Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Reaction of Criegee Intermediates with Acids and Enols
- Supporting information -

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Methodology: additional information

Quantum chemical calculations

The potential energy surface (PES) of each of the reactions is studied at the M06-2X/cc-pVDZ and M06-2X/aug-cc-pVTZ levels of theory,[1,2] identifying the relevant energetic minima and transition states, and obtaining their rovibrational characteristics. For key reactions, the transition states are further investigated by intrinsic reaction coordinate (IRC) calculations to obtain the minimum energy path, and to verify the reactants and products of the reaction. Vibrational wavenumbers and zero-point vibrational energy (ZPE) are scaled by 0.971.[3,4] The relative energies of minima and saddle points are then improved by single-point energy calculations at the CCSD(T)/aug-cc-pVTZ level of theory.[2,5] The CCSD(T) energies based on M06-2X/cc-pVDZ and M06-2X/aug-cc-pVTZ geometries differ on average by only 10 kJ mol^{-1}, averaged over 36 structures and TS, indicating that the geometries are well converged with respect to basis size. The largest differences are found for a carbene (HOOCH), a singlet biradical ($^{\bullet}OCH_2OCHOHO^{\bullet}$), and two related saddle points (**TS20**, **TS23**), none of which contribute significantly to the reaction flux, and are expected to be subject to larger uncertainties due to intrinsic multi-reference charactersinglet. Removing these four structures from the comparison set brings the CCSD(T) energies across the geometries obtained at the two employed methodologies in agreement within 1 kJ mol^{-1} (0.1 ± 1.0 kJ mol^{-1}, 1σ), indicating excellent geometry convergence with respect to basis set size. We did not perform systematic variations of the basis set at the CCSD(T) level of theory to estimate the complete basis set (CBS) limit, nor did we attempt post-CCSD(T) calculations. However, it has been documented for Criegee intermediate reactions that the CCSD(T)/aug-cc-pVTZ level of theory is within ~2 kJ mol^{-1} of HEAT and W3 post-CCSD(T) calculations,[6–12] which is sufficiently accurate to determine the reaction mechanism; the uncertainty induced on the predicted thermal rate coefficients at room temperature is then a factor of ~2.

For (near-)barrierless reactions, the energy profile and the rovibrational characteristics along this path are obtained by constrained optimization, typically fixing a bond length to several distances, thus probing the minimum energy pathway (MEP). This approach is not as rigorous as explicitly tracing the MEP, as the constraint is not identical to the reaction coordinate vector, biasing the geometry optimization. However, as long as the constraint vector is sufficiently close to the reaction coordinate vector, the accuracy remains very good. For the current reactions, the kinetic bottleneck lies in in the long-range region of the PES where the reaction coordinate consists mostly in the approach of the two reactants, i.e. the interaction between the reacting moieties has a minimal effect on their individual geometry as the attractive force is mostly due to charge and dipole, not chemical interaction. The pathways traced by constrained optimization should thus be very close to the true MEP. A second source of uncertainty is the calculation of the rovibrational characteristics, in particular the vibrational wavenumbers used to describe the transitional modes (i.e. those modes that correlate to relative translation and rotation of the reactants in the limit of infinite separation) as a vibration or internal rotation in the TS. These calculations have inherently large uncertainties, as the calculation of the Hessian is inaccurate due the flat PES. This leads to large relative errors on the predicted wavenumbers, and also manifests itself as noise on the prediction along the reaction coordinate. We remove the noise somewhat by (arbitrary) smoothing of the results; we can then

interpolate the wavenumbers along the reaction coordinate by Cspline interpolation. Other techniques exists, e.g. interpolation/smoothing at the level of the hessian, but none of these techniques can eliminate the intrinsic uncertainty on the PES derivatives at the chosen level of theory. Even small changes of the order of 20-30% on the values for the transitional modes has a very large impact on the predicted rate coefficient, and we estimate an uncertainty of a factor of 4 on the k(T) values due to methodological and computational errors on these characterizations. Below, we show a representative example of the evolution of the ZPE-corrected energy and vibrational wavenumbers along the reaction coordinate. The energy profile is improved by using CCSD(T)/aug-cc-pVTZ single point calculations, but especially for dissociation reactions to biradical products (e.g. HPMF -> OMF + OH), the energy profile retains a comparatively large uncertainty of several kJ mol^{-1} due to the intrinsic multi-reference character of the wavefunction of singlet biradical intermediate structures, which is not covered properly at the single-reference coupled cluster level of theory.

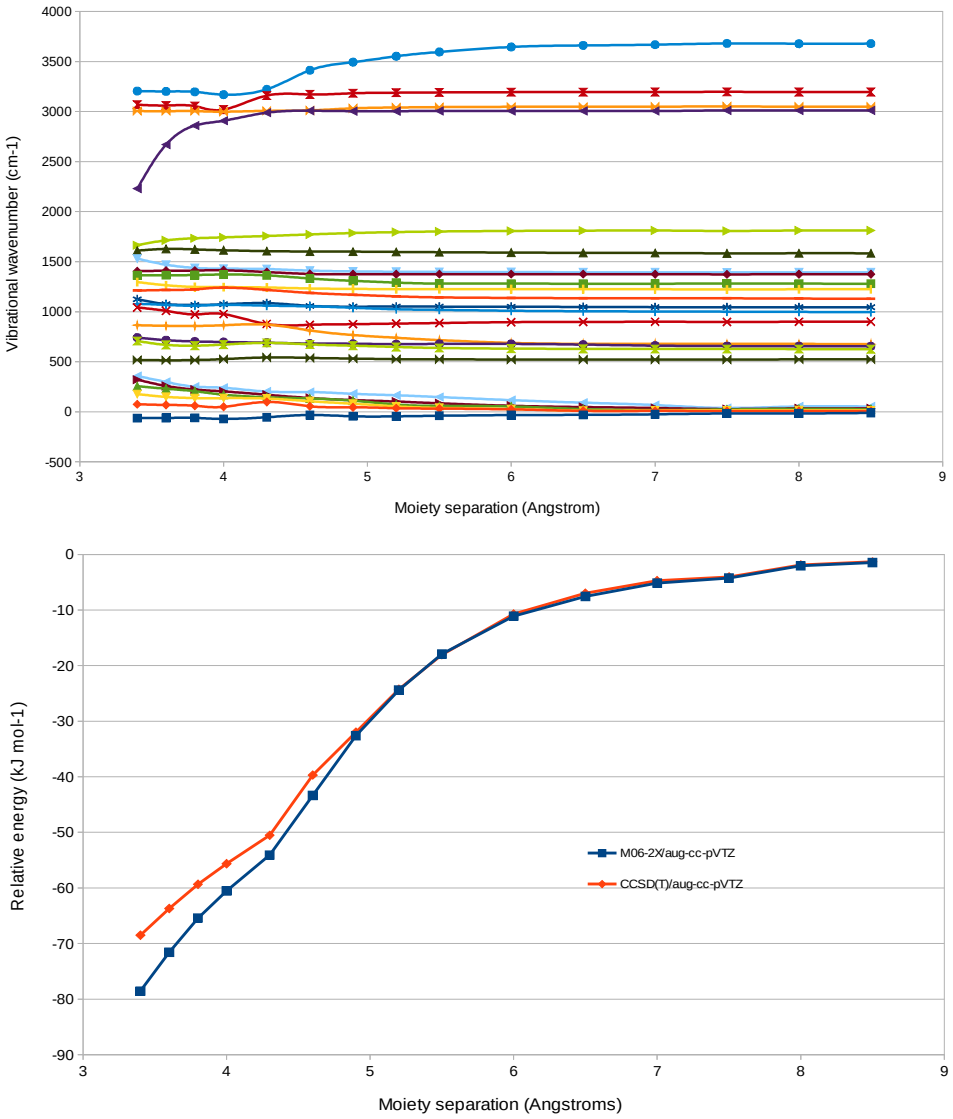

Figure S1: Vibrational wavenumbers at the M06-2X/aug-cc-pVTZ level of theory (top panel), and ZPE-corrected energy relative to the reactant energy limit (M06-2X/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ levels of theory) for the reaction of CH_2OO + HC(=O)OH.

Theoretical kinetic calculations

The rate coefficients of reactions with a clearly defined saddle point are predicted using multi-conformer canonical transition state theory (CTST),[13,14] accounting explicitly for multiple conformers of reactant and TS, and using a rigid rotor harmonic oscillator approximation based on the M06-2X rovibrational characteristics and CCSD(T) relative energies. The roaming transition states were treated identically as all other saddle points, i.e. we did not attempt to further improve the description of the PES in the region of these TS. The computational burden was deemed to high, as a large part of the uncertainty on our RRKM/ME product distribution predictions (see below) is due to the uncertainties on the collisional energy transfer parameters. Also, as described by Klippenstein et al.,[15] the reaction flux is partly determined by dynamic factors which can not be described by the statistical theories in use here.

For barrierless reactions, a *E*,*J*-micro-variational[16] approach is used based on quantum chemical characterization of many points along the reaction pathway obtained as described above. Using in-house software, the lowest state density $G^{\neq}(E,J)$ along the reaction coordinate is minimized explicitly as a function of energy *E* and rotational quantum number *J*. The minimization first performs a grid search along the reaction coordinate to determine the approximate position of the minimum $G^{\neq}(E,J)$. This is then further refined using a modified Brent algorithm,[17] reducing the bracketing of the minimum. When the sum of states for the TS becomes too low to assume a continuous function ($\leq 10^6$ states), the interval bracketing the minimum is sampled on at least 64 points to ensure that the sum of state function is indeed a constant integer across that interval. Several alternative minimization and interpolation strategies are used to verify that the rate constant prediction is viable, and to guard against overly large artifacts in the interpolation (e.g. overshoot, undershoot, oscillations and other haloing/ringing/echoing artifacts). The most rigorous calculation is the *E*,*J*-micro-variational minimization of the rate coefficient based on Cspline interpolated energies, wavenumbers, and moments of inertia; this is then supplemented by *E*-micro-variational and by variational minimization of the canonical TST rate coefficients (VCTST) based on the same data, on VCTST estimates interpolating the energies, and the vibrational and rotational partition functions, and on VCTST minimization interpolating the total partition function. These results are found to remain consistent with the E,J-μVTST predictions given in the paper, within a factor 2.5 on the predicted thermal rates for all cases.

The total *a priori* uncertainty on the rate coefficient estimates for the Cl + acid reactions is the convolution of the above-mentioned errors due to energies, rovibrational characteristics, minimization, interpolation, etc. However, some of these errors are correlated. One example is the energy profile and the vibrational wavenumbers for transitional modes: the latter depend on the shape of the PES, and a too-steep energy profile (=overestimation of the rate coefficient) also leads to more rigid structures with higher wavenumbers (=underestimation of the rate coefficient). Similar considerations also pertain when treating modes as (internal) rotors instead of vibrations. The minimization of predicted rate coefficient thus tends to cancel out some of the errors, as the optimum position along the reaction coordinate then also shifts. This cancellation of error is an important reason why this type of predictions typically gives very good results, typically within a factor of 2 to 3 of the experimental values.

The yield of the products are estimated by RRKM master equation analysis.[18] State densities are obtained in a rigid rotor, harmonic oscillator approximation; for barrierless reactions the energy-specific sum of states and thus k(E) are minimized along the reaction coordinate, similar to the micro-variational TST procedure described above. Multiple conformers are included explicitly by a multi-conformer approach accounting for the relative energy and rigidity of each conformer; this approach assumes that all conformers are present in ratios determined by their relative energy-specific density of states. For intermediates, these ratios are typically instated by rapid internal

rotations or fast re-arrangements. For some pre- and post-reactive complexes, and even more so for transition states, one can not necessarily assume a lifetime that is sufficient to equilibrate across all conformers. In some cases, for very low internal energies such as near the asymptotic energy limit in a barrierless dissociation, the barriers to internal rotation can even be similar or higher than the available energy. However, given the energy-specific equilibration across the conformers of the intermediates that act as reactants, it is assumed that the TS and complexes are formed initially in a conformer ratio that is sufficiently close to the statistical equilibrium ratios to minimize deviation of the rate predictions compared to a fully statistical re-distribution. Such an assumption can only be verified by computational dynamics studies, which is outside the scope of the present work. The Troe bi-exponential collisional energy transfer model[19] is used for all intermediates, with an average energy transfer of ΔE_{ave} = -2.9 kJ mol^{-1} in N_2 bath gas, and with Lennard-Jones collisional parameters of ε_{A-A} = 350 K and σ_{A-A} = 4.5 Å for HPMF, HPMN and $ClCH_2OOH$ intermediates.

The errors on these product yield predictions are determined mostly by uncertainties on the collisional energy transfer parameters, the treatment of the barrierless channels, and the treatment of the roaming channels, as applicable for the different PES. Quantitatively accurate *a priori* prediction of the competition between these different types of channels is difficult, and in this work we mostly aim to determine the dominant channels at room temperature and 1 atm, without necessarily endorsing a specific yield. While the (energy-specific) rates of reactions can be improved by more rigorous calculation of energy and state density, the energy transfer parameter ΔE_{ave} carries a large uncertainty, at least ±40%, as it is merely estimated based on similar molecules, with no tractable means to predict or improve its value using *a priori* calculations, and no experimental data available to calibrate the value. In the low- and high-pressure regime of the product yields, where virtually all or none of the initial adducts are collisionally stabilized, this has little impact on the reliability of the predictions, but for the reactions studied here the product formation is in the fall-off pressure region, with competing partial dissociation and partial thermalization. As such, we consider our product yield predictions as semi-quantitative only; experimental product studies are necessary to quantify the yield accurately.

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Rovibrational and energetic properties of reactants, products, intermediates and saddlepoint TS for the reaction of CH_2OO with formic acid, nitric acid, hydrogen chloride, and ethenol.

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CH2OO + HCOOH
M06-2X/aug-cc-pVTZ geometries
*****************************************

CH2OO
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059345
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649234
     T1 diagnostic:  0.041942
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(RHF/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

HCOOH
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.51744484
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.48986131
     T1 diagnostic:  0.016332
E(MP2/Aug-CC-pVTZ) (Hartree): -189.48638967
E(MP3/Aug-CC-pVTZ) (Hartree): -189.48384440
E(RHF/Aug-CC-pVTZ) (Hartree): -188.84523462
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.76956683
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.420940       0.000000
     O       1.152138      0.110702       0.000000
     O      -1.023538     -0.440647       0.000000
     H      -0.373433      1.449804       0.000000
     H      -0.655373     -1.335884       0.000000
Rotational constants (GHz):   78.0559900   12.2043700   10.5541800
Vibrational harmonic frequencies (cm-1):
      644.1645 (  A')           673.4757 (  A")           1075.4389 (  A")
     1161.5272 (  A')          1317.5161 (  A')           1414.0167 (  A')
     1868.4107 (  A')          3103.4645 (  A')           3792.3575 (  A')
Zero-point correction (Hartree): 0.034287

CI+acid complex a
-----------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85977757
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79783061
     T1 diagnostic:  0.030631
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78245752
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77931337
E(RHF/Aug-CC-pVTZ) (Hartree): -377.49006507
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.35866695
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.754901      0.714347       0.409779
     O       1.708147     -0.291164      -0.307558
     O       0.839040     -1.273870       0.051670
     H       1.152420      0.753567       1.307710
     H       2.422798      1.498366       0.077836
     C      -1.289734      0.132740      -0.456138
     O      -0.773390      1.190481      -0.201415
     O      -2.146959     -0.492641       0.346999
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     H      -1.161509     -0.416273      -1.389212
     H      -2.219410      0.019370       1.164247
Rotational constants (GHz):    6.5911300    2.2412700    1.8380600
Vibrational harmonic frequencies (cm-1):
       55.6802                  90.3001                 139.2607
      177.0805                 233.4388                 241.3325
      537.5579                 642.1394                 660.1788
      694.1837                 912.9241                1054.0804
     1059.9794                1171.7938                1258.9095
     1327.0584                1421.5869                1444.0805
     1654.6558                1810.4983                3152.0495
     3152.9938                3297.8446                3804.4743
Zero-point correction (Hartree): 0.068332

CI+acid complex b
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85925543
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79820600
     T1 diagnostic:  0.029776
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78175996
E(MP3/Aug-CC-pVTZ) (Hartree): -378.78005642
E(RHF/Aug-CC-pVTZ) (Hartree): -377.49351525
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.35786098
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.718612      0.944497       0.123349
     O      -1.830168     -0.137047      -0.458614
     O      -1.524745     -1.265871       0.256969
     H      -1.423817      0.956003       1.165078
     H      -1.931880      1.826608      -0.466428
     C       1.345045     -0.141848       0.035176
     O       0.942971      0.990475       0.113000
     O       2.631453     -0.455219      -0.109589
     H       0.701082     -1.025589       0.073426
     H       3.139933      0.368373      -0.137361
Rotational constants (GHz):    7.4486500    1.7083200    1.4420900
Vibrational harmonic frequencies (cm-1):
       42.0130                  49.2461                  77.7236
      119.5481                 133.2572                 214.8579
      526.5845                 648.8024                 679.0358
      697.1832                 882.2786                1076.9994
     1114.7683                1169.4587                1254.9571
     1321.0662                1421.6038                1444.4064
     1668.3057                1807.6312                3123.4463
     3149.2410                3293.2094                3788.0280
Zero-point correction (Hartree): 0.067670

Oxylmethylformate, OMF (most stable conformer)
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.20523968
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.16196264
     T1 diagnostic:  0.019346
E(MP2/Aug-CC-pVTZ) (Hartree): -303.14038976
E(MP3/Aug-CC-pVTZ) (Hartree): -303.15149762
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.14287329
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.15299589
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.15318553
E(UHF/Aug-CC-pVTZ) (Hartree): -302.14910569
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.61985820
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.238667      0.262358      -0.188570
     O      -1.404117     -0.858678       0.184290
     H      -2.009430      0.895544      -0.639321
     O      -0.083650      0.941569      -0.109192
     C       1.019858      0.211049       0.429269
     O       1.597637     -0.625937      -0.432469
     H       1.747885      0.968830       0.744062
     H       0.695447     -0.360451       1.310034
Rotational constants (GHz):   11.3891300    4.2103100    3.4478700
Vibrational harmonic frequencies (cm-1):
       82.1932                 250.8044                 319.1787
      574.3382                 736.0851                 864.4326
      960.4477                1064.8237                1120.2804
     1182.5742                1249.4250                1367.8435
     1395.1577                1416.5297                1853.2696
     2997.5257                3046.0689                3097.7874
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Zero-point correction (Hartree): 0.053716

OH
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree):  -75.64558510
E(CCSD/Aug-CC-pVTZ) (Hartree):  -75.63969539
     T1 diagnostic:  0.010035
E(MP2/Aug-CC-pVTZ) (Hartree):  -75.62633030
E(MP3/Aug-CC-pVTZ) (Hartree):  -75.63789504
E(PMP2/Aug-CC-pVTZ) (Hartree):  -75.62832143
E(PMP3/Aug-CC-pVTZ) (Hartree):  -75.63903850
E(PUHF/Aug-CC-pVTZ) (Hartree):  -75.42490330
E(UHF/Aug-CC-pVTZ) (Hartree):  -75.42155017
E(UM062X/Aug-CC-pVTZ) (Hartree):  -75.73381011
Point group : C*V
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.108021
     H       0.000000      0.000000      -0.864170
Rotational constants (GHz):    0.0000000  563.9825141  563.9825141
Vibrational harmonic frequencies (cm-1):
     3766.2002 (  SG)
Zero-point correction (Hartree): 0.008580

OMF+OH complex a
----------------
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.74318482
     T1 diagnostic:  0.033676
E(MP2/Aug-CC-pVTZ) (Hartree): -378.98890283
E(MP3/Aug-CC-pVTZ) (Hartree): -378.99778098
E(RHF/Aug-CC-pVTZ) (Hartree): -377.26330826
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.36292632
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.394202      0.519131      -0.097301
     O      -0.712953     -0.547281       0.353455
     H      -1.096644      1.242673      -0.521575
     O       0.852317      0.983796      -0.139237
     C       1.863397      0.097429       0.360981
     O       2.191705     -0.883250      -0.476386
     H       2.738262      0.732953       0.543794
     H       1.533169     -0.341569       1.312382
     H      -2.649023     -0.566088       0.132218
     O      -3.498686     -0.149180      -0.118945
Rotational constants (GHz):   10.2978700    1.3874700    1.2854600
Vibrational harmonic frequencies (cm-1):
       31.7247                   56.9894                   83.5054
      167.8693                  263.4662                  334.6999
      354.3975                  543.2845                  580.4246
      747.5893                  871.5358                  950.2527
     1079.9303                 1126.5899                 1203.1418
     1257.8887                 1367.8751                 1397.8742
     1424.0173                 1819.6194                 3000.8176
     3051.1202                 3114.1807                 3627.6608
Zero-point correction (Hartree): 0.064829

OMF+OH complex b
----------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.89355067
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.74432010
     T1 diagnostic:  0.057825
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78168606
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75625803
E(RHF/Aug-CC-pVTZ) (Hartree): -377.30924998
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.36236238
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.328576      1.228577       0.250720
     O       0.044950      1.551010      -0.861049
     H       1.118309      1.669931       0.862933
     O      -0.300545      0.257948       0.948587
     C      -1.313678     -0.435580       0.236893
     O      -0.850397     -1.350731      -0.624500
     H      -1.928974     -0.938438       0.993549
     H      -1.945440      0.270111      -0.321363
     H       1.287249     -1.328042      -0.507201
     O       2.028424     -1.012170       0.042763
Rotational constants (GHz):    3.4670300    3.3992800    2.2723000
```

```
Vibrational harmonic frequencies (cm-1):
       75.0346                  80.5902                 100.8031
      137.1377                 271.2958                 317.3290
      337.4305                 416.1308                 583.0140
      736.1994                 883.9286                 977.9969
     1058.4260                1096.8016                1168.1949
     1247.4811                1360.8199                1390.9056
     1414.1714                1854.4371                2992.1203
     3039.5775                3126.1397                3711.1742
Zero-point correction (Hartree): 0.064648

OMF+OH complex c
----------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.86337121
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.74382608
     T1 diagnostic:  0.033506
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78816136
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75645244
E(RHF/Aug-CC-pVTZ) (Hartree): -377.32205241
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.35473190
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.457722     -0.158006       0.140262
     O       2.176219     -1.062419      -0.128406
     H       1.795839      0.806791       0.546374
     O       0.119751     -0.230084      -0.029796
     C      -0.629594      0.932525       0.319952
     O      -0.332436      2.026420      -0.368200
     H      -1.685558      0.658726       0.152499
     H      -0.521157      1.146193       1.396349
     H      -1.486785     -1.803854      -0.284122
     O      -2.347422     -1.415788      -0.045147
Rotational constants (GHz):    3.6288500    2.3949100    1.4959000
Vibrational harmonic frequencies (cm-1):
       29.9134                  63.4349                 105.0916
      142.5869                 149.8815                 235.2885
      271.5880                 310.1996                 525.0800
      709.9292                 805.8709                1040.5823
     1051.8172                1127.5652                1136.8504
     1236.5278                1332.3833                1398.2834
     1441.1676                1899.0912                2937.3878
     2973.8287                3038.3880                3745.7867
Zero-point correction (Hartree): 0.063125

Formic acid anhydride, OCHOCHO
------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.67631476
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.62935773
     T1 diagnostic:  0.017114
E(MP2/Aug-CC-pVTZ) (Hartree): -302.62745852
E(MP3/Aug-CC-pVTZ) (Hartree): -302.61943396
E(RHF/Aug-CC-pVTZ) (Hartree): -301.61032721
E(RM062X/Aug-CC-pVTZ) (Hartree): -303.09123140
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.975989     -0.264664       0.000000
     O       2.117501      0.040025       0.000000
     H       0.570920     -1.278837       0.000000
     O       0.000000      0.712453       0.000000
     C      -1.307021      0.328347       0.000000
     O      -1.698420     -0.793166       0.000000
     H      -1.937372      1.222232       0.000000
Rotational constants (GHz):   22.4779700    3.2629100    2.8493000
Vibrational harmonic frequencies (cm-1):
       84.3840 (  A")           224.5284 (  A")           271.1521 (  A')
      556.9312 (  A')           805.2777 (  A')          1053.5484 (  A')
     1060.4765 (  A")          1070.4112 (  A")          1172.9966 (  A')
     1404.5589 (  A')          1421.7241 (  A')          1864.9973 (  A')
     1918.1383 (  A')          3113.5107 (  A')          3138.5375 (  A')
Zero-point correction (Hartree): 0.043652

H2O
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree):  -76.34228981
E(CCSD/Aug-CC-pVTZ) (Hartree):  -76.33365056
     T1 diagnostic:  0.010012
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E(MP2/Aug-CC-pVTZ) (Hartree):  -76.32895487
E(MP3/Aug-CC-pVTZ) (Hartree):  -76.33161592
E(RHF/Aug-CC-pVTZ) (Hartree):  -76.06050818
E(RM062X/Aug-CC-pVTZ) (Hartree):  -76.43010673
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.116391
     H       0.000000      0.762469      -0.465566
     H       0.000000     -0.762469      -0.465566
Rotational constants (GHz):  833.6147400  431.2787000  284.2297000
Vibrational harmonic frequencies (cm-1):
     1619.5331                3869.6314                3972.5789
Zero-point correction (Hartree): 0.021555

CH2O
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.34255830
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.32534109
     T1 diagnostic:  0.015260
E(MP2/Aug-CC-pVTZ) (Hartree): -114.31597316
E(MP3/Aug-CC-pVTZ) (Hartree): -114.32041411
E(RHF/Aug-CC-pVTZ) (Hartree): -113.91461119
E(RM062X/Aug-CC-pVTZ) (Hartree): -114.49897015
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C      -0.000001     -0.525317      -0.000000
     O      -0.000001      0.670465       0.000000
     H       0.938124     -1.105889      -0.000000
     H      -0.938105     -1.105933      -0.000000
Rotational constants (GHz):  284.8986600   39.4617000   34.6607800
Vibrational harmonic frequencies (cm-1):
     1213.9111 (  A")          1273.4438 (  A')          1540.3115 (  A')
     1870.5118 (  A')          2944.9633 (  A')          3014.6814 (  A')
Zero-point correction (Hartree): 0.027014

HCO
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.69211748
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.67456249
     T1 diagnostic:  0.021369
E(MP2/Aug-CC-pVTZ) (Hartree): -113.66827147
E(MP3/Aug-CC-pVTZ) (Hartree): -113.66790348
E(PMP2/Aug-CC-pVTZ) (Hartree): -113.67078678
E(PMP3/Aug-CC-pVTZ) (Hartree): -113.66926689
E(PUHF/Aug-CC-pVTZ) (Hartree): -113.29919493
E(UHF/Aug-CC-pVTZ) (Hartree): -113.29522699
E(UM062X/Aug-CC-pVTZ) (Hartree): -113.84942200
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.061713      0.580762       0.000000
     O       0.061713     -0.587049       0.000000
     H      -0.863978      1.211826       0.000000
Rotational constants (GHz):  721.1923700   45.4357100   42.7428700
Vibrational harmonic frequencies (cm-1):
     1101.8843 (  A')          1993.8124 (  A')          2727.4545 (  A')
Zero-point correction (Hartree): 0.013266

.OCH2O., singlet bisoxy
-----------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.35167429
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29391206
     T1 diagnostic:  0.027839
E(MP2/Aug-CC-pVTZ) (Hartree): -189.32428893
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.32428893
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.56751297
E(ROHF/Aug-CC-pVTZ) (Hartree): -188.56751297
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.60298789
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     O       1.164253     -0.280437       0.000000
     C       0.000000      0.388139       0.000000
     O      -1.164364     -0.279926       0.000000
     H       0.000444      1.077031       0.872697
```

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     H       0.000444      1.077031      -0.872697
Rotational constants (GHz):   62.4439800   11.2554000   10.1229500
Vibrational harmonic frequencies (cm-1):
      574.1120 (  A")           588.7092 (  A')           789.4961 (  A")
      961.4759 (  A')          1144.4944 (  A')          1225.5288 (  A')
     1291.6268 (  A')          2889.3307 (  A')          2918.1399 (  A")
Zero-point correction (Hartree): 0.028210

.OCH(OH)O., singlet bisoxy
--------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.48561213
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.40775745
     T1 diagnostic:  0.084036
E(MP2/Aug-CC-pVTZ) (Hartree): -264.40386284
E(MP3/Aug-CC-pVTZ) (Hartree): -264.38325943
E(RHF/Aug-CC-pVTZ) (Hartree): -263.45593242
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.82897954
Electronic state : 1-A
Cartesian coordinates (Angs):
     O      -0.075977      1.289393      -0.112656
     C      -0.080527     -0.025125       0.326294
     O      -1.161884     -0.669548      -0.181222
     O       1.161271     -0.531674      -0.008307
     H      -0.197107     -0.137266       1.417715
     H       1.292988     -0.417350      -0.957999
Rotational constants (GHz):   11.6606800   10.1015700    6.0469200
Vibrational harmonic frequencies (cm-1):
      220.6398                341.2493                464.4515
      560.8148                943.6787               1080.6486
     1119.2689               1240.2528               1294.1588
     1387.8437               2977.3370               3823.0310
Zero-point correction (Hartree): 0.035205

Hydroperoxymethylformate, HPMF (most stable conformer)
------------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.92535397
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.86765756
     T1 diagnostic:  0.015706
E(MP2/Aug-CC-pVTZ) (Hartree): -378.85600765
E(MP3/Aug-CC-pVTZ) (Hartree): -378.85711766
E(RHF/Aug-CC-pVTZ) (Hartree): -377.56092249
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.43021848
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.556763     -0.184854      -0.124251
     O      -1.059854     -1.249443       0.124171
     H      -2.600488     -0.057322      -0.426200
     O      -0.947513      0.990849      -0.079976
     C       0.424955      1.034390       0.362811
     O       1.280960      0.353213      -0.478244
     H       0.669864      2.090963       0.308560
     H       0.492300      0.640404       1.375252
     O       1.652299     -0.891472       0.094214
     H       0.822036     -1.396440       0.029707
Rotational constants (GHz):    6.0563100    3.3752000    2.3274000
Vibrational harmonic frequencies (cm-1):
      122.7991                195.4975                248.3853
      304.8545                464.6269                546.7243
      557.9150                802.1836                927.2742
      972.2527               1073.3346               1143.7765
     1175.1604               1246.9105               1327.7160
     1413.5180               1442.2091               1490.8671
     1498.8188               1823.0414               3107.8425
     3110.5152               3184.7734               3675.1787
Zero-point correction (Hartree): 0.072574

Hydroperoxyacetic acid, HOOCH2C(O)OH
------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.94065221
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.88377125
     T1 diagnostic:  0.014921
E(MP2/Aug-CC-pVTZ) (Hartree): -378.87244882
E(MP3/Aug-CC-pVTZ) (Hartree): -378.87438296
E(RHF/Aug-CC-pVTZ) (Hartree): -377.57678158
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.44497571
Electronic state : 1-A
Cartesian coordinates (Angs):
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     C      -0.858463      0.105768      -0.058471
     C       0.208572     -0.966836      -0.029694
     O       1.439639     -0.476948      -0.468322
     O       1.901818      0.447471       0.504754
     H       1.455667      1.259482       0.218080
     O      -0.663733      1.260804      -0.316884
     O      -2.060595     -0.391918       0.255945
     H      -2.698570      0.335121       0.240287
     H       0.273618     -1.375176       0.982162
     H      -0.068400     -1.768289      -0.715483
Rotational constants (GHz):    7.8119800    2.5686000    2.1261700
Vibrational harmonic frequencies (cm-1):
       84.0078                199.7882                287.9453
      393.9094                485.1614                504.4309
      531.6585                649.8228                696.5654
      888.2487                964.0371               1062.7367
     1159.2281               1191.6860               1290.7425
     1331.6703               1431.9265               1448.2091
     1456.3738               1868.1435               3069.1869
     3130.6077               3757.8350               3802.1011
Zero-point correction (Hartree): 0.072186

HOOCH2OCOH carbene
------------------
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.36732369
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.781504      1.001753      -0.216012
     O       1.527053      0.122925       0.522679
     O       1.666880     -1.091232      -0.205327
     H       1.014135      0.926359      -1.276441
     H       0.963822      1.994673       0.184592
     C      -1.052772     -0.453329      -0.073428
     O      -0.646457      0.797650      -0.055937
     O      -2.346261     -0.478368       0.087719
     H       0.751822     -1.440968      -0.152527
     H      -2.711888      0.421588       0.187951
Rotational constants (GHz):    8.1134400    2.3547600    1.9302500
Vibrational harmonic frequencies (cm-1):
      122.3259                186.1450                202.1375
      313.9369                444.7624                527.7599
      651.4778                721.2882                758.6319
      958.6991                984.7420               1137.9681
     1179.1298               1207.3451               1319.3829
     1334.3512               1396.0654               1465.6035
     1499.7870               1521.4031               3110.4453
     3186.5529               3515.8171               3629.9580
Zero-point correction (Hartree): 0.071479

Cycloadduct secondary ozonide (most stable conformer)
-----------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.91960220
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.86278872
     T1 diagnostic:  0.013905
E(MP2/Aug-CC-pVTZ) (Hartree): -378.85019157
E(MP3/Aug-CC-pVTZ) (Hartree): -378.85472631
E(RHF/Aug-CC-pVTZ) (Hartree): -377.55292573
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.42523398
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.372098     -0.503805      -0.090319
     O       1.012183      0.790843      -0.491664
     O       0.018029      1.071824       0.497124
     C      -0.772817     -0.101586       0.460474
     O       0.142651     -1.133108       0.183066
     H       1.870899     -0.989441      -0.925424
     H       1.992376     -0.469876       0.808322
     H      -1.224027     -0.206060       1.443745
     O      -1.778726     -0.063531      -0.463866
     H      -1.388030     -0.030496      -1.344852
Rotational constants (GHz):    6.9094800    3.9470100    3.1308400
Vibrational harmonic frequencies (cm-1):
      131.1797                295.3192                341.1371
      524.1663                580.4011                757.5103
      828.4634                942.3852                967.1670
      995.0952               1078.3312               1129.7930
     1170.7803               1189.7441               1251.3213
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     1308.6838                1325.7495                1421.8127
     1446.2805                1535.2192                3067.7123
     3161.6945                3163.5079                3839.5845
Zero-point correction (Hartree): 0.073933

Cycloadduct primary ozonide (most stable conformer)
---------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83442524
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77470302
     T1 diagnostic:  0.015541
E(MP2/Aug-CC-pVTZ) (Hartree): -378.76067393
E(MP3/Aug-CC-pVTZ) (Hartree): -378.76573432
E(RHF/Aug-CC-pVTZ) (Hartree): -377.45205798
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.33455455
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.022837     -0.824250      -0.480788
     O       1.489691      0.426679      -0.033847
     C       0.290023      1.167530       0.077782
     C      -0.755544      0.103598       0.460904
     O      -0.008612     -1.090263       0.458552
     H       0.445001      1.923017       0.842657
     H       0.002699      1.611550      -0.875051
     H      -1.146837      0.193533       1.474861
     O      -1.764330      0.134913      -0.493009
     H      -2.424432     -0.531504      -0.281844
Rotational constants (GHz):    6.8850300    3.7546600    2.9150700
Vibrational harmonic frequencies (cm-1):
      132.0239                 332.2201                 367.9968
      441.8764                 576.8002                 724.9424
      800.8208                 867.2374                 912.7267
      993.6489                1045.4710                1061.0572
     1083.9440                1160.1729                1231.4783
     1268.3122                1354.1250                1369.6860
     1434.4128                1504.4087                3096.1565
     3104.3794                3174.1173                3871.4326
Zero-point correction (Hartree): 0.072695

HOCH(O.)OCH2O. singlet biradical (most stable conformer)
---------------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.87300637
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.74762883
     T1 diagnostic:  0.032763
E(MP2/Aug-CC-pVTZ) (Hartree): -378.80848250
E(MP3/Aug-CC-pVTZ) (Hartree): -378.76828876
E(RHF/Aug-CC-pVTZ) (Hartree): -377.32214708
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.37031926
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       2.064558     -0.090629       0.724869
     C       1.464718     -0.009919      -0.469862
     O       0.178381     -0.574135      -0.534578
     C      -0.782373      0.072229       0.258503
     O      -0.968234      1.365585      -0.129043
     O      -1.917573     -0.701222       0.257265
     H      -0.437136      0.185118       1.302867
     H       1.438627      1.062481      -0.734459
     H       2.063615     -0.526353      -1.230476
     H      -2.016222     -1.091897      -0.617876
Rotational constants (GHz):    7.4745900    2.4278000    2.1771700
Vibrational harmonic frequencies (cm-1):
       67.3770                  122.5740                 157.5116
      275.4704                  451.3002                 504.2928
      557.2963                  662.6121                 816.2788
      908.0617                 1018.6907                1082.7530
     1125.0748                 1152.1055                1222.8385
     1301.5443                 1322.5942                1359.9899
     1373.6979                 1408.1786                2944.7907
     2955.7580                 3032.4203                3851.7159
Zero-point correction (Hartree): 0.067604

CH3OOOCHO (most stable conformer)
---------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83339787
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77301744
     T1 diagnostic:  0.017156
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75885484
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E(MP3/Aug-CC-pVTZ) (Hartree): -378.76047396
E(RHF/Aug-CC-pVTZ) (Hartree): -377.45752089
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.33324535
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.540568     -0.117118       0.254000
     O      -2.522475      0.525482       0.109725
     O      -0.524954     -0.045717      -0.663423
     H      -1.308984     -0.813746       1.067619
     O       0.520155     -0.904920      -0.257762
     O       1.302493     -0.188979       0.648961
     C       2.186880      0.644639      -0.091160
     H       1.623731      1.375098      -0.669978
     H       2.819030      0.039550      -0.738601
     H       2.786590      1.147044       0.663908
Rotational constants (GHz):   11.1310900    1.9295500    1.8671100
Vibrational harmonic frequencies (cm-1):
       79.3179                 139.2833                 190.3552
      222.3683                 341.9909                 484.0917
      561.1159                 687.6209                 912.7391
      991.3129                1050.7668                1073.3775
     1134.8820                1186.0699                1227.7957
     1388.6776                1457.7760                1481.6079
     1515.6149                1908.1884                3071.4400
     3092.8406                3155.3794                3173.2145
Zero-point correction (Hartree): 0.069548

CH3OOOCOH carbene
-----------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.76686500
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.70681892
     T1 diagnostic:  0.017814
E(MP2/Aug-CC-pVTZ) (Hartree): -378.68585899
E(MP3/Aug-CC-pVTZ) (Hartree): -378.69426080
E(RHF/Aug-CC-pVTZ) (Hartree): -377.39358026
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.26845328
Electronic state : 1-A
Cartesian coordinates (Angs):
     O      -0.619308      0.928364       0.408738
     O      -1.586614      0.367892      -0.407915
     C      -1.850802     -0.960327       0.035969
     C       1.259601     -0.341489       0.465443
     O       0.640036      0.634620      -0.189654
     O       2.416256     -0.490105      -0.126703
     H      -0.996139     -1.610034      -0.143721
     H       2.548635      0.131316      -0.868684
     H      -2.108497     -0.958308       1.093111
     H      -2.699761     -1.278257      -0.564907
Rotational constants (GHz):    9.2733300    2.1312500    1.8750100
Vibrational harmonic frequencies (cm-1):
       88.3931                 115.5918                 164.3895
      245.4817                 363.5116                 481.3959
      510.2347                 677.3435                 745.4796
      915.6546                 991.9265                1070.8483
     1112.8924                1182.5621                1225.3694
     1317.5017                1372.2397                1458.7009
     1480.5744                1511.7243                3074.2137
     3159.5094                3171.8297                3620.7647
Zero-point correction (Hartree): 0.068477

Hydroxymethylcarbonate, HOC(O)OCH2OH (most stable conformer)
------------------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -379.04872843
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.99396297
     T1 diagnostic:  0.014294
E(MP2/Aug-CC-pVTZ) (Hartree): -378.98598925
E(MP3/Aug-CC-pVTZ) (Hartree): -378.98535406
E(RHF/Aug-CC-pVTZ) (Hartree): -377.69850459
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.55782636
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.839597      0.070444       0.052095
     O       0.614454      1.222712       0.327762
     O       2.038711     -0.410401      -0.268655
     O      -0.054023     -0.903424       0.019388
     H       2.655429      0.331148      -0.247015
     C      -1.386097     -0.484402       0.380030
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     O      -1.923242      0.387222      -0.537148
     H      -1.484666      1.238925      -0.425974
     H      -1.966981     -1.399595       0.368080
     H      -1.331983     -0.055605       1.381391
Rotational constants (GHz):    8.4152900    2.6634400    2.2277100
Vibrational harmonic frequencies (cm-1):
      118.7382                176.4384                301.6991
      451.5583                544.0444                558.5160
      597.0065                727.7937                830.5120
      925.8125               1075.3954               1096.5389
     1168.9672               1233.8261               1316.3643
     1410.2097               1423.9542               1491.9072
     1525.5319               1830.5168               3089.6137
     3189.6915               3834.0251               3845.9034
Zero-point correction (Hartree): 0.074643

1,2-OH-insertion, TS2
---------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85261159
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79045768
     T1 diagnostic:  0.023492
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78043501
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77492878
E(RHF/Aug-CC-pVTZ) (Hartree): -377.47760232
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.35367093
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.885118      1.071357      -0.233036
     O      -1.781215      0.200717      -0.177047
     O      -1.389228     -0.861505       0.658024
     H      -1.051101      1.817696      -1.004134
     H      -0.078016      1.121064       0.499757
     O       0.609936     -0.676319      -0.724932
     H      -0.432042     -0.993820       0.181507
     C       1.714680     -0.230630      -0.224812
     O       1.805903      0.536904       0.720319
     H       2.620613     -0.587673      -0.740954
Rotational constants (GHz):    7.0252400    2.2985300    2.1281900
Vibrational harmonic frequencies (cm-1):
     i357.0226                88.3948                166.5086
      202.1044                347.7887                410.9287
      572.1037                769.5545                777.4296
      942.9651               1084.8002               1138.6305
     1164.0619               1263.2359               1296.6972
     1391.5857               1448.4779               1490.1982
     1631.3575               1741.7667               2171.8228
     3007.6437               3055.8540               3234.4131
Zero-point correction (Hartree): 0.066974

cycloaddition, TS3 (most stable conformer)
------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85378562
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.78970987
     T1 diagnostic:  0.029146
E(MP2/Aug-CC-pVTZ) (Hartree): -378.77820923
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77182787
E(RHF/Aug-CC-pVTZ) (Hartree): -377.47443025
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.35239467
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.446800      0.656680       0.471835
     O       1.550523     -0.370565      -0.233471
     O       0.525271     -1.254297       0.004916
     C      -1.037397      0.085476      -0.474968
     O      -0.435085      1.156219      -0.357614
     H       0.896501      0.614206       1.399992
     H       2.108965      1.473210       0.213640
     H      -1.125004     -0.456208      -1.412403
     O      -1.944934     -0.324845       0.415846
     H      -1.903080      0.263763       1.180155
Rotational constants (GHz):    6.7531100    2.9527900    2.3696400
Vibrational harmonic frequencies (cm-1):
     i347.2589                89.1740                195.0836
      306.8585               399.2628                422.4228
      559.1928               627.3125                642.0738
      793.2545               959.6132               1027.2458
     1094.0216              1155.4830               1244.3923
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     1320.4362                1395.8301                1430.8250
     1606.1258                1656.2930                3161.5570
     3182.1173                3297.9601                3822.9227
Zero-point correction (Hartree): 0.069232

1,3-CH-insertion reverse, TS4
-----------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83917887
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77825837
     T1 diagnostic:  0.020647
E(MP2/Aug-CC-pVTZ) (Hartree): -378.76636604
E(MP3/Aug-CC-pVTZ) (Hartree): -378.76479842
E(RHF/Aug-CC-pVTZ) (Hartree): -377.46612876
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.34217338
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.044152      0.963397       0.158486
     O      -1.529640     -0.049511      -0.512025
     O      -1.311338     -1.248570       0.278001
     H      -1.212562      0.933830       1.233087
     H      -1.236183      1.912928      -0.331824
     C       0.985742     -0.254317      -0.028797
     O       0.559285      0.922733       0.111023
     O       2.268910     -0.428145      -0.085147
     H       0.166481     -1.096670       0.005233
     H       2.734992      0.423377      -0.019436
Rotational constants (GHz):    7.5449900    2.5872300    2.0463700
Vibrational harmonic frequencies (cm-1):
     i273.4339                 174.3956                 186.5592
      307.1044                 398.5124                 469.1194
      635.6784                 718.9937                 733.9012
      877.8275                 916.9948                1120.8494
     1248.9018                1259.3235                1305.0084
     1338.8005                1358.6530                1501.3543
     1527.7162                1585.6448                2265.6334
     3106.4027                3199.9775                3709.7793
Zero-point correction (Hartree): 0.068225

1,3-CH-insertion, TS5 (most stable conformer)
---------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.82368671
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.75628386
     T1 diagnostic:  0.028955
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75378382
E(MP3/Aug-CC-pVTZ) (Hartree): -378.74042900
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.75378382
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.74042900
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.42297824
E(UHF/Aug-CC-pVTZ) (Hartree): -377.42297824
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.32176214
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.920895      0.172320      -0.134018
     C      -0.913292     -0.559254       0.919108
     O      -1.679841      0.240141       0.284153
     O      -1.479251      0.071167      -1.054649
     H      -0.200039      0.097179      -0.846238
     O       1.347053      1.214406       0.272233
     O       1.693617     -0.926895      -0.286756
     H       2.604512     -0.686699      -0.055618
     H      -0.683302     -1.527499       0.493465
     H      -0.819408     -0.351934       1.978000
Rotational constants (GHz):    6.1529600    2.2992300    2.2082100
Vibrational harmonic frequencies (cm-1):
    i1538.7808                 109.7711                 129.1381
      219.7168                 377.8746                 471.2293
      522.0651                 644.0631                 675.0089
      719.8424                 792.1322                1011.3780
     1080.0353                1139.8800                1242.2540
     1296.6249                1318.1047                1397.4544
     1555.2189                1704.6974                1825.7388
     3146.4581                3283.0810                3750.3641
Zero-point correction (Hartree): 0.064728

1,2-OH-insertion reverse, TS6
-----------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.81937690
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E(CCSD/Aug-CC-pVTZ) (Hartree): -378.75071555
     T1 diagnostic:  0.029186
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75030665
E(MP3/Aug-CC-pVTZ) (Hartree): -378.73467880
E(RHF/Aug-CC-pVTZ) (Hartree): -377.41554956
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.31741163
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.829052      0.099073      -0.223555
     O      -0.508573      0.004438       1.060100
     O      -1.556477      0.389840       0.279280
     C      -1.614807     -0.420646      -0.714514
     H      -0.084317     -0.210472      -0.983852
     O       1.297003      1.191654      -0.330973
     O       1.518751     -1.027094       0.051345
     H       2.435672     -0.764318       0.207799
     H      -1.389951     -1.467937      -0.544375
     H      -2.252496     -0.098541      -1.529180
Rotational constants (GHz):    6.4663000    2.6527100    2.4472100
Vibrational harmonic frequencies (cm-1):
     i813.6922                  81.4667                 247.7889
      276.0091                 396.8360                 480.1543
      521.6835                 654.6706                 682.1091
      773.0368                 887.6321                1030.9581
     1128.7523                1229.3878                1288.5374
     1312.0619                1348.4091                1469.1080
     1532.0386                1682.0112                1830.2471
     3129.6400                3262.3588                3812.8621
Zero-point correction (Hartree): 0.066198

cycloaddition reverse, TS7
--------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.80612055
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.73211099
     T1 diagnostic:  0.017378
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75456965
E(MP3/Aug-CC-pVTZ) (Hartree): -378.72533962
E(RHF/Aug-CC-pVTZ) (Hartree): -377.37052900
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.29454968
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.326981     -0.740594      -0.521598
     O       1.512462      0.344827       0.166413
     C       0.473423      1.154601       0.017723
     C      -0.888896     -0.023554       0.473339
     O      -0.327445     -1.150288       0.399067
     H       0.549545      2.023669       0.658530
     H       0.125653      1.296423      -0.999232
     H      -1.118497      0.372778       1.465872
     O      -1.903952      0.288796      -0.418893
     H      -1.928234     -0.421086      -1.071458
Rotational constants (GHz):    6.9441700    3.1685800    2.5637500
Vibrational harmonic frequencies (cm-1):
     i613.1933                 132.2887                 343.0393
      347.2845                 431.2623                 491.6700
      601.1911                 624.4556                 663.2129
      924.0967                 941.9764                1078.5269
     1108.1826                1175.2842                1261.6483
     1270.6081                1300.1839                1345.5849
     1496.1400                1509.4305                3076.2782
     3134.9850                3255.4873                3837.0536
Zero-point correction (Hartree): 0.069142

1,2-insertion reverse, TS8
--------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.78347944
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.72757754
     T1 diagnostic:  0.035102
E(MP2/Aug-CC-pVTZ) (Hartree): -378.68633328
E(MP3/Aug-CC-pVTZ) (Hartree): -378.70550097
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.71828363
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.73715196
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.49562476
E(UHF/Aug-CC-pVTZ) (Hartree): -377.46334177
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.28621706
Electronic state : 1-A
Cartesian coordinates (Angs):
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     O      -2.615037     -0.434949      -0.536418
     O      -2.059739      0.170158       0.463247
     C      -0.771092      0.655079       0.159878
     O       1.264875     -1.130486       0.210923
     H      -0.047549     -0.213072       0.261757
     C       2.192781     -0.256626      -0.061792
     O       2.110912      0.924315      -0.235087
     H       3.147353     -0.829576      -0.110616
     H      -0.723519      1.015950      -0.862733
     H      -0.514504      1.403668       0.901752
Rotational constants (GHz):    8.5858800    1.3985500    1.2731100
Vibrational harmonic frequencies (cm-1):
     i356.0912                 47.3544                  62.4954
      110.0518                172.3315                 234.1588
      316.2339                533.2578                 599.6448
      977.0396               1005.7679                1062.4131
     1136.7786               1181.7415                1255.1818
     1288.6452               1346.4130                1393.7702
     1451.3671               1784.1331                2088.5394
     2883.2305               3132.3974                3222.0742
Zero-point correction (Hartree): 0.062160

1,4-insertion reverse, TS9
--------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.78744795
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.70739965
     T1 diagnostic:  0.034860
E(MP2/Aug-CC-pVTZ) (Hartree): -378.72193334
E(MP3/Aug-CC-pVTZ) (Hartree): -378.68747059
E(RHF/Aug-CC-pVTZ) (Hartree): -377.34754131
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.27226891
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       0.993830     -1.136604       0.247847
     O       1.493479     -0.197188      -0.409999
     C       1.336689      1.050673       0.146130
     O      -1.269899      1.166650       0.003286
     H       0.093187      1.229210       0.020299
     C      -1.677730     -0.021933      -0.037057
     O      -1.055458     -1.090793      -0.010574
     H      -2.773194     -0.122679      -0.115112
     H       1.497146      1.034291       1.221133
     H       1.933494      1.750224      -0.425232
Rotational constants (GHz):    5.8652000    2.9717100    2.0629200
Vibrational harmonic frequencies (cm-1):
    i1454.8910                 59.6253                 155.6117
      273.7087                334.8621                 498.3658
      523.7708                575.0224                 661.5672
      806.6285               1041.8085                1072.3576
     1103.5644               1241.0537                1314.6860
     1342.6937               1379.9957                1398.7274
     1462.5305               1517.5157                1714.5031
     3003.9706               3116.8954                3236.9083
Zero-point correction (Hartree): 0.063416

OMF---OH to FAA+H2O, TS11 (most stable conformer)
------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85948449
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.80783410
     T1 diagnostic:  0.022304
E(MP2/Aug-CC-pVTZ) (Hartree): -378.77232660
E(MP3/Aug-CC-pVTZ) (Hartree): -378.79365435
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.79991468
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.82098270
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.59342743
E(UHF/Aug-CC-pVTZ) (Hartree): -377.56557410
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.36413465
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.236578      1.433860      -0.096207
     O       0.640411      1.237476       0.695721
     H      -0.562894      2.426518      -0.420230
     O      -0.949088      0.495011      -0.718880
     C      -0.715507     -0.868674      -0.338430
     O      -1.205263     -1.211411       0.824359
     H      -1.109721     -1.476267      -1.162921
     H       0.393084     -1.081133      -0.314654
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     O       2.128142     -0.912852      -0.275631
     H       2.078422     -0.126022       0.301070
Rotational constants (GHz):    3.6228300    3.1428900    2.1248700
Vibrational harmonic frequencies (cm-1):
     i163.3458                  53.5846                 104.9107
      187.4774                 259.1392                 298.2839
      423.1593                 534.3009                 577.5846
      735.9436                 857.3356                 934.0553
     1073.5286                1122.4810                1179.5597
     1223.6958                1307.9574                1384.3205
     1421.2613                1830.0017                2422.2956
     3031.0009                3109.7791                3692.2237
Zero-point correction (Hartree): 0.063251

HPMF to HCOOH + HOOCH, TS14 (most stable conformer)
---------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.84469838
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.78148555
     T1 diagnostic:  0.021274
E(MP2/Aug-CC-pVTZ) (Hartree): -378.77192268
E(MP3/Aug-CC-pVTZ) (Hartree): -378.76715429
E(RHF/Aug-CC-pVTZ) (Hartree): -377.46236633
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.34476183
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.774790      0.502163      -0.126510
     O      -1.984776     -0.759297      -0.137483
     H      -2.622238      1.137810      -0.401239
     O      -0.685269      1.004842       0.172083
     C       0.435435     -0.646125       0.525130
     O       1.328891     -0.581037      -0.381747
     H       0.742174     -0.206663       1.475018
     H      -0.962168     -1.116330       0.152115
     O       2.436679      0.323985      -0.048067
     H       2.114163      1.141010      -0.455903
Rotational constants (GHz):    9.4262600    1.9749500    1.7356200
Vibrational harmonic frequencies (cm-1):
     i690.6872                  92.3842                 111.9360
      194.9497                 247.8056                 291.8000
      396.3136                 598.0069                 668.5860
      799.3526                 916.5494                1087.2157
     1108.2637                1225.7607                1342.7478
     1352.1266                1354.7770                1403.5919
     1419.6644                1731.4308                1926.4512
     3097.2011                3117.4481                3794.4857
Zero-point correction (Hartree): 0.064424

cycloadduct to HPMF, TS15
---------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.84490912
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.78219407
     T1 diagnostic:  0.017354
E(MP2/Aug-CC-pVTZ) (Hartree): -378.77824984
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77103004
E(RHF/Aug-CC-pVTZ) (Hartree): -377.45449541
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.34891727
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.349379     -0.535312       0.063428
     O      -0.119187     -1.152038      -0.178840
     C       0.879313     -0.385484       0.382915
     O       0.040271      1.132250       0.332051
     O      -1.176894      0.814632      -0.321185
     H      -2.110358     -0.967747      -0.577798
     H      -1.615908     -0.585460       1.123258
     H       1.031009     -0.579750       1.446903
     O       1.822323      0.035492      -0.362483
     H       0.983552      1.015046      -0.426770
Rotational constants (GHz):    7.0440100    3.9586400    2.8703100
Vibrational harmonic frequencies (cm-1):
    i1785.6705                 159.2045                 315.5809
      455.9774                 550.6264                 612.4638
      711.1698                 738.9343                 952.3787
     1033.0587                1071.1390                1085.2103
     1179.6334                1204.8843                1266.7852
     1323.0990                1349.3746                1414.8365
     1518.8100                1556.5355                1972.1656
```

```
     3059.0161                3114.6048                3188.7611
Zero-point correction (Hartree): 0.067967

HPFM to FAA+H2O, TS16 (most stable conformer)
---------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83602234
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.76540281
     T1 diagnostic:  0.020985
E(MP2/Aug-CC-pVTZ) (Hartree): -378.76932443
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75253980
E(RHF/Aug-CC-pVTZ) (Hartree): -377.41728363
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32421246
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       0.662408     -0.846354      -0.374470
     C      -0.398555     -0.523352       0.508399
     O      -1.561836     -0.790343       0.068099
     H      -0.175623     -0.750443       1.553833
     O      -1.834683      0.991741      -0.244329
     H      -2.539936      1.558646      -0.617772
     H      -0.596635      0.735880       0.467921
     C       1.730710     -0.038698      -0.329469
     O       1.837612      0.922884       0.369863
     H       2.491249     -0.395209      -1.030870
Rotational constants (GHz):    7.0596000    2.3077200    1.9234800
Vibrational harmonic frequencies (cm-1):
    i1970.9121                36.3534                 160.6927
      248.6008                281.7376                 338.1930
      514.2386                577.0169                 651.6659
      804.3068                982.0562                1011.6336
     1061.9123               1134.9466                1216.2847
     1242.2021               1301.5075                1403.8248
     1422.9242               1744.1746                1847.2848
     3088.5198               3101.3817                3644.7808
Zero-point correction (Hartree): 0.063370

HPMF to CH2O+HC(O)OOH, TS17 (most stable conformer)
---------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.81478052
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.74886981
     T1 diagnostic:  0.020222
E(MP2/Aug-CC-pVTZ) (Hartree): -378.74909580
E(MP3/Aug-CC-pVTZ) (Hartree): -378.73551283
E(RHF/Aug-CC-pVTZ) (Hartree): -377.41973872
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.31735974
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.387691     -0.442353      -0.293697
     H      -0.981555     -1.443682      -0.407918
     O      -2.468496      0.011578      -0.207722
     O      -0.221014     -0.035876       0.993543
     C       0.243795      0.715033       0.057080
     H      -0.487042      0.230106      -1.037895
     O       1.547595      0.608315      -0.307998
     H      -0.056720      1.760997      -0.046878
     O       1.974103     -0.736843      -0.202661
     H       1.731182     -0.960892       0.711095
Rotational constants (GHz):    9.9522000    2.0344700    1.9718000
Vibrational harmonic frequencies (cm-1):
    i1148.6260                92.5674                 191.1717
      275.9400                328.6625                 349.2603
      435.4070                626.9635                 713.0961
      819.2716                960.6291                1048.5991
     1165.8647               1222.3960                1258.9943
     1311.3865               1433.3318                1470.5744
     1515.7501               1753.7287                1882.4372
     3104.9130               3172.0038                3732.8512
Zero-point correction (Hartree): 0.065761

cycloadduct ringopening, TS20 (most stable conformer)
-----------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.87398718
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79693926
     T1 diagnostic:  0.021822
E(MP2/Aug-CC-pVTZ) (Hartree): -378.80196879
E(MP3/Aug-CC-pVTZ) (Hartree): -378.78722400
E(RHF/Aug-CC-pVTZ) (Hartree): -377.43612725
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E(UM062X/Aug-CC-pVTZ) (Hartree): -379.36874111
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.418683     -0.395597      -0.057638
     O      -1.234536      0.719533       0.685438
     O       0.350426      1.113878      -0.682874
     C       0.850073     -0.129347      -0.410754
     O      -0.206030     -1.063587      -0.292000
     H      -2.061420     -1.058542       0.541080
     H      -1.923987     -0.159980      -1.001025
     H       1.445584     -0.386923      -1.296749
     O       1.686499     -0.185471       0.678380
     H       1.180609      0.080283       1.455496
Rotational constants (GHz):    6.2418300    3.4193900    3.0264600
Vibrational harmonic frequencies (cm-1):
     i211.3370                  98.0526                 278.8688
      303.4497                 516.0025                 532.8810
      607.0491                 770.5069                 912.7368
      961.2763                1006.6819                1058.3173
     1105.4673                1149.3974                1210.3111
     1281.3849                1284.1075                1372.7294
     1403.1651                1431.5303                2993.6676
     3032.8472                3047.5430                3836.4525
Zero-point correction (Hartree): 0.068788

HOCH(O.)OCH2O. 1,4-Hshift, TS21
-------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85139521
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79739335
     T1 diagnostic:  0.032228
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75607236
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77991474
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.79150016
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.81476250
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.57330191
E(UHF/Aug-CC-pVTZ) (Hartree): -377.53738364
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.35869709
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.669855     -0.241431       0.891655
     C       1.485187      0.119266      -0.400983
     O       0.238847     -0.352808      -0.854243
     C      -0.731541      0.104234       0.062985
     O      -1.060636      1.334384       0.081965
     O      -1.715901     -0.823949       0.190967
     H      -0.057561      0.169849       1.089436
     H       1.547634      1.207183      -0.528423
     H       2.275222     -0.360680      -0.993944
     H      -1.344495     -1.686920      -0.021827
Rotational constants (GHz):    6.6144100    2.7690100    2.5266500
Vibrational harmonic frequencies (cm-1):
    i1329.7979                 117.7667                 267.2219
      380.2699                 396.6741                 492.3648
      578.7328                 633.2256                 748.2314
      860.4500                 984.9634                1048.5495
     1069.3753                1107.3955                1130.3255
     1216.1314                1285.0814                1368.3964
     1410.3742                1438.2752                1729.8839
     3004.5474                3047.5528                3861.1287
Zero-point correction (Hartree): 0.064192

HOCH(O.)OCH2O. - HCOOH + .OCH2O., TS22
--------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.84822465
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.79372021
     T1 diagnostic:  0.028352
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75205436
E(MP3/Aug-CC-pVTZ) (Hartree): -378.77492185
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.82337769
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.84462181
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.60697431
E(UHF/Aug-CC-pVTZ) (Hartree): -377.53440054
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.35292055
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       2.004639     -0.158727       0.806105
     C       1.554024      0.006853      -0.442733
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     O       0.281060     -0.456643      -0.727607
     C      -0.940041      0.087111       0.403795
     O      -0.876507      1.250402      -0.075402
     O      -1.991410     -0.704127       0.165061
     H      -0.457141     -0.175998       1.344071
     H       1.659932      1.074401      -0.699690
     H       2.215880     -0.544409      -1.137671
     H      -2.444821     -0.365021      -0.618337
Rotational constants (GHz):    7.6546500    2.2714300    2.1667900
Vibrational harmonic frequencies (cm-1):
     i609.8331                 69.8773                147.5696
      223.8093                337.0588                408.2395
      551.9294                606.3957                650.5755
      724.2266                976.6465               1080.7841
     1136.3906               1159.1258               1163.7495
     1303.0528               1319.8321               1334.2555
     1363.1613               1520.5321               2936.4830
     2975.8730               3146.3700               3812.3721
Zero-point correction (Hartree): 0.065949

cycloadduct to 2 HCOOH, TS23
----------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.85043502
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77866788
     T1 diagnostic:  0.027674
E(MP2/Aug-CC-pVTZ) (Hartree): -378.78198987
E(MP3/Aug-CC-pVTZ) (Hartree): -378.76180995
E(RHF/Aug-CC-pVTZ) (Hartree): -377.43750697
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.34527608
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.416213      0.339072      -0.058602
     O       1.082850     -0.795696       0.554819
     O      -0.352033     -1.083365      -0.576890
     C      -0.920956      0.050037      -0.465005
     O       0.464523      1.196996      -0.141595
     H       2.043769      0.272071       0.973272
     H       2.134356      0.250144      -0.883662
     H      -1.206161      0.580656      -1.369318
     O      -1.747875      0.292247       0.557473
     H      -1.523223     -0.318985       1.270903
Rotational constants (GHz):    6.4307600    3.5270400    2.8863700
Vibrational harmonic frequencies (cm-1):
    i1279.9501                146.6267                264.2973
      344.7380                428.0540                452.8498
      528.3973                630.7459                703.9334
      766.7128                929.7361               1080.1725
     1150.5079               1206.5436               1245.9162
     1315.6408               1336.1685               1353.5056
     1463.4119               1527.8211               2352.2206
     3037.0485               3172.0307               3822.2618
Zero-point correction (Hartree): 0.066658

cycloadduct to CH2O + HOC(O)OH, TS24
------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.84367138
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77272845
     T1 diagnostic:  0.025169
E(MP2/Aug-CC-pVTZ) (Hartree): -378.77843226
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75794121
E(RHF/Aug-CC-pVTZ) (Hartree): -377.43127922
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.33968746
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.468560     -0.484354      -0.065023
     O       1.265519      0.661329      -0.629706
     O      -0.152794      1.127092       0.504331
     C      -0.757002     -0.021075       0.317392
     O       0.002751     -1.059975       0.472675
     H       1.697664     -1.299583      -0.754868
     H       2.030334     -0.506521       0.871263
     H      -1.165611      0.607581       1.333477
     O      -1.747034     -0.077384      -0.599868
     H      -1.779265     -0.977408      -0.943540
Rotational constants (GHz):    6.6152700    3.5074100    2.9586300
Vibrational harmonic frequencies (cm-1):
    i1422.2838                157.2584                247.0799
```

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      345.6614                380.2548                516.9346
      572.5205                650.3993                673.5673
      859.2572                948.1374               1040.4185
     1041.6675               1194.7169               1200.5134
     1258.8294               1345.8877               1409.5331
     1519.3001               1544.6402               2165.8727
     3043.7479               3118.5382               3854.3123
Zero-point correction (Hartree): 0.066270

HOCH(O.)OCH2O. to H2CO + .OCH(OH)O., TS25
----------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.81714764
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.76460806
     T1 diagnostic:  0.027418
E(MP2/Aug-CC-pVTZ) (Hartree): -378.71581617
E(MP3/Aug-CC-pVTZ) (Hartree): -378.74480728
E(PMP2/Aug-CC-pVTZ) (Hartree): -378.79947303
E(PMP3/Aug-CC-pVTZ) (Hartree): -378.82656562
E(PUHF/Aug-CC-pVTZ) (Hartree): -377.60274702
E(UHF/Aug-CC-pVTZ) (Hartree): -377.51776782
E(UM062X/Aug-CC-pVTZ) (Hartree): -379.31962740
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.917347      0.154363       0.717031
     C       1.797849     -0.152150      -0.477153
     O       0.057861     -0.838791      -0.257242
     C      -0.824380      0.108850       0.278525
     O      -0.748082      1.318808      -0.334552
     O      -2.066232     -0.497818       0.206441
     H      -0.605550      0.332382       1.332675
     H       1.542546      0.609836      -1.221181
     H       2.206162     -1.095868      -0.854621
     H      -2.271124     -0.679039      -0.718535
Rotational constants (GHz):    7.6705000    2.3419600    2.0884500
Vibrational harmonic frequencies (cm-1):
     i599.3456                90.0694                139.1698
      185.6023               271.4588                326.6360
      465.8551               482.9129                562.4462
      762.2020               938.8751               1052.1551
     1118.9469              1182.3986               1243.6448
     1246.9340              1289.9468               1372.8197
     1471.2760              1607.2248               3016.3118
     3019.1599              3103.5996               3835.3275
Zero-point correction (Hartree): 0.065577
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*******************************************
Oxylmethylformate subsequent chemistry
M06-2X/aug-cc-pVTZ geometries
*******************************************

HCOOH
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.51744484
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.48986131
     T1 diagnostic:  0.016332
E(MP2/Aug-CC-pVTZ) (Hartree): -189.48638967
E(MP3/Aug-CC-pVTZ) (Hartree): -189.48384440
E(RHF/Aug-CC-pVTZ) (Hartree): -188.84523462
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.76956683
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.420940       0.000000
     O       1.152138      0.110702       0.000000
     O      -1.023538     -0.440647       0.000000
     H      -0.373433      1.449804       0.000000
     H      -0.655373     -1.335884       0.000000
Rotational constants (GHz):   78.0559900   12.2043700   10.5541800
Vibrational harmonic frequencies (cm-1):
      644.1645 (  A')          673.4757 (  A")          1075.4389 (  A")
     1161.5272 (  A')         1317.5161 (  A')          1414.0167 (  A')
     1868.4107 (  A')         3103.4645 (  A')          3792.3575 (  A')
Zero-point correction (Hartree): 0.034287

HCO
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -113.69211748
E(CCSD/Aug-CC-pVTZ) (Hartree): -113.67456249
     T1 diagnostic:  0.021369
E(MP2/Aug-CC-pVTZ) (Hartree): -113.66827147
E(MP3/Aug-CC-pVTZ) (Hartree): -113.66790348
E(PMP2/Aug-CC-pVTZ) (Hartree): -113.67078678
E(PMP3/Aug-CC-pVTZ) (Hartree): -113.66926689
E(PUHF/Aug-CC-pVTZ) (Hartree): -113.29919493
E(UHF/Aug-CC-pVTZ) (Hartree): -113.29522699
E(UM062X/Aug-CC-pVTZ) (Hartree): -113.84942200
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.061713      0.580762       0.000000
     O       0.061713     -0.587049       0.000000
     H      -0.863978      1.211826       0.000000
Rotational constants (GHz):  721.1923700   45.4357100   42.7428700
Vibrational harmonic frequencies (cm-1):
     1101.8843 (  A')          1993.8124 (  A')          2727.4545 (  A')
Zero-point correction (Hartree): 0.013266

HOCH2OC.O
---------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.21709541
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.17151177
     T1 diagnostic:  0.018431
E(MP2/Aug-CC-pVTZ) (Hartree): -303.16145153
E(MP3/Aug-CC-pVTZ) (Hartree): -303.16105873
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.16375746
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.16237172
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.14353131
E(UHF/Aug-CC-pVTZ) (Hartree): -302.13992220
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.63151290
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.066694      0.166321       0.234893
     H      -1.420614      1.412320       0.313955
     O       2.203853      0.275830      -0.032219
     O       0.166117     -0.635384      -0.309551
     C      -1.164430     -0.496060       0.229844
     H      -1.093807     -0.568550       1.315450
     H      -1.713827     -1.331690      -0.188169
     O      -1.768137      0.667848      -0.186938
Rotational constants (GHz):   18.4129700    2.9853700    2.7133900
```

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Vibrational harmonic frequencies (cm-1):
      106.0696                 220.3714                 294.4852
      420.7237                 500.9493                 684.6123
      998.6539                1060.4064                1121.3912
     1176.1738                1308.5897                1402.0903
     1453.6117                1527.9565                1945.5856
     3089.0508                3192.9016                3856.4770
Zero-point correction (Hartree): 0.055496

HOC.HOCHO
---------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.21047619
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.16610758
     T1 diagnostic:  0.017733
E(MP2/Aug-CC-pVTZ) (Hartree): -303.15414763
E(MP3/Aug-CC-pVTZ) (Hartree): -303.15638476
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.15566533
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.15728252
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.14212765
E(UHF/Aug-CC-pVTZ) (Hartree): -302.13959766
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.62637001
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.037909     -0.217984       0.252384
     H       0.633099     -0.913946       0.998396
     O       2.152911     -0.207431      -0.145991
     O       0.114067      0.681352      -0.184782
     C      -1.167793      0.505865       0.250926
     H      -1.759089      1.409860       0.168692
     H      -2.611543     -0.739666       0.097617
     O      -1.702375     -0.659363      -0.204797
Rotational constants (GHz):   19.2927000    3.0762800    2.7716400
Vibrational harmonic frequencies (cm-1):
      112.9870                 145.1878                 285.8411
      343.2471                 530.2830                 689.4076
      901.8811                1048.7629                1076.5543
     1132.4365                1226.4274                1302.9392
     1410.1888                1425.9408                1901.5360
     3063.5228                3176.1170                3882.4355
Zero-point correction (Hartree): 0.053892

CH2O
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.34255830
E(CCSD/Aug-CC-pVTZ) (Hartree): -114.32534109
     T1 diagnostic:  0.015260
E(MP2/Aug-CC-pVTZ) (Hartree): -114.31597316
E(MP3/Aug-CC-pVTZ) (Hartree): -114.32041411
E(RHF/Aug-CC-pVTZ) (Hartree): -113.91461119
E(RM062X/Aug-CC-pVTZ) (Hartree): -114.49897015
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C      -0.000001     -0.525317      -0.000000
     O      -0.000001      0.670465       0.000000
     H       0.938124     -1.105889      -0.000000
     H      -0.938105     -1.105933      -0.000000
Rotational constants (GHz):  284.8986600   39.4617000   34.6607800
Vibrational harmonic frequencies (cm-1):
     1213.9111 (  A")          1273.4438 (  A')          1540.3115 (  A')
     1870.5118 (  A')          2944.9633 (  A')          3014.6814 (  A')
Zero-point correction (Hartree): 0.027014

OMF -> HCOOH + CHO, TS44
------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.17941529
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.12715738
     T1 diagnostic:  0.030828
E(MP2/Aug-CC-pVTZ) (Hartree): -303.11464528
E(MP3/Aug-CC-pVTZ) (Hartree): -303.11008910
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.11998716
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.11321444
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.08547697
E(UHF/Aug-CC-pVTZ) (Hartree): -302.07765661
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.59216326
Electronic state : 2-A
Cartesian coordinates (Angs):
```

```
     C      -1.293384      0.303207      -0.131600
     O      -1.281488     -0.945391      -0.015722
     H      -2.229970      0.801595      -0.396679
     O      -0.268398      1.011233       0.044611
     C       1.017059     -0.148772       0.417226
     O       1.889836     -0.170195      -0.411239
     H       1.148161      0.105293       1.476044
     H       0.020158     -0.998675       0.265686
Rotational constants (GHz):   12.1776000    3.8631600    3.2073400
Vibrational harmonic frequencies (cm-1):
     i793.2751                 168.7008                 287.4403
      414.9059                 558.1697                 628.5966
      861.0649                 978.8680                1081.8503
     1154.1145                1286.9738                1340.8797
     1418.2629                1633.4672                1673.8304
     1721.9430                3026.5481                3112.1766
Zero-point correction (Hartree): 0.048634

OMF -> HOCH2OCO, TS45
---------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.14256547
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.09192113
     T1 diagnostic:  0.046288
E(MP2/Aug-CC-pVTZ) (Hartree): -303.06016040
E(MP3/Aug-CC-pVTZ) (Hartree): -303.06954691
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.07627321
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.08036889
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.06597914
E(UHF/Aug-CC-pVTZ) (Hartree): -302.04610017
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.55568116
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.340542     -0.125102      -0.064226
     O      -0.248112     -1.025656      -0.001712
     C       0.662815     -0.004086       0.236859
     O      -0.606153      1.060883      -0.066222
     H      -1.877757     -0.244859      -1.010819
     H      -2.010574     -0.228958       0.791175
     H       0.539923      0.422201       1.292910
     O       1.781112      0.068116      -0.195699
Rotational constants (GHz):   12.6073800    5.2122300    3.9600200
Vibrational harmonic frequencies (cm-1):
     i877.3566                 228.4867                 431.2304
      600.2353                 729.3374                 850.4220
      952.9691                1039.8023                1067.9315
     1130.3555                1138.4668                1151.2544
     1360.4473                1521.9469                1663.4190
     2497.4589                3036.7337                3100.1704
Zero-point correction (Hartree): 0.051260

OMF -> FAA + H, TS46
--------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.16129228
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.11357836
     T1 diagnostic:  0.024791
E(MP2/Aug-CC-pVTZ) (Hartree): -303.10074217
E(MP3/Aug-CC-pVTZ) (Hartree): -303.09791141
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.10985887
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.10427195
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.09589661
E(UHF/Aug-CC-pVTZ) (Hartree): -302.08493104
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.57599264
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.219142      0.275993      -0.180687
     O      -1.394211     -0.841889       0.173743
     H      -1.974863      0.933728      -0.619933
     O      -0.052024      0.965984      -0.054276
     C       1.123497      0.268385       0.222423
     O       1.471996     -0.699747      -0.389781
     H       1.770481      0.896148       0.843911
     H       0.572160     -0.490932       1.688115
Rotational constants (GHz):   11.1036300    4.4309100    3.5066100
Vibrational harmonic frequencies (cm-1):
     i956.0168                 144.5791                 219.6223
      252.7989                 529.7698                 553.3242
      599.0121                 827.8797                 982.9199
```

```
     1048.3703                1075.9183                1154.7748
     1381.4545                1412.1108                1742.5751
     1886.2094                3085.4052                3105.8394
Zero-point correction (Hartree): 0.045569

OMF -> HOCHOCHO, TS47
---------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.14812004
E(CCSD/Aug-CC-pVTZ) (Hartree): -303.10094027
     T1 diagnostic:  0.020131
E(MP2/Aug-CC-pVTZ) (Hartree): -303.08819808
E(MP3/Aug-CC-pVTZ) (Hartree): -303.08903446
E(PMP2/Aug-CC-pVTZ) (Hartree): -303.09397065
E(PMP3/Aug-CC-pVTZ) (Hartree): -303.09236091
E(PUHF/Aug-CC-pVTZ) (Hartree): -302.06933859
E(UHF/Aug-CC-pVTZ) (Hartree): -302.06131110
E(UM062X/Aug-CC-pVTZ) (Hartree): -303.56410718
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.006762     -0.280406       0.161008
     H       0.551657     -1.163785       0.622229
     O       2.153130     -0.157724      -0.105075
     O       0.114811      0.724392      -0.083074
     C      -1.214753      0.485267       0.134188
     H      -1.793453      1.394628       0.001370
     H      -1.736221     -0.359553       0.942328
     O      -1.739696     -0.704225      -0.228988
Rotational constants (GHz):   18.8600400    3.1193600    2.7597800
Vibrational harmonic frequencies (cm-1):
    i1843.4995                 106.4792                 151.2192
      282.2820                 533.7512                 694.2339
      771.8702                 994.8566                1045.6210
     1068.6520                1188.9094                1252.8215
     1383.8201                1431.0728                1903.7240
     2367.6741                3091.8753                3159.1247
Zero-point correction (Hartree): 0.048817

OMF + O2 -> FAA + HO2
---------------------
E(UM062X/Aug-CC-pVTZ) (Hartree): -453.92410978
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.432764      1.496816      -0.326155
     O       0.910466      1.518029       0.768319
     H       0.774825      2.093835      -1.177031
     O      -0.606547      0.729781      -0.697224
     C      -1.213455     -0.056056       0.321965
     H      -1.213876      0.470788       1.288754
     O      -2.146439     -0.795874      -0.026880
     H      -0.256660     -0.874714       0.595678
     O       0.964703     -1.553289       0.430033
     O       1.550300     -1.190456      -0.559531
Rotational constants (GHz):    2.8062500    2.5345100    1.5922100
Vibrational harmonic frequencies (cm-1):
    i2033.2116                  72.9566                  97.4699
      116.4867                 165.2853                 235.4969
      270.5268                 391.9664                 481.1177
      533.3114                 791.5570                 862.5079
      978.7681                1062.1189                1151.5170
     1195.7914                1287.4894                1337.0430
     1410.3656                1558.3892                1664.6220
     1842.3648                2997.9526                3104.6927
Zero-point correction (Hartree): 0.053787
```

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*****************************************
CH2OO + HNO3
M06-2X/aug-cc-pVTZ geometries
*****************************************

CH2OO
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059345
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649234
     T1 diagnostic:  0.041942
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(RHF/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

HNO3
----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -280.54402243
E(CCSD/Aug-CC-pVTZ) (Hartree): -280.49740022
     T1 diagnostic:  0.018108
E(MP2/Aug-CC-pVTZ) (Hartree): -280.51317330
E(MP3/Aug-CC-pVTZ) (Hartree): -280.48824959
E(RHF/Aug-CC-pVTZ) (Hartree): -279.56683406
E(RM062X/Aug-CC-pVTZ) (Hartree): -280.89732773
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     N       0.000000      0.145325       0.000000
     O       1.164907      0.437371       0.000000
     O      -0.959120      0.842455       0.000000
     O      -0.280304     -1.204622       0.000000
     H       0.596132     -1.618912       0.000000
Rotational constants (GHz):   13.3046700   12.4594900    6.4341100
Vibrational harmonic frequencies (cm-1):
      496.2155 (  A")           621.6413 (  A')           706.6031 (  A')
      825.3552 (  A")           983.8557 (  A')          1359.2234 (  A')
     1416.0794 (  A')          1809.2843 (  A')          3785.4692 (  A')
Zero-point correction (Hartree): 0.027347

HC(O)OOH, peracetic acid
------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.55388215
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.51349546
     T1 diagnostic:  0.018216
E(MP2/Aug-CC-pVTZ) (Hartree): -264.51049726
E(MP3/Aug-CC-pVTZ) (Hartree): -264.50489512
E(RHF/Aug-CC-pVTZ) (Hartree): -263.62462081
E(RM062X/Aug-CC-pVTZ) (Hartree): -264.89723288
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.758185      0.458537      -0.000162
     O      -1.219842     -0.644942       0.000051
     O       0.548967      0.724812       0.000246
     H      -1.311125      1.401734      -0.000420
     O       1.323479     -0.454858      -0.000228
     H       0.639394     -1.153059       0.000835
Rotational constants (GHz):   21.0129500    7.6770400    5.6227700
Vibrational harmonic frequencies (cm-1):
      334.7494                  365.8434                  458.4415
      870.7977                  966.8680                 1034.0207
     1226.8698                 1376.9276                 1514.9791
     1836.2620                 3119.6819                 3622.4221
```

Zero-point correction (Hartree): 0.038109

trans-HONO

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -205.45113499
E(CCSD/Aug-CC-pVTZ) (Hartree): -205.41767135
T1 diagnostic: 0.020536
E(MP2/Aug-CC-pVTZ) (Hartree): -205.42018442
E(MP3/Aug-CC-pVTZ) (Hartree): -205.40914647
E(RHF/Aug-CC-pVTZ) (Hartree): -204.72866693
E(RM062X/Aug-CC-pVTZ) (Hartree): -205.70918527
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):

H	1.753035	-0.148500	0.000000
N	-0.000000	0.507661	0.000000
O	0.882522	-0.566865	0.000000
O	-1.101651	0.141224	0.000000

Rotational constants (GHz): 97.1747900 13.0282200 11.4880200
Vibrational harmonic frequencies (cm-1):

578.9048 (A")	700.9305 (A')	906.1602 (A')
1343.0818 (A')	1841.5251 (A')	3830.3272 (A')

Zero-point correction (Hartree): 0.020961

OCH2OOH

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -265.07057676
E(CCSD/Aug-CC-pVTZ) (Hartree): -265.03520335
T1 diagnostic: 0.018326
E(MP2/Aug-CC-pVTZ) (Hartree): -265.01074185
E(MP3/Aug-CC-pVTZ) (Hartree): -265.02672318
E(PMP2/Aug-CC-pVTZ) (Hartree): -265.01320590
E(PMP3/Aug-CC-pVTZ) (Hartree): -265.02821113
E(PUHF/Aug-CC-pVTZ) (Hartree): -264.15890537
E(UHF/Aug-CC-pVTZ) (Hartree): -264.15485437
E(UM062X/Aug-CC-pVTZ) (Hartree): -265.41391801
Electronic state : 2-A
Cartesian coordinates (Angs):

C	0.701757	0.465507	0.226172
H	1.261922	1.359626	-0.080884
H	0.636488	0.447697	1.327626
O	-0.572987	0.621170	-0.334190
O	1.354666	-0.648511	-0.139437
O	-1.391447	-0.406049	0.200146
H	-1.230804	-1.133247	-0.415923

Rotational constants (GHz): 19.0313900 6.2812400 5.2322300
Vibrational harmonic frequencies (cm-1):

168.8540	310.8469	403.2996
638.9836	843.9612	957.3949
1076.4341	1117.0888	1231.8782
1353.6119	1376.7485	1418.9356
2956.8787	3029.9514	3805.4920

Zero-point correction (Hartree): 0.047136

NO2

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -204.81609875
E(CCSD/Aug-CC-pVTZ) (Hartree): -204.77945274
T1 diagnostic: 0.023733
E(MP2/Aug-CC-pVTZ) (Hartree): -204.79452861
E(MP3/Aug-CC-pVTZ) (Hartree): -204.76835378
E(PMP2/Aug-CC-pVTZ) (Hartree): -204.79825908
E(PMP3/Aug-CC-pVTZ) (Hartree): -204.77013239
E(PUHF/Aug-CC-pVTZ) (Hartree): -204.12249154
E(UHF/Aug-CC-pVTZ) (Hartree): -204.11641281
E(UM062X/Aug-CC-pVTZ) (Hartree): -205.07463512
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):

O	1.090261	-0.137560	0.000000
N	0.000000	0.314396	0.000000
O	-1.090261	-0.137537	0.000000

Rotational constants (GHz): 254.0398200 13.2905900 12.6298400
Vibrational harmonic frequencies (cm-1):

783.4540 (A')	1465.3073 (A')	1775.7005 (A')

Zero-point correction (Hartree): 0.009168

Oxymethylnitrate, OMN (most stable conformer)

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -394.23379279
E(CCSD/Aug-CC-pVTZ) (Hartree): -394.17073599
T1 diagnostic: 0.020198
E(MP2/Aug-CC-pVTZ) (Hartree): -394.16960737
E(MP3/Aug-CC-pVTZ) (Hartree): -394.15671655
E(PMP2/Aug-CC-pVTZ) (Hartree): -394.17208558
E(PMP3/Aug-CC-pVTZ) (Hartree): -394.15821280
E(PUHF/Aug-CC-pVTZ) (Hartree): -392.87429448
E(UHF/Aug-CC-pVTZ) (Hartree): -392.87024018
E(UM062X/Aug-CC-pVTZ) (Hartree): -394.74882939
Electronic state : 2-A
Cartesian coordinates (Angs):

N	0.937134	0.067840	0.014884
O	1.974172	-0.409656	-0.305990
O	0.661906	1.206348	0.263169
O	-0.087769	-0.872968	0.116457
C	-1.370905	-0.299457	0.397272
O	-1.929606	0.341529	-0.625703
H	-1.977744	-1.173151	0.667720
H	-1.306400	0.372988	1.261004

Rotational constants (GHz): 9.0917800 2.7701600 2.3820600
Vibrational harmonic frequencies (cm-1):

90.0505	123.3026	351.7995
486.1988	657.8730	701.3692
816.1559	858.7931	922.7964
1015.5156	1129.1816	1232.4611
1355.0727	1364.1738	1433.0206
1779.4573	3011.9701	3057.0117

Zero-point correction (Hartree): 0.046443

Formylnitrate, FN (most stable conformer)

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.70494676
E(CCSD/Aug-CC-pVTZ) (Hartree): -393.63651504
T1 diagnostic: 0.019449
E(MP2/Aug-CC-pVTZ) (Hartree): -393.65836196
E(MP3/Aug-CC-pVTZ) (Hartree): -393.62191490
E(RHF/Aug-CC-pVTZ) (Hartree): -392.32378716
E(RM062X/Aug-CC-pVTZ) (Hartree): -394.21792689
Electronic state : 1-A
Cartesian coordinates (Angs):

N	0.855381	-0.000101	0.052121
O	1.235131	1.081827	-0.224127
O	1.236265	-1.079635	-0.231791
O	-0.284694	-0.003931	0.971647
C	-1.461473	-0.001390	0.280965
O	-1.554541	0.003439	-0.898498
H	-2.276117	-0.004555	1.011523

Rotational constants (GHz): 7.3252300 3.1288900 3.0215800
Vibrational harmonic frequencies (cm-1):

61.4092	205.0437	255.6672
569.2432	625.9072	683.4889
844.5985	930.4228	1038.8002
1083.0925	1372.2513	1423.1903
1845.7156	1889.9784	3111.0330

Zero-point correction (Hartree): 0.036314

CI+acid complex (most stable conformer)

E(RM062X/Aug-CC-pVTZ) (Hartree): -470.54860235
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.830643	1.028963	-0.368705
O	1.613380	0.343757	0.524786
O	1.919332	-0.949589	0.013292
H	0.978964	0.654748	-1.379941
H	1.074028	2.087095	-0.273043
N	-1.212523	-0.164512	-0.030244
O	-0.540283	1.029345	-0.016760
O	-2.352022	-0.054651	0.266745
O	-0.593435	-1.174454	-0.268878
H	1.075032	-1.319296	-0.076559

Rotational constants (GHz): 5.9240900 2.0907400 1.6490200
Vibrational harmonic frequencies (cm-1):

i730.4856	i44.2626	54.6818

```
      230.1512                 318.0609                 429.2330
      534.0417                 667.9968                 736.1316
      818.1884                 935.9817                 965.3262
     1078.0449                1162.1475                1182.3579
     1312.2408                1347.6334                1388.9176
     1448.8816                1485.8303                1772.2472
     3097.8528                3166.6614                4313.1206
Zero-point correction (Hartree): 0.064804

Hydroperoxymethylnitrate, HPMN (most stable conformer)
------------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.95036473
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.87337363
     T1 diagnostic:  0.017018
E(MP2/Aug-CC-pVTZ) (Hartree): -469.88123192
E(MP3/Aug-CC-pVTZ) (Hartree): -469.85925584
E(RHF/Aug-CC-pVTZ) (Hartree): -468.27998532
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.55598267
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.790471      0.971272       0.419003
     O       1.612927      0.379445      -0.521859
     O       2.108601     -0.857258      -0.037312
     H       0.876807      0.469400       1.378805
     H       1.029516      2.030849       0.474631
     H       1.367469     -1.457466      -0.206122
     O      -0.580695      1.022986      -0.009399
     N      -1.259207     -0.178772       0.012961
     O      -0.643129     -1.161590       0.337762
     O      -2.397975     -0.085960      -0.300700
Rotational constants (GHz):    6.1121200    1.9296300    1.5749300
Vibrational harmonic frequencies (cm-1):
       80.7623                  126.9085                 180.2415
      299.6654                  380.5689                 422.5859
      529.9798                  655.6767                 722.0016
      823.6276                  926.6116                 981.1170
     1012.1124                 1151.9866                1172.7405
     1324.1314                 1380.0858                1440.3152
     1451.8619                 1483.8899                1768.5657
     3118.3638                 3190.1985                3775.3764
Zero-point correction (Hartree): 0.064699

Cycloadduct (most stable conformer)
-----------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.88953075
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.80988951
     T1 diagnostic:  0.018340
E(MP2/Aug-CC-pVTZ) (Hartree): -469.81711908
E(MP3/Aug-CC-pVTZ) (Hartree): -469.79588279
E(RHF/Aug-CC-pVTZ) (Hartree): -468.20194954
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.49184091
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.543901      0.577614       0.036033
     O       1.392453     -0.815283       0.077987
     O       0.233380     -0.942199      -0.687857
     N      -0.688697      0.101820      -0.095381
     O       0.274600      1.070167       0.406923
     H       2.266509      0.873891       0.791103
     H       1.804494      0.904149      -0.971575
     O      -1.498363      0.485445      -0.903481
     O      -1.202897     -0.457691       1.083891
     H      -2.106918     -0.679973       0.812243
Rotational constants (GHz):    5.0192500    2.7306500    2.5674800
Vibrational harmonic frequencies (cm-1):
       89.0630                  255.6779                 325.0519
      426.1669                  486.3418                 499.3203
      594.3205                  682.0447                 700.3262
      747.3068                  851.5898                 993.0381
     1042.9667                 1061.3615                1111.4961
     1178.6704                 1269.9137                1362.4223
     1407.2094                 1519.7142                1565.6174
     3087.3376                 3183.0069                3780.1638
Zero-point correction (Hartree): 0.064290

OMN+HO complex (most stable conformer)
--------------------------------------
```

```
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.88529495
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.81573847
     T1 diagnostic:  0.024205
E(MP2/Aug-CC-pVTZ) (Hartree): -469.79594111
E(MP3/Aug-CC-pVTZ) (Hartree): -469.79722853
E(PMP2/Aug-CC-pVTZ) (Hartree): -469.83078833
E(PMP3/Aug-CC-pVTZ) (Hartree): -469.83158524
E(PUHF/Aug-CC-pVTZ) (Hartree): -468.32798223
E(UHF/Aug-CC-pVTZ) (Hartree): -468.29279675
E(UM062X/Aug-CC-pVTZ) (Hartree): -470.49091025
Electronic state : 1-A
Cartesian coordinates (Angs):
     N      -0.667185     -0.718889       0.096550
     O      -0.628140     -0.027032       1.080438
     O      -1.491876     -1.505771      -0.230208
     O       0.376686     -0.609513      -0.802514
     C       1.406409      0.314208      -0.402303
     O       2.190726     -0.120071       0.574209
     H       1.982036      0.448108      -1.327230
     H       0.957290      1.278090      -0.124556
     H      -1.680001      2.129467       0.477973
     O      -1.075831      2.173801      -0.282952
Rotational constants (GHz):    2.9201900    2.3220500    1.6304100
Vibrational harmonic frequencies (cm-1):
       28.1853                  71.2603                  91.4046
      117.1567                 139.5447                 172.5655
      277.6667                 353.1874                 480.8281
      665.1356                 697.3735                 816.9505
      853.7531                 937.2868                 998.5294
     1136.1011                1236.0830                1344.7398
     1353.7612                1432.9206                1761.8159
     2985.6154                3044.2766                3760.8128
Zero-point correction (Hartree): 0.056400

1,2-insertion, TS28
-------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.88712380
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.80757664
     T1 diagnostic:  0.022820
E(MP2/Aug-CC-pVTZ) (Hartree): -469.81376011
E(MP3/Aug-CC-pVTZ) (Hartree): -469.78922291
E(RHF/Aug-CC-pVTZ) (Hartree): -468.21479831
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.49053505
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.401972      1.008892      -0.386186
     O      -2.154430      0.018645      -0.295645
     O      -1.700160     -0.895496       0.675397
     H      -1.644867      1.663316      -1.218215
     H      -0.634322      1.211514       0.364900
     O       0.392980     -0.567207      -0.611592
     H      -0.716045     -0.955614       0.321251
     N       1.405125     -0.021317       0.008867
     O       1.143094      0.723244       0.960258
     O       2.514915     -0.257104      -0.380029
Rotational constants (GHz):    6.3176200    1.5097900    1.4650200
Vibrational harmonic frequencies (cm-1):
     i243.3734                 61.2526                 113.0834
      189.0074                288.6068                 373.9268
      561.8122                722.7173                 740.3397
      771.2565                863.7673                 935.1076
     1045.4661               1075.4177                1180.8953
     1274.6195               1346.1874                1465.5726
     1596.7841               1638.8609                1652.3850
     2459.1639               3032.2844                3230.8573
Zero-point correction (Hartree): 0.060643

1,4-insertion, TS29
-------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.89811236
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.81875015
     T1 diagnostic:  0.022892
E(MP2/Aug-CC-pVTZ) (Hartree): -469.82438182
E(MP3/Aug-CC-pVTZ) (Hartree): -469.80043657
E(RHF/Aug-CC-pVTZ) (Hartree): -468.22742907
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.50271451
Electronic state : 1-A
```

```
Cartesian coordinates (Angs):
     C       1.695521     -1.055465       0.108073
     O       1.892588      0.010824      -0.484054
     O       1.565994      1.133411       0.300916
     H       1.486241     -1.052105       1.169184
     H       1.843027     -1.955655      -0.478013
     N      -1.360962     -0.063610       0.002315
     O      -0.604642     -1.033689       0.161378
     O      -0.838431      1.131053      -0.069022
     O      -2.546374     -0.158043      -0.093757
     H       0.271257      1.117371       0.120500
Rotational constants (GHz):    5.9046400    1.7363300    1.3980600
Vibrational harmonic frequencies (cm-1):
     i230.4344                  56.6688                  91.1747
      196.5019                 326.6665                 387.4907
      524.3226                 676.9178                 722.6194
      754.3822                 846.5635                 897.5647
     1052.2495                1098.9975                1176.4614
     1235.5197                1259.1119                1450.8457
     1519.9260                1651.9874                1685.6366
     1796.8493                3153.4360                3295.2277
Zero-point correction (Hartree): 0.058907

HPMN -> HC(O)OOH + HONO, TS31 (most stable conformer)
-----------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.88125089
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.79124193
     T1 diagnostic:  0.021904
E(MP2/Aug-CC-pVTZ) (Hartree): -469.82032336
E(MP3/Aug-CC-pVTZ) (Hartree): -469.77625333
E(RHF/Aug-CC-pVTZ) (Hartree): -468.15710165
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.47637678
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.933388     -0.927429       0.126464
     H      -0.087574     -0.509710       1.049606
     H      -1.264975     -1.884920       0.538077
     O      -2.011086     -0.027473       0.156017
     N       1.394888      0.027545      -0.004274
     O       1.099689      0.063797       1.171463
     O      -0.117020     -0.896479      -0.833363
     O       2.379125      0.399119      -0.531004
     O      -1.513689      1.270375      -0.117196
     H      -1.507492      1.291677      -1.083888
Rotational constants (GHz):    5.1523300    1.7224000    1.6269600
Vibrational harmonic frequencies (cm-1):
    i1674.2788                  98.2909                 110.7183
      218.9661                 286.2040                 352.7688
      382.2403                 459.2239                 560.3802
      636.4945                 739.1975                 843.1859
      942.5268                1056.9864                1096.6773
     1207.2869                1308.1995                1398.4501
     1422.8919                1517.3867                1655.5231
     1866.5715                3086.4757                3800.2945
Zero-point correction (Hartree): 0.057061

HPMN -> HCOOH + HNO3, TS32 (most stable conformer)
--------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.87477116
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.79388246
     T1 diagnostic:  0.022039
E(MP2/Aug-CC-pVTZ) (Hartree): -469.80069546
E(MP3/Aug-CC-pVTZ) (Hartree): -469.77570951
E(RHF/Aug-CC-pVTZ) (Hartree): -468.19446559
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.47649259
Electronic state : 1-A
Cartesian coordinates (Angs):
     N       1.576744     -0.145001      -0.006186
     O       1.386759      1.144681      -0.087960
     O       0.588894     -0.839330       0.307455
     O       2.658809     -0.588659      -0.229832
     C      -1.008525      0.637932       0.480690
     O      -1.835551      0.384831      -0.431403
     H      -1.268850      0.212635       1.451907
     H       0.235725      1.213387       0.148453
     O      -2.896559     -0.521590      -0.005589
     H      -3.171762     -0.878064      -0.862566
```

```
Rotational constants (GHz):    8.0130800    1.2409500    1.1276900
Vibrational harmonic frequencies (cm-1):
     i900.1953                   66.1337                   97.1363
      106.2566                  125.7080                  290.0252
      309.0092                  451.0217                  611.1535
      736.2568                  812.9882                  849.9024
      857.3239                 1021.7980                 1081.1936
     1245.9017                 1327.0503                 1389.3525
     1451.5258                 1507.7831                 1636.9584
     1798.2719                 3117.7645                 3808.3287
Zero-point correction (Hartree): 0.056268

HPMN -> cycloadduct, TS33
-------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.86685754
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.78328607
     T1 diagnostic:  0.025279
E(MP2/Aug-CC-pVTZ) (Hartree): -469.79160877
E(MP3/Aug-CC-pVTZ) (Hartree): -469.76540175
E(RHF/Aug-CC-pVTZ) (Hartree): -468.17218969
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.46781641
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.312871     -0.833241       0.021399
     O       1.678614      0.467410      -0.055201
     O       0.618027      1.113177       0.628024
     N      -0.905186     -0.169717      -0.029961
     O       0.012890     -0.940892      -0.666733
     H       1.981483     -1.460531      -0.560241
     H       1.153157     -1.174828       1.045740
     O      -1.571458     -0.631629       0.809785
     O      -1.272492      0.914556      -0.713265
     H      -0.400211      1.441850      -0.425046
Rotational constants (GHz):    4.8120000    2.6868700    2.2386700
Vibrational harmonic frequencies (cm-1):
     i925.6455                  118.7407                  244.7484
      355.6784                  402.0070                  519.6805
      561.3424                  668.1461                  685.7659
      762.2047                  872.5799                  986.1153
     1024.4220                 1053.6313                 1168.9173
     1181.5132                 1294.9108                 1307.1683
     1398.9907                 1498.0419                 1758.4086
     2433.7350                 3085.8417                 3195.4544
Zero-point correction (Hartree): 0.060549

HPMN -> FN + H2O, TS34
----------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.85958301
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.77043775
     T1 diagnostic:  0.022438
E(MP2/Aug-CC-pVTZ) (Hartree): -469.79385269
E(MP3/Aug-CC-pVTZ) (Hartree): -469.75268805
E(RHF/Aug-CC-pVTZ) (Hartree): -468.13716674
E(RM062X/Aug-CC-pVTZ) (Hartree): -470.45255296
Electronic state : 1-A
Cartesian coordinates (Angs):
     O      -0.306321     -0.717787       0.340001
     C       0.765666      0.127328       0.662153
     O       1.382318      0.690104      -0.329845
     H       0.623413      0.725471       1.558841
     O       2.685182     -0.475920      -0.339737
     H       3.543588     -0.034673      -0.212098
     H       1.875639     -0.653377       0.694191
     N      -1.478566     -0.021003      -0.051290
     O      -1.421143      1.171013      -0.063756
     O      -2.375869     -0.749205      -0.313515
Rotational constants (GHz):    7.5590900    1.4899300    1.3460000
Vibrational harmonic frequencies (cm-1):
    i2574.5828                  87.5386                   88.7084
      160.6172                 271.9400                  352.1499
      474.4871                 517.3365                  644.4907
      664.4059                 776.2414                  811.3115
      874.0596                 924.9016                  932.8563
     1089.9319                1270.7736                 1320.5975
     1337.4577                1424.1542                 1713.4079
     1789.0174                3144.7083                 3740.7443
Zero-point correction (Hartree): 0.055614
```

```
OMN---OH -> FN + H2O, TS37 (most stable conformer)
--------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -469.88486776
E(CCSD/Aug-CC-pVTZ) (Hartree): -469.81352989
     T1 diagnostic:  0.027368
E(MP2/Aug-CC-pVTZ) (Hartree): -469.79207657
E(MP3/Aug-CC-pVTZ) (Hartree): -469.79266364
E(PMP2/Aug-CC-pVTZ) (Hartree): -469.83395581
E(PMP3/Aug-CC-pVTZ) (Hartree): -469.83374131
E(PUHF/Aug-CC-pVTZ) (Hartree): -468.32561824
E(UHF/Aug-CC-pVTZ) (Hartree): -468.28321604
E(UM062X/Aug-CC-pVTZ) (Hartree): -470.49004227
Electronic state : 1-A
Cartesian coordinates (Angs):
     N      -1.119766      0.178357       0.060183
     O      -0.512753      0.752658       0.925455
     O      -2.272019      0.236120      -0.207317
     O      -0.405509     -0.671450      -0.769373
     C       0.953887     -0.917165      -0.363962
     O       1.104178     -1.600817       0.734018
     H       1.397281     -1.392279      -1.249104
     H       1.506323      0.063655      -0.246935
     O       1.839722      1.729743      -0.318336
     H       1.182479      2.013088       0.342951
Rotational constants (GHz):    3.1578700    2.1556700    1.5807800
Vibrational harmonic frequencies (cm-1):
     i219.1317                  54.1330                  93.2309
      146.8438                 165.4901                 319.3117
      333.0031                 486.8611                 510.6331
      660.0905                 703.9206                 809.6585
      852.3100                 931.3216                 986.2954
     1097.6638                1199.4365                1290.1369
     1340.7142                1421.6687                1770.2606
     2316.2640                3031.4845                3736.3481
Zero-point correction (Hartree): 0.055262
```

```
*****************************************
CH2OO + HCl
M06-2X/aug-cc-pVTZ geometries
*****************************************

HCl
---
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -460.34324110
E(CCSD/Aug-CC-pVTZ) (Hartree): -460.33472213
     T1 diagnostic:  0.006077
E(MP2/Aug-CC-pVTZ) (Hartree): -460.31512054
E(MP3/Aug-CC-pVTZ) (Hartree): -460.33545881
E(RHF/Aug-CC-pVTZ) (Hartree): -460.10755138
E(RM062X/Aug-CC-pVTZ) (Hartree): -460.80750693
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
     H       0.000000      0.000000      -1.207655
    Cl       0.000000      0.000000       0.071039
Rotational constants (GHz):    0.0000000  315.5287808  315.5287808
Vibrational harmonic frequencies (cm-1):
     2991.1156 (  SG)
Zero-point correction (Hartree): 0.006814

ClCH2O.
-------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -574.03044193
E(CCSD/Aug-CC-pVTZ) (Hartree): -574.00576311
     T1 diagnostic:  0.019819
E(MP2/Aug-CC-pVTZ) (Hartree): -573.96923863
E(MP3/Aug-CC-pVTZ) (Hartree): -574.00213643
E(PMP2/Aug-CC-pVTZ) (Hartree): -573.97181030
E(PMP3/Aug-CC-pVTZ) (Hartree): -574.00371958
E(PUHF/Aug-CC-pVTZ) (Hartree): -573.41388435
E(UHF/Aug-CC-pVTZ) (Hartree): -573.40971506
E(UM062X/Aug-CC-pVTZ) (Hartree): -574.65811913
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.644503      0.497306      -0.000028
     O      -1.582324     -0.435227      -0.000024
     H      -0.754476      1.133364      -0.887753
     H      -0.754768      1.132994       0.888047
    Cl       1.060874     -0.104022       0.000004
Rotational constants (GHz):   48.4462500    5.8047800    5.3583500
Vibrational harmonic frequencies (cm-1):
      403.4646                 666.1336                 710.1918
     1064.7767                1121.6379                1283.2814
     1348.7683                2988.6614                3033.1917
Zero-point correction (Hartree): 0.028751

OH
--
E(CCSD(T)/Aug-CC-pVTZ) (Hartree):  -75.64558510
E(CCSD/Aug-CC-pVTZ) (Hartree):  -75.63969539
     T1 diagnostic:  0.010035
E(MP2/Aug-CC-pVTZ) (Hartree):  -75.62633030
E(MP3/Aug-CC-pVTZ) (Hartree):  -75.63789504
E(PMP2/Aug-CC-pVTZ) (Hartree):  -75.62832143
E(PMP3/Aug-CC-pVTZ) (Hartree):  -75.63903850
E(PUHF/Aug-CC-pVTZ) (Hartree):  -75.42490330
E(UHF/Aug-CC-pVTZ) (Hartree):  -75.42155017
E(UM062X/Aug-CC-pVTZ) (Hartree):  -75.73381011
Point group : C*V
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.108021
     H       0.000000      0.000000      -0.864170
Rotational constants (GHz):    0.0000000  563.9825141  563.9825141
Vibrational harmonic frequencies (cm-1):
     3766.2002 (  SG)
Zero-point correction (Hartree): 0.008580

ClCHO
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -573.50100832
E(CCSD/Aug-CC-pVTZ) (Hartree): -573.47210921
     T1 diagnostic:  0.015681
```

```
E(MP2/Aug-CC-pVTZ) (Hartree): -573.45675014
E(MP3/Aug-CC-pVTZ) (Hartree): -573.46906011
E(RHF/Aug-CC-pVTZ) (Hartree): -572.86769340
E(RM062X/Aug-CC-pVTZ) (Hartree): -574.12861063
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.674269      0.422769      -0.000009
     O       1.571230     -0.336318       0.000000
     H       0.744716      1.514409       0.000044
    Cl      -1.021187     -0.080028       0.000001
Rotational constants (GHz):   78.5368000    6.1679000    5.7187800
Vibrational harmonic frequencies (cm-1):
      467.7809                754.2822                969.6152
     1338.6354               1891.0664               3092.3194
Zero-point correction (Hartree): 0.019396

ClCH2OOH
--------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -649.75100907
E(CCSD/Aug-CC-pVTZ) (Hartree): -649.71256270
     T1 diagnostic:  0.012533
E(MP2/Aug-CC-pVTZ) (Hartree): -649.68664600
E(MP3/Aug-CC-pVTZ) (Hartree): -649.70897422
E(RHF/Aug-CC-pVTZ) (Hartree): -648.82412658
E(RM062X/Aug-CC-pVTZ) (Hartree): -650.46865024
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.005861      0.849992       0.257565
     O       1.126781      0.475491      -0.427418
     O       1.671821     -0.664884       0.211135
     H       0.153624      0.857815       1.331443
     H      -0.296106      1.817675      -0.137810
     H       1.202826     -1.387374      -0.231252
    Cl      -1.377294     -0.286642      -0.045736
Rotational constants (GHz):   14.6449300    3.6309200    3.1365400
Vibrational harmonic frequencies (cm-1):
      163.4725                301.1994                383.3143
      521.8939                720.2731                949.9351
     1032.1966               1147.4318               1287.6198
     1341.7928               1431.4200               1473.7580
     3122.2110               3203.2852               3780.7551
Zero-point correction (Hartree): 0.047524

ClCH2O+HO complex (most stable conformer)
-----------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -649.68140374
E(CCSD/Aug-CC-pVTZ) (Hartree): -649.64963180
     T1 diagnostic:  0.020287
E(MP2/Aug-CC-pVTZ) (Hartree): -649.60002483
E(MP3/Aug-CC-pVTZ) (Hartree): -649.64369842
E(PMP2/Aug-CC-pVTZ) (Hartree): -649.62335076
E(PMP3/Aug-CC-pVTZ) (Hartree): -649.66692702
E(PUHF/Aug-CC-pVTZ) (Hartree): -648.85284596
E(UHF/Aug-CC-pVTZ) (Hartree): -648.82936201
E(UM062X/Aug-CC-pVTZ) (Hartree): -650.39995546
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.662630     -0.615302       0.017873
     O       1.974928     -0.666592      -0.020763
    Cl      -0.051341      1.067266       0.002427
     H       0.223910     -1.136296      -0.842999
     H       0.274754     -1.095919       0.925300
     H      -2.627998     -0.049179      -0.109123
     O      -2.096633     -0.854697       0.005554
Rotational constants (GHz):    7.5263600    3.4450600    2.3992400
Vibrational harmonic frequencies (cm-1):
       70.2813                 110.7792                 155.2289
      167.8393                 371.8375                 398.0221
      678.3281                 708.8506                1077.0904
     1136.1847                1276.2206                1334.4863
     2992.5229                3031.6413                3773.1742
Zero-point correction (Hartree): 0.039372

ClCH2OOH -> ClCH2O+HO, TS41
---------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -649.68026365
E(CCSD/Aug-CC-pVTZ) (Hartree): -649.64895167
```

```
     T1 diagnostic:  0.024447
E(MP2/Aug-CC-pVTZ) (Hartree): -649.59926662
E(MP3/Aug-CC-pVTZ) (Hartree): -649.64340836
E(PMP2/Aug-CC-pVTZ) (Hartree): -649.62189919
E(PMP3/Aug-CC-pVTZ) (Hartree): -649.66594612
E(PUHF/Aug-CC-pVTZ) (Hartree): -648.85331124
E(UHF/Aug-CC-pVTZ) (Hartree): -648.83053198
E(UM062X/Aug-CC-pVTZ) (Hartree): -650.39855508
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.335534      0.893675       0.409714
     O       0.628084      1.303343      -0.406189
    Cl      -1.178589     -0.617098      -0.104456
     H       0.080353      0.701021       1.405229
     H      -1.099386      1.676815       0.490887
     O       1.984141     -0.894703       0.172036
     H       2.170450     -0.518341      -0.705416
Rotational constants (GHz):    6.7943500    3.7867600    2.6372500
Vibrational harmonic frequencies (cm-1):
     i148.5695                 103.0936                 133.8814
      170.2661                 297.7991                 406.3078
      707.2572                 728.9650                1099.0182
     1110.7990                1286.5917                1352.9891
     3003.6483                3054.9500                3757.8440
Zero-point correction (Hartree): 0.039215

ClCH2OOH -> ClCHO + H2O, TS43
-----------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -649.66308570
E(CCSD/Aug-CC-pVTZ) (Hartree): -649.61147693
     T1 diagnostic:  0.021706
E(MP2/Aug-CC-pVTZ) (Hartree): -649.60079360
E(MP3/Aug-CC-pVTZ) (Hartree): -649.60504850
E(RHF/Aug-CC-pVTZ) (Hartree): -648.68152468
E(RM062X/Aug-CC-pVTZ) (Hartree): -650.36483997
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.012851      0.524010       0.440727
     O       0.879263      0.816784      -0.445889
     H      -0.162517      1.236855       1.247014
     O       1.886418     -0.607361       0.071356
     H       2.662021     -1.095657      -0.272159
     H       0.739495     -0.414156       0.903588
    Cl      -1.496562     -0.267440      -0.089796
Rotational constants (GHz):   15.0978000    3.0940100    2.8003100
Vibrational harmonic frequencies (cm-1):
    i2032.2364                 176.1973                 213.4354
      416.2936                 566.6830                 627.1558
      744.2539                 877.0062                1091.2713
     1233.7765                1264.9250                1358.2245
     1773.1924                3104.6348                3646.7270
Zero-point correction (Hartree): 0.038942
```

```
*****************************************
CH2OO + CH2CHOH
M06-2X/aug-cc-pVTZ geometries
*****************************************

CH2OO
-----
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059345
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649234
     T1 diagnostic:  0.041942
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(RHF/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

CH2=CHOH,
---------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -153.58054121
E(CCSD/Aug-CC-pVTZ) (Hartree): -153.55517337
     T1 diagnostic:  0.012426
E(MP2/Aug-CC-pVTZ) (Hartree): -153.53587195
E(MP3/Aug-CC-pVTZ) (Hartree): -153.55238821
E(RHF/Aug-CC-pVTZ) (Hartree): -152.95669470
E(RM062X/Aug-CC-pVTZ) (Hartree): -153.80587832
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.219253     -0.180276      -0.000035
     C       0.037664      0.411843      -0.000033
     H       1.303090     -1.257404      -0.000097
     H       2.115217      0.418739       0.000122
     H      -0.064302      1.491296       0.000130
     O      -1.127368     -0.293244       0.000029
     H      -1.876564      0.303921       0.000020
Rotational constants (GHz):   64.4792800   10.5381100    9.0577600
Vibrational harmonic frequencies (cm-1):
      296.9962                  483.3678                  726.4621
      888.7454                  968.7835                  995.1580
     1157.4689                 1295.1385                 1353.9305
     1438.7429                 1757.3358                 3179.3193
     3197.8802                 3293.5055                 3917.4984
Zero-point correction (Hartree): 0.056841

CI+CH2CHOH complex
------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -342.92997017
E(CCSD/Aug-CC-pVTZ) (Hartree): -342.86989793
     T1 diagnostic:  0.027183
E(MP2/Aug-CC-pVTZ) (Hartree): -342.84167729
E(MP3/Aug-CC-pVTZ) (Hartree): -342.85633061
E(RHF/Aug-CC-pVTZ) (Hartree): -341.60558522
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40360226
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.356384      1.039519      -0.433361
     O      -1.423808     -0.193805      -0.422898
     O      -1.283767     -0.801504       0.809338
     H      -1.284010      1.575949       0.503728
     H      -1.421722      1.508468      -1.407401
     C       1.660621      0.052140      -0.277138
     C       1.353029      1.001186       0.611911
     O       1.138127     -1.173327      -0.351655
     H       2.401124      0.221805      -1.050659
```

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     H       0.377508     -1.260405       0.265475
     H       1.855712      1.954544       0.566359
     H       0.683373      0.791656       1.435744
Rotational constants (GHz):    5.1878600    2.5398700    2.1165500
Vibrational harmonic frequencies (cm-1):
      103.0136                 111.0952                 149.0345
      201.7623                 240.2419                 279.0855
      517.3297                 530.7867                 698.5054
      748.4924                 857.9073                 884.5844
      898.5136                 989.9346                1049.5649
     1072.2650                1211.1017                1249.8447
     1344.4996                1414.8470                1442.8274
     1462.6650                1659.0652                1695.8870
     3150.4148                3174.7726                3188.0447
     3278.7248                3294.8948                3411.5965
Zero-point correction (Hartree): 0.091836

1,4-insertion TS
----------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -342.92744929
E(CCSD/Aug-CC-pVTZ) (Hartree): -342.86581206
     T1 diagnostic:  0.025229
E(MP2/Aug-CC-pVTZ) (Hartree): -342.84188755
E(MP3/Aug-CC-pVTZ) (Hartree): -342.85345582
E(RHF/Aug-CC-pVTZ) (Hartree): -341.59686652
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40228204
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.083833      1.099977      -0.359240
     O      -1.304513     -0.119220      -0.507792
     O      -1.302926     -0.837159       0.706217
     H      -1.225411      1.550869       0.612386
     H      -0.992361      1.675960      -1.272374
     C       1.560167     -0.009284      -0.235655
     C       1.185091      0.995111       0.587744
     O       1.037958     -1.210839      -0.272206
     H       2.333568      0.137668      -0.983749
     H       0.197783     -1.259510       0.294333
     H       1.689915      1.946597       0.524866
     H       0.583795      0.771342       1.457696
Rotational constants (GHz):    5.1854300    3.0068200    2.3475400
Vibrational harmonic frequencies (cm-1):
     i211.5485                 147.0566                 200.1634
      253.6278                 310.6034                 366.8650
      510.9476                 541.7775                 758.2784
      777.6120                 871.1081                 887.7217
     1011.8775                1019.2378                1053.6915
     1138.6416                1234.4666                1263.7028
     1340.3992                1424.9406                1443.4236
     1498.2247                1603.6695                1673.4351
     2785.4968                3154.8195                3171.4286
     3182.2704                3281.4250                3293.7753
Zero-point correction (Hartree): 0.091584

3-hydroxy-propanal (most stable conformer characterized)
--------------------------------------------------------
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -343.01343789
E(CCSD/Aug-CC-pVTZ) (Hartree): -342.95837468
     T1 diagnostic:  0.014192
E(MP2/Aug-CC-pVTZ) (Hartree): -342.93293798
E(MP3/Aug-CC-pVTZ) (Hartree): -342.94963403
E(RHF/Aug-CC-pVTZ) (Hartree): -341.69630570
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.48706287
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.489567      0.148976      -0.222383
     O      -1.554269     -1.045770      -0.092664
     H      -2.113407      0.655566      -0.980321
     C      -0.541358      1.001052       0.573768
     C       0.806658      1.078932      -0.157442
     O       1.224256     -0.174143      -0.649093
     O       1.332990     -1.063294       0.452666
     H       0.470045     -1.509248       0.422320
     H      -0.936497      2.008619       0.700431
     H      -0.398368      0.541064       1.549284
     H       0.739053      1.697157      -1.053511
     H       1.560955      1.498732       0.510864
```

```
Rotational constants (GHz):    5.3350600    3.1948800    2.3829600
Vibrational harmonic frequencies (cm-1):
       89.4057                  147.3352                  223.2800
      236.5922                  383.5587                  511.1711
      526.6140                  562.8198                  830.7220
      894.6164                  951.3866                 1000.6565
     1027.1569                 1124.8708                 1159.3287
     1236.8997                 1271.9131                 1341.2210
     1392.5947                 1427.4218                 1460.3028
     1479.1276                 1492.5346                 1845.2229
     2970.2095                 3066.6711                 3096.2029
     3121.0205                 3156.9831                 3717.9731
Zero-point correction (Hartree): 0.095104

3-oxo-1-propoxyl (most stable conformer characterized)
------------------------------------------------------
E(UM062X/Aug-CC-pVTZ) (Hartree): -267.67280223
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.094731     -0.089030       0.359516
     O       2.123691     -0.355456      -0.191812
     H       0.872683     -0.501613       1.364445
     C       0.037094      0.820083      -0.214455
     C      -1.363570      0.365830       0.169643
     O      -1.653358     -0.916877      -0.210739
     H       0.215440      1.824649       0.181983
     H       0.158567      0.862229      -1.295653
     H      -1.481234      0.355543       1.268684
     H      -2.137656      1.056555      -0.187272
Rotational constants (GHz):   12.7632600    2.9880200    2.6475100
Vibrational harmonic frequencies (cm-1):
       64.4698                  122.9380                  253.6223
      426.1323                  565.3704                  648.9623
      752.5865                  945.1193                 1000.7239
     1064.9955                 1087.0289                 1179.7949
     1231.5828                 1322.6824                 1373.5397
     1384.7482                 1437.4894                 1450.0143
     1871.4959                 2930.7056                 2944.4386
     3022.0378                 3060.4086                 3137.5666
Zero-point correction (Hartree): 0.075814

propanedial
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -266.75372159
E(CCSD/Aug-CC-pVTZ) (Hartree): -266.70987404
     T1 diagnostic:  0.015527
E(MP2/Aug-CC-pVTZ) (Hartree): -266.69188741
E(MP3/Aug-CC-pVTZ) (Hartree): -266.70172567
E(RHF/Aug-CC-pVTZ) (Hartree): -265.73790026
E(RM062X/Aug-CC-pVTZ) (Hartree): -267.13737778
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.391919      0.328222      -0.088912
     O      -1.671854     -0.837619      -0.072561
     H      -2.172438      1.094573      -0.245339
     C       0.007709      0.857646       0.093923
     C       1.029682     -0.233232       0.298993
     O       2.078223     -0.261086      -0.280703
     H       0.760249     -1.010976       1.032100
     H       0.286390      1.479129      -0.758658
     H       0.002013      1.511095       0.973986
Rotational constants (GHz):   14.4778200    3.1494600    2.7331100
Vibrational harmonic frequencies (cm-1):
       67.5311                  110.0831                  246.4078
      470.4596                  655.9543                  696.4091
      870.1035                  934.6797                 1081.0926
     1107.9255                 1227.1283                 1324.5476
     1417.7267                 1424.4123                 1441.6093
     1856.0048                 1871.0774                 2967.2044
     3002.8260                 3049.3855                 3113.7125
Zero-point correction (Hartree): 0.065922
```