744.0154	852.3682	946.9682
989.7127	998.1956	1059.8116
1095.3362	1335.7720	1379.6367
1418.6500	1463.1957	1474.3703
1530.3984	1570.1370	1889.0225
2277.4902	3074.2227	3118.7252
3140.5666	3174.9022	3230.5304

Zero-point correction (Hartree): 0.090376

propeneO0

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.22424418

E(CCSD/Aug-CC-pVTZ) (Hartree): -267.17962543

T1 diagnostic: 0.028510

E(MP2/Aug-CC-pVTZ) (Hartree): -267.13931173

E(MP3/Aug-CC-pVTZ) (Hartree): -267.16637519

E(PMP2/Aug-CC-pVTZ) (Hartree): -267.14641126

E(PMP3/Aug-CC-pVTZ) (Hartree): -267.17149638

E(PUHF/Aug-CC-pVTZ) (Hartree): -266.20230995

E(UHF/Aug-CC-pVTZ) (Hartree): -266.19374692

E(UM062X/Aug-CC-pVTZ) (Hartree): -267.60868612
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.493583	-0.029548	-0.000014
O	-0.663236	-0.812355	0.000410
O	-1.776014	-0.138997	-0.000343
C	0.307287	1.442430	0.000109
C	1.625981	-0.717282	-0.000179
H	-0.257678	1.756957	0.876485
H	-0.257567	1.757194	-0.876256
H	1.281989	1.921926	0.000174
H	1.613175	-1.797329	0.000029
H	2.572973	-0.201523	-0.000475

Rotational constants (GHz): 8.9298200 4.7845700 3.1759800
 Vibrational harmonic frequencies (cm-1):

129.1710	248.0690	340.8048
412.0830	476.5127	608.5540
724.5858	824.2907	918.8823
940.3776	1026.4535	1069.7546
1262.7457	1299.8754	1400.0920
1441.7869	1471.0035	1484.8389
1743.1184	3081.9105	3143.8609
3178.0165	3197.2856	3294.9349

Zero-point correction (Hartree): 0.076818

vinylperformate.cpc

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.04707391
 E(CCSD/Aug-CC-pVTZ) (Hartree): -380.98127539
 T1 diagnostic: 0.015499
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.95705838
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.97168752
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.57605682
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.59140283
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.018171	1.414196	-0.423523
C	1.103111	0.172403	0.022170
C	2.242373	-0.773651	-0.155351
O	0.131104	-0.486093	0.747541
O	-1.019101	0.306062	0.917050
C	-1.925428	0.060427	-0.064206
O	-1.786664	-0.660015	-0.992605
H	1.846166	1.818126	-0.983276
H	0.158317	2.039330	-0.248686
H	3.046555	-0.282562	-0.695208
H	1.914671	-1.650699	-0.712889
H	2.612129	-1.108079	0.813757
H	-2.809900	0.663994	0.175880

Rotational constants (GHz): 5.1061800 1.8444000 1.7619100
 Vibrational harmonic frequencies (cm-1):

70.5939	72.5285	173.6649
232.3520	329.1445	381.7021
421.1202	509.7176	573.0865
742.3337	838.5728	873.2652
893.9089	954.5383	996.3313
1035.0583	1038.7446	1076.7025
1140.2790	1289.3499	1389.9660
1406.1398	1441.7826	1475.2766
1493.6602	1765.0077	1894.9837
3074.8841	3076.5982	3137.3960
3177.3911	3212.5408	3302.1602

Zero-point correction (Hartree): 0.099079

 Formic Acid Anhydride : M06-2X/aug-cc-pVTZ geometries

FAA

E(RM062X/Aug-CC-pVTZ) (Hartree): -303.08598507

Point group : C2V

Electronic state : 1-A1

Cartesian coordinates (Angs):

C	0.000000	1.172874	-0.319758
O	0.000000	0.000000	0.380670
C	0.000000	-1.172874	-0.319758
O	0.000000	2.220350	0.225666
H	0.000000	1.033612	-1.409456
O	0.000000	-2.220350	0.225666
H	0.000000	-1.033612	-1.409456

Rotational constants (GHz): 49.0677100 2.6202100 2.4873900

Vibrational harmonic frequencies (cm-1):

130.4601	187.2671	287.8518
554.8718	722.2851	1043.2717
1051.4922	1136.0081	1179.9823
1404.2826	1467.5850	1876.9298
1958.3253	3041.5044	3064.1495

Zero-point correction (Hartree): 0.043527

bicycFAA

E(RM062X/Aug-CC-pVTZ) (Hartree): -302.90585963

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.365259	-0.716994	0.371714
O	0.955493	-0.728643	-0.129325
O	0.955497	0.728640	-0.129323
H	-0.742589	-1.570911	0.909030
H	-0.742586	1.570918	0.909021
C	-0.365257	0.716997	0.371711
O	-1.177456	0.000000	-0.526177

Rotational constants (GHz): 11.4452300 7.7078600 5.6151500

Vibrational harmonic frequencies (cm-1):

497.5828	638.5588	782.7204
818.5699	936.2963	964.8515
979.6752	1048.6282	1063.8463
1118.2903	1228.8658	1265.7739
1480.6770	3262.2091	3281.2599

Zero-point correction (Hartree): 0.044123

TS.FAA.bicycFAA

E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86908700

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.342514	-0.720428	0.362307
O	0.932568	-0.931527	-0.128676
O	0.932568	0.931527	-0.128676
H	-0.774075	-1.488182	0.988822
H	-0.774075	1.488182	0.988822
C	-0.342514	0.720428	0.362307
O	-1.157847	0.000000	-0.533314

Rotational constants (GHz): 9.2270300 7.9707700 5.1574000

Vibrational harmonic frequencies (cm-1):

i924.2068	450.9131	622.0293
655.6369	833.5687	846.8215

982.6452	1017.6389	1041.4235
1080.9925	1240.2270	1254.9558
1403.9788	3214.5742	3229.9873

Zero-point correction (Hartree): 0.040723

TS.bicycFAA.CH2O+CO2

E(UM062X/Aug-CC-pVTZ) (Hartree): -302.82114702

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.488985	0.728181	0.258366
O	-0.833503	0.815378	-0.149060
O	-1.022019	-0.608620	-0.102252
H	0.984156	1.638400	0.572231
H	0.319613	-0.121514	1.338817
C	0.244599	-0.995849	0.356774
O	1.142362	-0.195617	-0.448923

Rotational constants (GHz): 10.9616600 8.1995500 5.5228500

Vibrational harmonic frequencies (cm-1):

i1080.4235	512.7960	629.1447
734.4051	788.9773	889.0636
943.4690	984.3368	1076.6431
1123.4372	1247.0954	1373.9250
1412.3461	2107.0548	3217.5537

Zero-point correction (Hartree): 0.038821