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

Theoretical study of the OH-initiated atmospheric oxidation mechanism of perfluoro methyl vinyl ether, $CF_3OCF=CF_2$

– Supporting Information –

L.Vereecken, J. N. Crowley, D. Amedro

Table of content

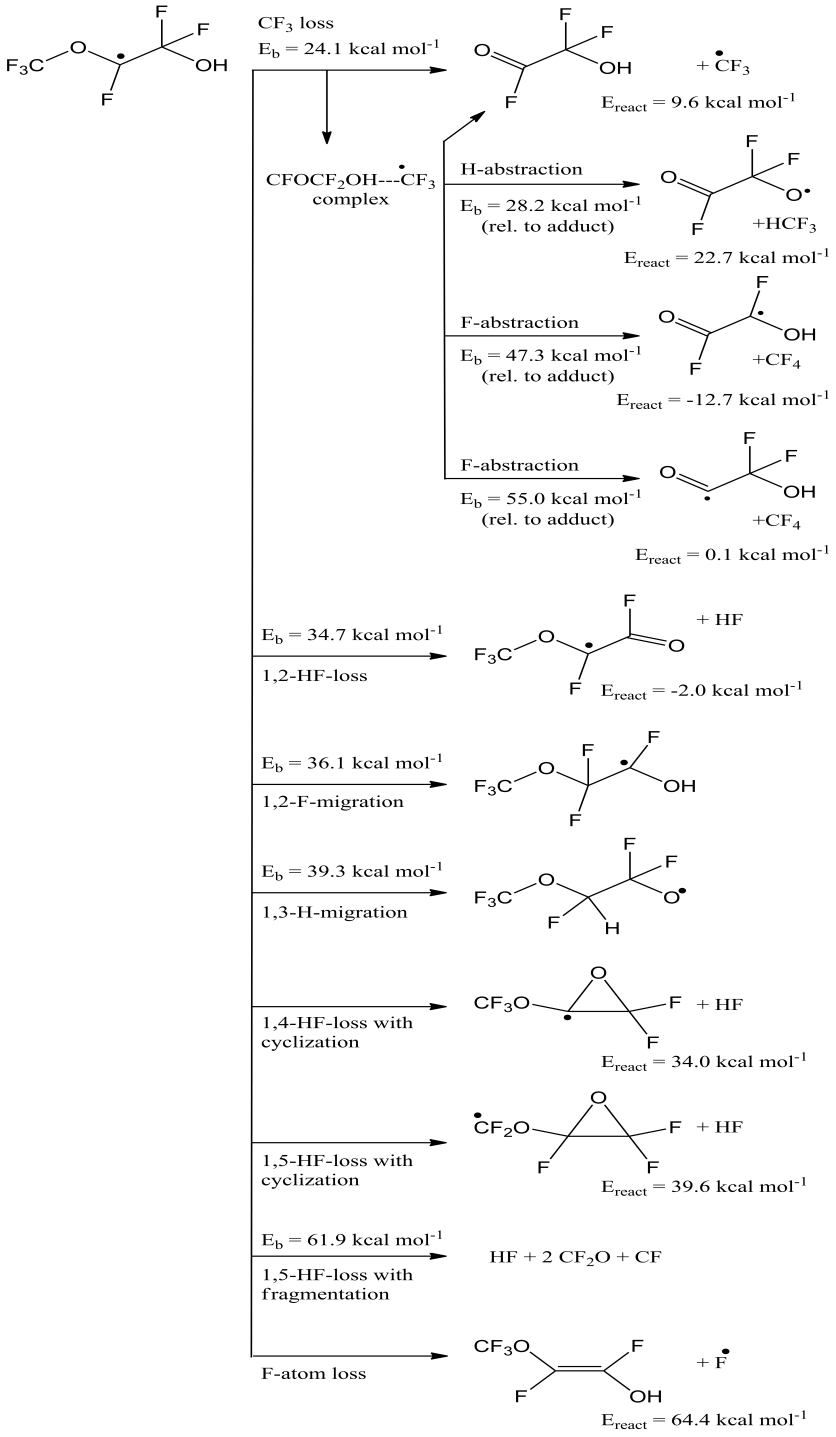

Figure SI - 1: All pathways considered for the main adduct, at the M06-2X/aug-cc-pVTZ level of theory.

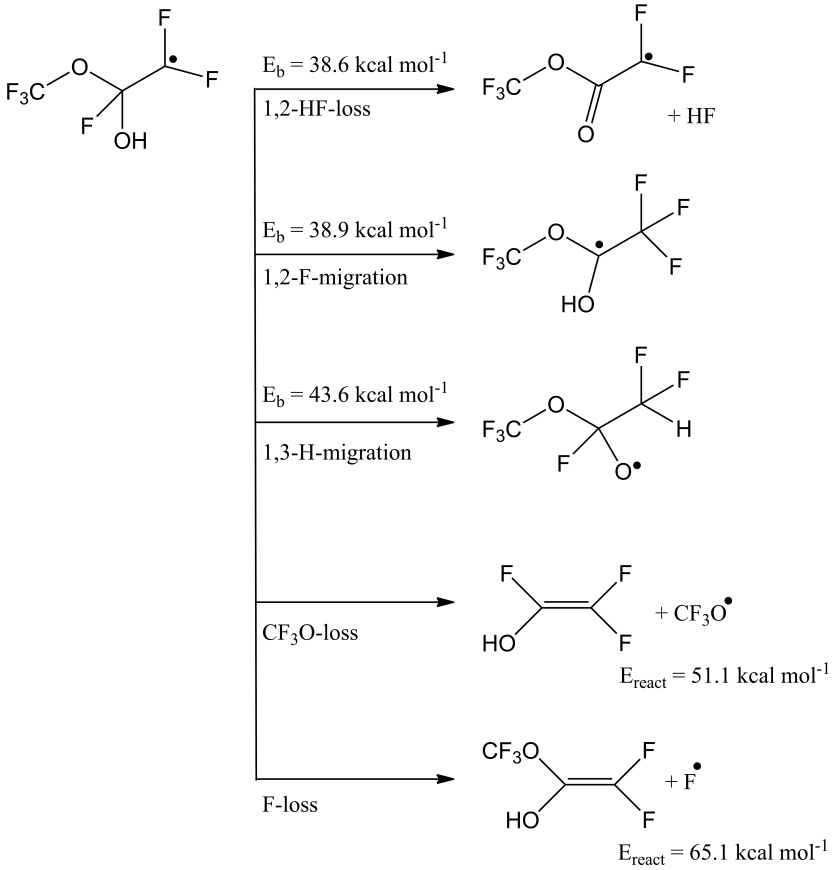

Figure SI - 2: All pathways considered for the minor adduct, at the M06-2X/aug-cc-pVTZ level of theory.

CCSD(T) a*b initio* calculations

To assess the robustness of the M06-2X/aug-cc-pVTZ calculations, we compared these against single point energy calculations at the CCSD(T)/6-311++G(d,p), CCSD(T)/aug-cc-pVDZ, and CCSD(T)-F12a/aug-cc-pVDZ levels of theory (see Table SI-1); the raw data on all compounds discussed in the paper are listed further in this supporting information. The CCSD(T) calculations were obtained using Gaussian-09, the CCSD(T)-F12 results with Molpro 2010.1. While these calculations are based on coupled cluster theory, they are not *a priori* more reliable than the M06-2X calculations, as the CC predictions still carry uncertainties of several kcal/mol due to the small size of the basis set, which limits the flexibility in accounting for electron correlation. 6-311++G(d,p) and aug-cc-pVDZ basis sets are similar in size, where the first basis set is rather small but reasonably balanced due to its use of split valence orbitals, while the latter has ~20% more Gaussian primitives and is part of a systematic series of basis sets that allows for extrapolation to the complete basis set. For basis sets of this size, errors on absolute CCSD(T) atomization energies are reported of up to several tens of kcal/mol (see e.g. D. Feller, K. A. Peterson, J. Chem. Phys., 2007, 126, 114105 ; K. A. Peterson, D. Feller, D. A. Dixon, Theor. Chem. Acc., 2012, 131, 1079). Cancellation of error leads to *relative* energies that are significantly more reliable, but non-negligible uncertainties remain especially for free products/reactants or for barrier heights for bimolecular reactions, where the cancellation of error is least effective due to significant differences in bond types and bonding partners on either side of the chemical equation. For example, the predicted relative energy of some sets of products differs as much as 7 kcal mol^{-1} among the CC levels of theory, despite using the same geometry and a similarly sized basis set. For the unimolecular reactions listed in Table SI-1, the average unsigned difference (MUE) between the M06-2X barrier height and the CCSD(T)/6-311++G(d,p) barrier height is 2.5 kcal/mol, against CCSD(T)/aug-cc-pVDZ it is 2.1 kcal/mol. In these values, the "$CF_3OC^{\bullet}FCF_2OH$ 1,5-HF-loss with fragmentation" reaction (see figure SI-1) has a disproportionate impact; it leads to 4 fragments in a single decomposition TS and thus represents an extreme change in bonding. Without this reaction M06-2X and CCSD(T) with a small basis set agree on average within ~2 kcal/mol on the barrier heights.

Preferably one would use larger basis sets in the coupled cluster calculations, such as aug-cc-pVTZ and beyond, and extrapolate the energies to the basis set limit. Unfortunately, with up to 12 non-hydrogen atoms and open shell wave functions, these calculations are beyond our computational capabilities. CCSD(T)-F12 explicitly correlated methodologies converge significantly faster to the complete basis set limit, but CCSD(T)-F12/aug-cc-pVDZ still shows sizable uncertainties even when these are up to an order of magnitude smaller than for traditional CCSD(T) calculations with a similar small basis set (See e.g. Peterson et al., 2012). Also, such calculations again strain our computational resources to the maximum, and we had to limit our calculations to the smaller fragments, and a few select reactions. Composite methods, such as G2, G3SX or CBS-QB3, have reported uncertainties of a few kcal/mol, and are likewise not a sufficient improvement over the current set of data to warrant the computational cost. Reaching chemical accuracy, i.e. with uncertainties of 1 kcal/mol, is thus computationally too costly, while more tractable calculations do not result in a meaningful increase in

the *a priori* reliability compared to the results reported here. As such, we consider higher level calculations than those considered here or available in the literature to be beyond our reach at this time.

As argued in the main paper, however, our analysis of the reaction mechanism driving the $CF_3OCF=CF_2$ + OH reaction is not sensitive even to large uncertainties of several kcal/mol on the energy predictions, due to the sizable energy differences predicted for competing channels. Comparing M06-2X and CCSD(T) results for the critical points on the potential energy surface, we conclude that :

- The relative energy of the addition transition states indicates that the OH-addition to the outer carbon has an energetic advantage, and is expected to be the main entrance channel with a contribution of 80±15% (see below).
- The energy of the addition transition states is below the energy of the separated reactants, allowing for a negative temperature-dependence of the rate coefficient (see below). Protruding barriers for addition would lead to rate coefficients that are significantly lower than the experimental values, and are considered unlikely.
- The CF_3 loss channel is the only reaction channel for the adducts that has a sufficiently low barrier to allow for prompt decomposition at 1 atm. The HF elimination channel has a significantly higher barrier and concomitantly a negligible contribution.
- The reaction mechanism proposed earlier by Li et al. and Mashino et al., i.e. leading to formation of glyoxal directly by a process of HF elimination and C–O bond scission in the alkoxy radicals subsequently formed, is not viable as several steps in this mechanism have competing reactions with significantly lower energy barriers.
- The products of the reaction are predicted to be (per)fluorinated methylformate, glycolaldehyde, and formaldehyde. Direct glyoxal formation is unsupported by the available theoretical data, and glyoxal is predicted to be a secondary product.
- An *a priori* estimation of the yield of prompt decomposition has only limited reliability due to the uncertainties on the collisional energy transfer parameters. A yield of ~40% prompt decomposition by CF_3 loss from the $CF_3OC^{\bullet}FCF_2OH$ radical can be reproduced using physically viable collisional parameters. A significant yield of HF-loss from the initial adducts requires physically highly unlikely collision characteristics, as well as the removal of the CF_3 loss channel from the calculations.

These main conclusions of the paper are thus supported in full within the uncertainties of the theoretical calculations available at this time, *i.e.* in the current paper and in the cited literature.

Table SI-1 : Barrier heights or (in brackets) reaction energies for critical reactions in the CF_3OCFCF_2 + OH reaction. The table is subdivided in sections corresponding to Figures 1 through 3 (main text), Figures SI-1 and SI-2 (supporting information), and miscellaneous reactions. The table compares the energies obtained using M06-2X/aug-cc-pVTZ (designated as M06-2X), CCSD(T)/6-311+ +G(d,p)//M06-2X (CC/311), CCSD(T)/aug-cc-pVDZ//M06-2X (CC/aVDZ), and ROHF-UCCSD(T)-F12a/aug-cc-pVDZ//M06-2X (CCF12/aVDZ).

Reaction	M06-2X	CC/311	CC/aVDZ	CCF12/aVDZ	
$CF_3OC^{\bullet}FCFO$: CF_3 loss	30.1	25.1	25.8	29.8	Figure 1
$CF_3OCF(O^{\bullet})CFO$: OCF_3 loss	17.8	13.8	14.1		
$CF_3OCF(O^{\bullet})CFO$: F-loss	24.2	24.9	24.4		
$CF_3OCF(O^{\bullet})CFO$: FCO loss	0.29	2.0	3.7		
$CFOCF_2OH$: 1,2-HF-loss	45.5	44.6	43.0	48.0	
$CF_3OCF=CF_2 + {}^{\bullet}OH \rightarrow CF_3OC^{\bullet}F–CF_2OH$	-2.1	-0.03	-2.1		Figure 2
$CF_3OC^{\bullet}FCF_2OH$: CF_3-loss	24.1	21.4	22.1		
$CF_3OC^{\bullet}FCF_2OH$: 1,2-HF-loss	34.7	35.6	34.0		
$CF_3OC^{\bullet}F(O^{\bullet})CF_2OH$: F-loss	26.4	20.6	20.4		
$CF_3OC^{\bullet}F(O^{\bullet})CF_2OH$: OCF_3 loss	19.5	15.1	15.2		
$CF_3OC^{\bullet}F(O^{\bullet})CF_2OH$: CF_2OH loss	< 1.5	< 1.5	< 1.5		
$CF_3OCF=CF_2 + {}^{\bullet}OH \rightarrow CF_3OCFOH–C^{\bullet}F_2$	-1.5	1.2	-1.3		Fig. 3
$CF_3OCFOHC^{\bullet}F_2$: 1,2-HF-loss	38.6	39.6	37.9		
$CF_3OC^{\bullet}FCF_2OH$: CF_3 loss	24.1	21.4	22.1		Figure SI-1
$CF_3OC^{\bullet}FCF_2OH$: 1,2-HF-loss	34.7	35.6	34.0		
$CF_3OC^{\bullet}FCF_2OH$: 1,2-F-migration	36.1	37.1	35.7		
$CF_3OC^{\bullet}FCF_2OH$: 1,3-H-migration	39.3	37.5	36.7		
$CF_3OC^{\bullet}FCF_2OH$: 1,4-HF-loss with cyclization	(34.0)	(30.0)	(33.9)		
$CF_3OC^{\bullet}FCF_2OH$: 1,5-HF-loss with cyclization	(39.6)	(35.6)	(39.8)		
$CF_3OC^{\bullet}FCF_2OH$: 1,5-HF-loss with fragmentation	61.9	53.6	55.6		
$CF_3OC^{\bullet}FCF_2OH$: F-atom loss	(64.4)	(57.3)	(60.5)		
$CF_3OCFOHC^{\bullet}F_2$: 1,2-HF-loss	38.6	39.6	37.9		Figure SI-2
$CF_3OCFOHC^{\bullet}F_2$: 1,2-F-migration	38.9	40.6	38.4		
$CF_3OCFOHC^{\bullet}F_2$: 1,3-H-migration	43.6	41.9	41.0		
$CF_3OCFOHC^{\bullet}F_2$: CF_3O-loss	(51.1)	(46.4)	(50.1)		
$CF_3OCFOHC^{\bullet}F_2$: F-atom loss	(65.1)	(57.2)	(61.0)		
$CFOCF_2O^{\bullet}$: C–C scission	0.97	3.1	4.3	2.4	Misc. React.
$CFOCF_2OH$---H_2O : 1,2-HF-loss	14.4	15.6	12.8	15.0	
$CFOCF_2OH + {}^{\bullet}CF_3$ -> $CF_4 + CFOC^{\bullet}FOH$	47.3	47.5	41.6		
$CFOCF_2OH + {}^{\bullet}CF_3$ -> $HCF_3 + CFOCF_2O^{\bullet}$	28.2	20.6	21.8		
$CFOCF_2OH + {}^{\bullet}CF_3$ -> $CF_4 + OC^{\bullet}CF_2OH$	55.0	47.2	47.8		

Rate coefficient predictions

Three experimental determination for the rate coefficient of the $CF_3OCF=CF_2$ + OH reaction are available in the literature :

Li et al. : k(253-348K) = $(6.41 \pm 0.82)\times10^{-11}$ exp((-868±40)/T) cm^3 $molecule^{-1}$ s^{-1}

Tokuhashi et al. : k(250-430K) = $(1.01 \pm 0.04)\times10^{-12}$ exp((320±10)/T) cm^3 $molecule^{-1}$ s^{-1}

Mashino et al. : k(296K) = $(2.6 \pm 0.3)\times10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}

Near room temperature these rate coefficients differ by less than 30%, but the opposite sign of the temperature dependence for the expressions by Li et al. versus Tokuhashi et al. leads to larger differences at higher and lower temperatures.

The accurate prediction of the absolute rate coefficient of the $CF_3OCF=CF_2$ + OH reaction is difficult, as the value depends critically on the absolute barrier heights of the entrance transition states, on the interplay between the initial complex formation and the OH addition step, and on the description of the degrees of freedom for internal rotation, non-harmonic vibration, etc. along the addition process. Such complex calculations are beyond the scope of the current paper. Hence, we will not attempt a highly accurate prediction of the rate coefficient, but rather limit ourselves to assess the temperature dependence, and the relative contribution of the different entrance channels leading to addition on the inner or outer carbon atom.

To this end we performed simplified canonical transition state theory calculations (CTST), where we assume that (i) the formation and redissociation of the pre-reactive complex is fast enough compared to the addition reaction to ensure canonical equilibrium between the free reactants and the complex; (ii) that the impact of anharmonicities, internal rotation, etc. is sufficiently similar between all of the reactants, complex formation TS, complex, and the addition transition states, to mostly cancel out relative to a harmonic oscillator treatment; (iii) that the predicted relative energy of the two addition transition states is sufficiently accurate; (iv) that tunneling is negligible; and (v) that the addition reaction is irreversible.

If the approximations above hold, the impact of the pre-reactive complex cancels out of the rate equations, and the absolute rate coefficient can be predicted based on the rigid-rotor, harmonic oscillator approximation for reactants and addition transition states, where we use the M06-2X/aug-cc-pVTZ rovibrational and energetic characteristics. For OH we use the experimental spin-orbit splitting value of 126.23 cm^{-1} :

$$k(T)=\frac{k_b T}{h}\times\frac{Q^{\neq}(T)}{Q_{CF_3OCFCF_2(T)}\times Q_{OH}(T)}\times\exp\left(\frac{-E_b}{k_b T}\right)$$

Figure SI-3 shows the result of this calculation, compared to the available experimental data. The submerged barriers as predicted by M06-2X//aug-cc-pVDZ and CCSD(T)/aVDZ lead to a negative temperature dependence in fair agreement with the results of Tokuhashi et al., and in strong disagreement with the results of Li et al. The excellent level of agreement of the absolute rate

coefficients between theory and experiment must be considered fortuitous, in view of the uncertainties on the underlying data and the methodology used. Raising the barrier heights by only 0.4 kcal/mol is sufficient to shift our rate coefficient predictions below the k(T) values of Tokuhashi et al. and Mashino et al. To obtain a temperature-neutral rate coefficient, the barriers must be raised by 1.5 kcal/mol above the M06-2X values, while a positive temperature dependence similar to Li et al. requires barriers higher by 3.5 kcal/mol. The predicted k(T) in these latter two cases are found to be a factor of 10 to 350 below the experimental rate coefficient, respectively. Using the CCSD(T)/6-311++G(d,p) addition barrier heights, which are 2 to 2.7 kcal/mol higher than the M06-2X and CCSD(T)/aVDZ results, yields a nearly temperature-neutral k(T) that is a factor 25 below all experimental data.

The current rate analysis thus supports a negative temperature dependence, resulting from submerged barriers ~ 2 kcal/mol below the free reactants. The predicted absolute rate coefficient carries an *a priori* uncertainty of at least a factor of 5, and we recommend the use of the k(T) expression by Tokuhashi et al. instead.

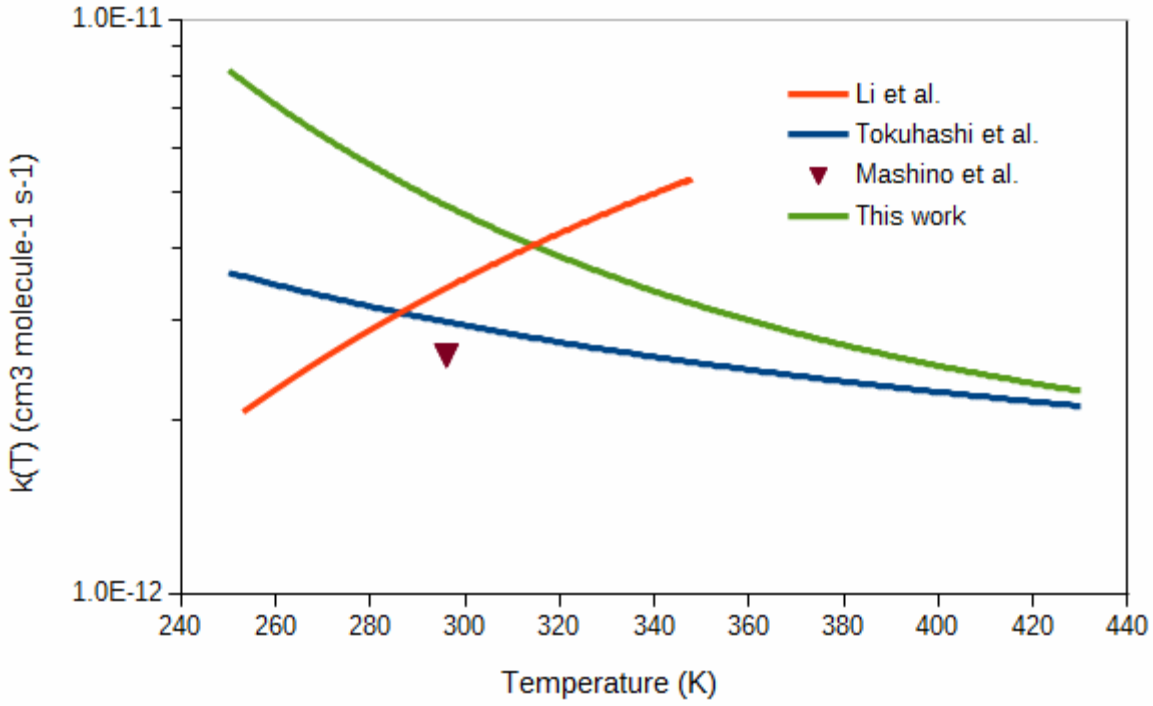

Figure SI-3 : Rate coefficients for the reaction of $CF_3OCF=CF_2$ + OH (cm^3 $molecule^{-1}$ s^{-1}), as reported in the literature, and as estimated in this work based on a rigid-rotor harmonic-oscillator CTST approximation using addition barrier heights of -2.1 and -1.5 kcal/mol relative to the free reactants, for addition on the outer and inner carbon atom, respectively.

The relative contribution of the two entrance channels can be estimated with fairly good accuracy, owing to the excellent error cancellation between the two addition transition states. The energy difference between the two TS at the M06-2X level of theory is 0.56 kcal/mol, leading to a ratio

of 83:17 at 300K for addition on the outer:inner carbon atom, using the RRHO approximation as detailed above, and changing only by ~4% absolute over the 240-400K T-range. Averaging the energy difference of the two TS over the levels of theory listed in Table SI-1 yields ΔE=0.88 kcal/mol, leading to a ratio of 88:12. We thus estimate a contribution of 85±15% for addition on the outer carbon. The dominance of addition to the outer carbon is in agreement with literature data on OH addition on alkenes, where formation of the most substituted carbon radical is found to be favored. As discussed in the main text, the experimental observation of 69±8% of glyoxal by Mashino et al. at 10 Torr can be interpreted as indicative of a ratio of ~70:30, which remains within the uncertainties of the enthalpy and entropy calculations in the current theoretical work.

Quantum chemical data on reactants, products, and TS

```
*********************************************
CF3OCF=CF2 + OH : M06-2X/cc-pVDZ geometry
*********************************************

CF3
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -337.47101834
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.000124     -0.000500       0.328762
     F      -1.104936     -0.593425      -0.073108
     F       1.066832     -0.659480      -0.073081
     F       0.038187      1.253238      -0.072987
Rotational constants (GHz):   10.8935400   10.8810600    5.6380500
Vibrational harmonic frequencies (cm-1):
      516.3667                 517.5031                 705.8909
     1128.4593                1335.8732                1337.8613
Zero-point correction (Hartree): 0.012626

CF3O
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -412.67717517
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.006460      0.000842       0.035029
     F      -0.779589     -1.067848      -0.006813
     F       0.850511     -0.027021      -0.989646
     F      -0.766167      1.075572      -0.051728
     O       0.777306      0.021078       1.152939
Rotational constants (GHz):    6.0538100    5.8749700    5.6235700
Vibrational harmonic frequencies (cm-1):
      240.4554                 418.9718                 588.5250
      605.1949                 631.2607                 929.9720
     1282.4225                1310.5443                1349.1661
Zero-point correction (Hartree): 0.016759

CFOCF2
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -450.77929161
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):
     C      -0.155187     -0.776621       0.000000
     C       0.000000      0.643315       0.000000
     F       1.039144     -1.385753       0.000000
     O      -1.195392     -1.365263       0.000000
     F       1.152115      1.248269       0.000000
     F      -1.025230      1.439922       0.000000
Rotational constants (GHz):    5.6894300    3.4267300    2.1386300
Vibrational harmonic frequencies (cm-1):
      132.1384 (  A")           217.1530 (  A")           220.6489 (  A')
      413.2745 (  A')           537.0718 (  A')           612.8043 (  A')
      644.8228 (  A")           829.7127 (  A')          1174.1349 (  A')
     1467.7187 (  A')          1586.2871 (  A')          1848.7504 (  A')
Zero-point correction (Hartree): 0.022063

CFOCF2OH
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -526.65681872
Electronic state : 1-A
Cartesian coordinates (Angs):
```

```
     C      -0.926111      0.130406      -0.008977
     C       0.607752      0.021858      -0.004372
     F      -1.509247     -1.052336      -0.016036
     O      -1.519767      1.154825       0.003548
     F       0.994365     -0.765495      -1.022032
     F       0.969090     -0.614287       1.130834
     O       1.186037      1.229197      -0.097212
     H       0.492125      1.903303      -0.005491
Rotational constants (GHz):    3.8048500    2.5444800    2.0810400
Vibrational harmonic frequencies (cm-1):
       41.3475                212.8340                 240.9736
      327.6125                404.0623                 441.2731
      530.3607                614.9684                 700.1705
      783.2171                837.9568                1117.0883
     1217.7955               1280.0455                1375.8275
     1485.0529               1983.0320                3779.6643
Zero-point correction (Hartree): 0.039579

CFOCFO
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -426.22630863
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.765117       0.000000
     C      -0.000037     -0.765141       0.000000
     O      -0.955673      1.453999       0.000000
     O       0.955652     -1.453890       0.000000
     F       1.243061      1.217279       0.000000
     F      -1.243018     -1.217360       0.000000
Rotational constants (GHz):    5.9645800    3.5797300    2.2371000
Vibrational harmonic frequencies (cm-1):
       66.6815 (  A")           245.8273 (  A')           423.0977 (  A')
      457.7500 (  A")           535.3851 (  A')           691.0305 (  A')
      835.6805 (  A")           841.6858 (  A')          1189.9163 (  A')
     1367.2170 (  A')          1997.2040 (  A')          2001.6342 (  A')
Zero-point correction (Hartree): 0.024270

CFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -213.03922496
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.000000      0.423726       0.000000
     F      -1.012660     -0.432460       0.000000
     O       1.139243      0.168723       0.000000
Rotational constants (GHz):  186.9101500   11.5713600   10.8967600
Vibrational harmonic frequencies (cm-1):
      648.7703 (  A')          1106.6095 (  A')          1996.4126 (  A')
Zero-point correction (Hartree): 0.008547

F
-------------------------
E(UM062X/CC-pVDZ) (Hartree):  -99.69555398
Point group : OH
Cartesian coordinates (Angs):
     F       0.000000      0.000000       0.000000
Zero-point correction (Hartree): 0.000000

HF
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -100.40278281
Point group : C*V
Electronic state : 1-SG
Cartesian coordinates (Angs):
     F       0.000000      0.000000       0.092245
     H       0.000000      0.000000      -0.830203
Rotational constants (GHz):    0.0000000  620.5790284  620.5790284
Vibrational harmonic frequencies (cm-1):
     4129.9553 (  SG)
```

Zero-point correction (Hartree): 0.009409

O2

E(UM062X/CC-pVDZ) (Hartree): -150.27726911
Point group : D*H
Electronic state : 3-SGG
Cartesian coordinates (Angs):

O	0.000000	0.000000	0.595738
O	0.000000	0.000000	-0.595738

Rotational constants (GHz): 0.0000000 44.5138317 44.5138317
Vibrational harmonic frequencies (cm-1):
1777.0525 (SGG)
Zero-point correction (Hartree): 0.004048

OH

E(UM062X/CC-pVDZ) (Hartree): -75.70046613
Point group : C*V
Cartesian coordinates (Angs):

O	0.000000	0.000000	0.108808
H	0.000000	0.000000	-0.870468

Rotational constants (GHz): 0.0000000 555.8514600 555.8514600
Vibrational harmonic frequencies (cm-1):
3717.8362 (SG)
Zero-point correction (Hartree): 0.008470

FO2

E(UM062X/CC-pVDZ) (Hartree): -249.97293613
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):

F	-0.993949	-0.608359	0.000000
O	0.000000	0.551603	0.000000
O	1.118193	0.132801	0.000000

Rotational constants (GHz): 80.6488800 11.3173200 9.9246100
Vibrational harmonic frequencies (cm-1):
419.2663 (A') 663.7730 (A') 1532.8411 (A')
Zero-point correction (Hartree): 0.005959

CF4

E(RM062X/CC-pVDZ) (Hartree): -437.38085819
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):

C	-0.000033	0.000063	0.000000
F	-0.439754	1.243945	0.000000
F	1.319283	-0.000044	0.000000
F	-0.439754	-0.621972	1.077250
F	-0.439754	-0.621972	-1.077250

Rotational constants (GHz): 5.7310400 5.7308400 5.7304800
Vibrational harmonic frequencies (cm-1):
440.0897 (A") 440.1489 (A') 636.6912 (A')
637.3753 (A") 637.7396 (A') 943.4989 (A')
1358.9491 (A') 1359.7896 (A') 1359.8307 (A")
Zero-point correction (Hartree): 0.017802

HCF3

E(RM062X/CC-pVDZ) (Hartree): -338.14538978
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.000092	0.000010	0.339330
F	0.905846	-0.858935	-0.128586
F	0.291058	1.213742	-0.128692
F	-1.196961	-0.354893	-0.128593
H	-0.000033	0.000711	1.436860

Rotational constants (GHz): 10.3655400 10.3611000 5.6902300
Vibrational harmonic frequencies (cm-1):

```
      516.8866                 517.1093                 710.5043
     1174.9865                1225.7947                1226.5443
     1420.4163                1420.7385                3178.1038
Zero-point correction (Hartree): 0.025951

FNO
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -229.64021922
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     F      -0.945958     -0.556648       0.000000
     N       0.000000      0.547666       0.000000
     O       1.064203      0.147021       0.000000
Rotational constants (GHz):   97.1319400   12.5341900   11.1016100
Vibrational harmonic frequencies (cm-1):
      606.1782 (  A')          865.1589 (  A')         1991.8551 (  A')
Zero-point correction (Hartree): 0.007890

NO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -129.85561078
Point group : C*V
Cartesian coordinates (Angs):
     N       0.000000      0.000000      -0.609646
     O       0.000000      0.000000       0.533441
Rotational constants (GHz):    0.0000000   51.8018810   51.8018810
Vibrational harmonic frequencies (cm-1):
     2101.9361 (  SG)
Zero-point correction (Hartree): 0.004789

CF2O
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -312.93589312
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     C       0.000000      0.000000       0.141679
     O       0.000000      0.000000       1.313238
     F       0.000000      1.060818      -0.630888
     F       0.000000     -1.060818      -0.630888
Rotational constants (GHz):   11.8192200   11.7736000    5.8981800
Vibrational harmonic frequencies (cm-1):
      588.0028                 629.2054                 794.4039
     1013.0912                1333.8831                2055.8938
Zero-point correction (Hartree): 0.014613

H2O
-------------------------
E(RM062X/CC-pVDZ) (Hartree):  -76.38877424
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.120151
     H       0.000000      0.755011      -0.480605
     H       0.000000     -0.755011      -0.480605
Rotational constants (GHz):  782.2606700  439.8404600  281.5396300
Vibrational harmonic frequencies (cm-1):
     1648.4950                3842.0977                3943.2940
Zero-point correction (Hartree): 0.021492

CF3OH
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -413.36940150
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.004235      0.023024      -0.000064
     F       0.247193     -0.741912      -1.071102
     F       0.251023     -0.732751       1.076428
     F       0.833123      1.045907      -0.005726
     O      -1.261230      0.497464       0.000289
```

```
     H      -1.866800     -0.259049       0.001667
Rotational constants (GHz):    5.7304900    5.6603700    5.6243900
Vibrational harmonic frequencies (cm-1):
      254.9522                447.1666                460.1038
      608.7028                629.8676                643.5574
      934.3151               1155.9023               1266.7147
     1370.1402               1458.1360               3838.1555
Zero-point correction (Hartree): 0.029770

CF3OCFCF2
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -788.35463805
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.672616     -0.287932      -0.068459
     C       0.694091      0.564996      -0.335089
     O      -0.488561      0.168681      -0.874721
     F       0.823924      1.869870      -0.148821
     C      -1.471733     -0.111240       0.043085
     F      -1.683853      0.918544       0.854497
     F      -1.141887     -1.159607       0.790339
     F      -2.570402     -0.380072      -0.628547
     F       1.566372     -1.581829      -0.246295
     F       2.843472      0.072607       0.396666
Rotational constants (GHz):    2.3475600    0.9395300    0.7772000
Vibrational harmonic frequencies (cm-1):
       42.7445                 67.2912                118.5448
      192.6827                210.7831                341.5436
      369.1534                452.4712                469.3770
      546.3894                554.7824                607.0276
      641.9512                652.4408                726.3140
      856.0562                946.8563               1225.8433
     1270.7324               1303.7518               1382.7947
     1388.7653               1429.0729               1961.5734
Zero-point correction (Hartree): 0.040458

CF3OCFCF2OH.b
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.15280338
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.502030     -0.252021      -0.021838
     C       0.534407      0.774244      -0.585957
     O      -0.714846      0.384491      -0.972365
     F       0.556457      1.932774       0.051753
     C      -1.579501     -0.094752      -0.028635
     F      -1.607587      0.664494       1.058163
     F      -1.223854     -1.332989       0.362502
     F      -2.775371     -0.157696      -0.565521
     F       1.413833     -1.359640      -0.788736
     O       1.312176     -0.555740       1.292582
     F       2.735018      0.253939      -0.128970
     H       0.593268     -1.202761       1.354128
Rotational constants (GHz):    1.9696800    0.8478200    0.7506500
Vibrational harmonic frequencies (cm-1):
       34.0092                 57.7252                130.6047
      166.3854                196.9071                218.3432
      300.4147                330.8038                364.7875
      430.5164                485.7505                511.8767
      558.3645                586.8435                632.2428
      637.7359                687.4308                764.8264
      824.3453                921.6583               1140.6732
     1141.4601               1226.2863               1263.6132
     1279.1272               1347.5469               1386.6135
     1410.4939               1440.3405               3841.3603
Zero-point correction (Hartree): 0.055403

CF3OCFCF2OH
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.15271486
Electronic state : 2-A
```

```
Cartesian coordinates (Angs):
     C       1.500508     -0.282034      -0.043294
     C       0.538221      0.729093      -0.626795
     O      -0.721638      0.391282      -0.972266
     F       0.640371      1.923976      -0.036838
     C      -1.584319     -0.096976      -0.008336
     F      -1.441210      0.554633       1.138165
     F      -1.375259     -1.386552       0.206145
     F      -2.809080      0.070498      -0.463405
     F       1.528887     -1.365365      -0.820154
     O       2.758734      0.204735       0.060467
     F       1.040946     -0.677631       1.180618
     H       2.714872      1.055345       0.524159
Rotational constants (GHz):    1.9624500    0.8637900    0.7603500
Vibrational harmonic frequencies (cm-1):
       31.1296                  71.9159                 109.6047
      151.8585                 196.0286                 216.7416
      280.2610                 341.3362                 359.5651
      428.2155                 473.3544                 521.8439
      554.3154                 590.7160                 632.1368
      636.9499                 686.3507                 766.1424
      819.7463                 922.6191                1096.5140
     1135.6155                1218.4450                1288.1493
     1313.9371                1341.1435                1369.4645
     1399.4842                1475.4214                3828.9544
Zero-point correction (Hartree): 0.055264

CF3OCFCFOH
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -764.35221643
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.682358     -0.319785      -0.070948
     C       0.689821      0.521001      -0.348632
     O      -0.508046      0.163192      -0.880570
     F       0.864540      1.841022      -0.167272
     C      -1.486363     -0.096591       0.044836
     F      -1.671217      0.936875       0.860975
     F      -1.177893     -1.153370       0.789486
     F      -2.599475     -0.338905      -0.616260
     F       1.551738     -1.617250      -0.237490
     O       2.889670      0.009563       0.393260
     H       2.922873      0.974845       0.481991
Rotational constants (GHz):    2.3447800    0.9509600    0.7844900
Vibrational harmonic frequencies (cm-1):
       45.7715                  68.7031                 110.0883
      191.9706                 209.4577                 340.8296
      351.6364                 370.1612                 437.5304
      468.8086                 548.0042                 559.8556
      624.6288                 642.2215                 654.0201
      717.0477                 855.6679                 946.9498
     1152.5390                1271.5632                1296.5798
     1308.2966                1369.0874                1379.4009
     1481.6466                1934.6331                3825.0868
Zero-point correction (Hartree): 0.052767

CF3OCFCFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -763.73876235
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.826660     -0.306897      -0.011068
     C       0.733990      0.588808      -0.292829
     O      -0.429580      0.206207      -0.843029
     F       0.902570      1.874515      -0.141163
     C      -1.445694     -0.103548       0.043163
     F      -1.752313      0.948446       0.789716
     F      -1.082193     -1.091046       0.848178
     F      -2.485288     -0.465587      -0.670284
     F       1.475239     -1.576069      -0.251364
     O       2.903096      0.008480       0.391610
```

```
Rotational constants (GHz):    2.3575000    0.9821800    0.8048500
Vibrational harmonic frequencies (cm-1):
       34.6011                   49.7698                   74.2047
      142.3748                  209.5242                  327.5129
      354.0007                  382.2282                  466.1603
      534.6876                  564.6519                  638.6468
      665.7959                  669.2335                  702.1340
      838.0330                  946.0423                 1165.2849
     1239.1636                 1317.6725                 1390.8386
     1429.3370                 1529.3187                 1864.1480
Zero-point correction (Hartree): 0.039949

CF3OCFOCF2OH
------------------------
E(UM062X/CC-pVDZ) (Hartree): -939.35055168
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.351517     -0.530633      -0.022931
     C       0.567815      0.867204       0.000152
     O      -0.721303      0.810099      -0.541184
     F       1.228040      1.676829      -0.848812
     C      -1.661809     -0.048858      -0.043660
     F      -1.657106     -0.107965       1.282132
     F      -1.488873     -1.280349      -0.514410
     F      -2.835868      0.395782      -0.453244
     F       1.188648     -1.045071      -1.233854
     O       2.667337     -0.371922       0.199876
     F       0.773628     -1.347700       0.877370
     H       2.787159      0.100392       1.038901
     O       0.652902      1.255524       1.263445
Rotational constants (GHz):    1.5663200    0.7911300    0.7189700
Vibrational harmonic frequencies (cm-1):
       62.6395                   79.8852                  116.8089
      169.5713                  200.9001                  225.4360
      274.5833                  315.1010                  339.9183
      357.4456                  381.3601                  433.9029
      471.4822                  517.9227                  536.1759
      585.0397                  624.8445                  660.6677
      687.7100                  734.4103                  768.9161
      874.5457                  977.2055                 1095.3918
     1173.5591                 1228.1175                 1289.0952
     1300.1688                 1312.2486                 1335.9739
     1382.4719                 1439.5061                 3818.5755
Zero-point correction (Hartree): 0.058712

CF3OCFOCFO
------------------------
E(UM062X/CC-pVDZ) (Hartree): -838.92025750
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.542186     -0.562552       0.161134
     C       0.724132      0.727279      -0.152791
     O      -0.503760      0.456203      -0.771156
     F       1.409853      1.413435      -1.087698
     C      -1.472993     -0.127597      -0.002901
     F      -2.052376      0.741183       0.811521
     F      -0.964218     -1.115729       0.742746
     F      -2.377289     -0.623474      -0.819367
     F       1.403667     -1.413816      -0.844425
     O       2.215047     -0.749146       1.106257
     O       0.596629      1.388297       1.007694
Rotational constants (GHz):    1.7516400    0.9239000    0.8419900
Vibrational harmonic frequencies (cm-1):
       39.2746                   58.6082                   91.7071
      165.0382                  215.6815                  232.5666
      334.0522                  356.4422                  376.2570
      433.2546                  483.9399                  520.5625
      622.1618                  646.5482                  677.6836
      714.0592                  786.4851                  821.2214
      942.2781                 1071.3351                 1186.8303
     1218.5876                 1289.7746                 1304.0120
```

```
     1318.3689                1389.1805                2000.5364
Zero-point correction (Hartree): 0.043961

CF3OCFOHCF2
------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.15090431
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.468539      0.672877       0.102535
     C      -0.895448     -0.724242      -0.011581
     O       0.398115     -0.803145      -0.588518
     F      -0.811504     -1.233597       1.243742
     C       1.399895     -0.005914      -0.118907
     F       1.512324     -0.046088       1.202785
     F       1.208681      1.265951      -0.472754
     F       2.524617     -0.431574      -0.664141
     F      -1.504108      1.340980      -1.031352
     F      -0.976741      1.395671       1.089820
     O      -1.716115     -1.448424      -0.799620
     H      -1.250861     -2.265873      -1.040083
Rotational constants (GHz):    1.5597400    1.0000600    0.8848400
Vibrational harmonic frequencies (cm-1):
       52.1003                  99.6120                 130.5446
      157.2650                 204.2146                 218.4213
      305.6484                 349.5107                 365.3784
      406.8178                 449.6697                 507.2350
      550.7400                 582.1924                 613.4673
      659.0262                 683.4816                 752.4771
      833.6755                 937.8475                1080.2086
     1145.7284                1262.9880                1299.3164
     1314.5774                1347.5755                1364.6519
     1378.1792                1508.8686                3804.1409
Zero-point correction (Hartree): 0.055509

CF3OCFOOCF2OH.a
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -1014.49166116
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.086260      0.885992      -0.003508
     C      -0.498625     -0.552614       0.091905
     O       0.715372     -0.742217      -0.518433
     F      -0.494074     -0.944337       1.368922
     C       1.870826     -0.123141      -0.086517
     F       1.842099      0.151874       1.207544
     F       2.084549      0.992476      -0.763168
     F       2.860159     -0.960825      -0.332803
     F      -1.310368      1.118156      -1.314485
     O      -2.176623      1.085897       0.753225
     F      -0.143939      1.744367       0.406341
     O      -1.299367     -1.485605      -0.652266
     O      -2.548723     -1.423096      -0.303101
     H      -2.786748      0.343351       0.602162
Rotational constants (GHz):    1.3350000    0.6682700    0.5838000
Vibrational harmonic frequencies (cm-1):
       31.4599                  78.3334                  90.5647
      120.5422                 169.1334                 217.1604
      229.1803                 287.9877                 328.7751
      347.7605                 367.6370                 399.3712
      442.9937                 446.5259                 477.1721
      543.9579                 568.8980                 606.2962
      624.1929                 683.5254                 708.9546
      763.6965                 815.8179                 951.7727
     1076.3876                1171.8793                1193.4084
     1236.1015                1287.8150                1310.5447
     1314.9903                1336.0462                1364.9986
     1399.9767                1455.9734                3771.0607
Zero-point correction (Hartree): 0.064292

CF3OCFOOCF2OH.b
-------------------------
```

E(UM062X/CC-pVDZ) (Hartree): -1014.49039045
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-0.992171	0.939396	-0.024246
C	-0.541969	-0.545378	0.031186
O	0.688170	-0.832431	-0.501728
F	-0.649540	-0.958162	1.304024
C	1.826264	-0.183361	-0.073707
F	1.870331	-0.081596	1.246036
F	1.919481	1.027385	-0.600656
F	2.842126	-0.910726	-0.491756
F	-0.749942	1.416015	-1.245293
O	-2.297579	1.115552	0.251363
F	-0.207615	1.613173	0.850007
H	-2.561557	0.510998	0.963705
O	-1.388872	-1.352621	-0.787318
O	-2.553566	-1.521717	-0.227862

Rotational constants (GHz): 1.3084300 0.6908800 0.5936000
Vibrational harmonic frequencies (cm-1):

64.6053	82.1346	105.4384
149.8109	155.0087	210.1429
216.7138	227.3207	276.5627
331.5791	354.0653	368.8438
402.2195	438.7321	476.2832
546.8789	572.0087	598.0006
631.7293	697.3217	715.2341
765.3362	815.8198	952.8177
1079.3707	1156.6953	1194.9612
1232.1090	1270.4203	1294.6427
1312.8804	1329.2816	1366.3555
1393.0315	1453.2218	3812.5026

Zero-point correction (Hartree): 0.063903

CF3OCFOOHCF2O

E(UM062X/CC-pVDZ) (Hartree): -1014.45407928
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.594121	-0.730088	-0.040296
C	0.368272	0.247894	0.069703
O	-0.686573	-0.405477	-0.522742
F	0.144359	0.502683	1.366196
C	-1.960605	-0.102773	-0.091876
F	-2.221414	-0.675785	1.072848
F	-2.787211	-0.578536	-1.000766
F	-2.140996	1.204284	0.031345
F	1.703775	-1.102319	-1.331634
O	2.688275	-0.119405	0.408674
F	1.303895	-1.834177	0.669361
O	0.563465	1.415477	-0.640991
O	1.641331	2.085787	-0.016372
H	2.315618	2.053399	-0.719885

Rotational constants (GHz): 1.3195100 0.6285400 0.5485000
Vibrational harmonic frequencies (cm-1):

42.8522	49.2126	74.7488
123.3936	161.0846	209.7715
223.9721	260.5212	306.2218
340.3914	354.9138	365.3602
385.5199	428.5558	500.7852
548.7252	562.8610	595.1564
632.2285	654.9522	715.8977
744.1175	851.1434	934.3263
1047.9762	1062.1653	1155.4691
1226.5319	1237.0957	1250.5931
1317.1305	1323.3292	1336.5852
1388.2496	1446.7462	3747.1922

Zero-point correction (Hartree): 0.062891

CF3OCOHCF2

E(RM062X/CC-pVDZ) (Hartree): -764.35149549

```
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.664350     -0.289644      -0.061357
     C       0.700557      0.578653      -0.346123
     O      -0.483577      0.102792      -0.892531
     C      -1.449568     -0.135391       0.029921
     F      -1.638320      0.941352       0.818407
     F      -1.142101     -1.151746       0.829778
     F      -2.572987     -0.402550      -0.600661
     F       2.833911      0.053771       0.422852
     F       1.567040     -1.582533      -0.264814
     O       0.845215      1.912211      -0.231304
     H       0.186973      2.233624       0.405987
Rotational constants (GHz):    2.3594500    0.9482300    0.7873400
Vibrational harmonic frequencies (cm-1):
       56.3819                   73.8533                  130.0879
      203.8369                  214.2157                  325.5031
      362.1713                  370.6758                  453.0713
      480.9830                  543.2033                  561.7109
      620.8788                  645.0231                  654.6573
      719.0532                  850.7701                  940.0746
     1179.7084                 1239.4897                 1294.3232
     1324.6848                 1368.6271                 1387.3415
     1419.5866                 1945.3410                 3784.9508
Zero-point correction (Hartree): 0.052740

CH3OCHCH2
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -193.03591470
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.434143      0.568648       0.000003
     C       0.732832     -0.568565      -0.000005
     O      -0.609584     -0.716963       0.000013
     H       1.217255     -1.547108      -0.000025
     C      -1.357855      0.478097      -0.000007
     H      -1.138226      1.081005      -0.897020
     H      -1.138307      1.080989       0.897037
     H      -2.413629      0.186560      -0.000054
     H       0.974108      1.555502       0.000027
     H       2.520750      0.509679      -0.000013
Rotational constants (GHz):   18.2889000    6.4601700    4.9248000
Vibrational harmonic frequencies (cm-1):
      256.0947                  280.8650                  341.4340
      596.2423                  728.0034                  847.8294
      942.1595                 1009.1841                 1057.3613
     1171.9543                 1217.2540                 1278.5429
     1351.5511                 1406.9691                 1465.9034
     1467.7104                 1487.6039                 1736.6951
     3036.3770                 3106.2853                 3180.9864
     3203.9581                 3223.2741                 3303.1601
Zero-point correction (Hartree): 0.085881

CH3OCHCH2OH
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -268.78646623
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.950174     -0.394724       0.318576
     C      -0.039447      0.740023      -0.035034
     O       1.310180      0.668494       0.075055
     H      -0.401361      1.754792       0.146213
     C       1.903455     -0.595498      -0.139550
     H       1.587391     -1.023122      -1.105581
     H       1.657706     -1.303593       0.668569
     H       2.987015     -0.432705      -0.153471
     H      -1.055311     -0.512357       1.414269
     O      -2.252888     -0.134008      -0.159411
     H      -0.557859     -1.355553      -0.065077
     H      -2.158923      0.097838      -1.094021
Rotational constants (GHz):   14.4439400    2.6519400    2.3869200
```

Vibrational harmonic frequencies (cm-1):

78.0753	160.9798	249.6241
261.3442	372.0982	385.3998
548.6671	643.6833	941.1431
1012.2734	1116.1845	1131.0510
1160.5391	1190.4572	1203.5872
1318.6425	1322.3098	1388.0796
1446.9464	1473.4654	1477.6533
1487.2814	1497.1383	3003.6716
3031.3064	3041.4855	3108.8984
3172.9491	3202.9570	3823.7039

Zero-point correction (Hartree): 0.100813

CH3OCHOHCH2

E(UM062X/CC-pVDZ) (Hartree): -268.79105185
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-0.746925	1.395192	-0.111862
C	-0.464829	-0.008616	0.308975
O	0.659940	-0.540309	-0.362533
H	-0.266310	-0.050024	1.402914
C	1.874678	0.006341	0.088825
H	2.019375	-0.167479	1.171916
H	1.929814	1.093358	-0.099047
H	2.680780	-0.491940	-0.462591
H	-0.816033	1.591653	-1.182673
H	-1.093970	2.142602	0.600009
O	-1.555343	-0.803955	-0.040507
H	-1.267978	-1.721560	0.078161

Rotational constants (GHz): 8.5975000 4.0586800 3.0513600
Vibrational harmonic frequencies (cm-1):

64.4565	121.6963	208.7737
285.1803	320.1088	380.3213
472.6788	529.8539	597.2581
871.4363	1045.9035	1103.3912
1161.8142	1174.7358	1190.1219
1236.6008	1282.2993	1368.5716
1399.2550	1455.6505	1465.1359
1486.7515	1495.5145	2953.5102
3011.8079	3074.2263	3166.0398
3177.4365	3300.4756	3816.8991

Zero-point correction (Hartree): 0.098458

complex.CF3OCFCF2.OH.a

E(UM062X/CC-pVDZ) (Hartree): -864.06225948
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.508895	-0.741170	-0.098708
C	0.676475	0.217200	0.277209
O	-0.468236	0.497055	-0.411411
F	0.912975	1.009484	1.307922
C	-1.581220	-0.187689	0.018678
F	-1.791635	-0.000474	1.315632
F	-1.452800	-1.490744	-0.194850
F	-2.607631	0.271514	-0.666953
F	1.281534	-1.528877	-1.121609
F	2.638978	-1.001352	0.509560
H	0.174459	2.620018	-0.924354
O	1.139217	2.792192	-0.914344

Rotational constants (GHz): 1.2933600 0.8178700 0.6594800
Vibrational harmonic frequencies (cm-1):

25.1118	40.2045	55.5376
71.9722	89.0994	117.3545
145.5216	195.4270	215.2323
335.5326	343.8949	370.7291
460.3984	469.9556	547.1884
555.4644	609.5410	644.3089
652.8220	727.7043	855.5684
949.6319	1225.4701	1270.2020

```
     1310.7071                1375.6679                1383.1856
     1430.0651                1969.1764                3709.0402
Zero-point correction (Hartree): 0.050465

complex.CF3OCFCF2.OH.b
------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.06520395
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.580719     -0.369306      -0.371650
     C       0.583567      0.455330      -0.676246
     O      -0.639913     -0.002858      -1.056408
     F       0.733549      1.765442      -0.707633
     C      -1.568594     -0.110326      -0.055349
     F      -1.727867      1.027812       0.600363
     F      -1.205146     -1.046558       0.831888
     F      -2.705125     -0.471362      -0.609008
     F       1.437861     -1.672310      -0.336831
     F       2.793910      0.025486      -0.100555
     H       0.326080     -0.279005       2.198820
     O       0.909303      0.473886       1.970987
Rotational constants (GHz):    1.7056800    0.7952200    0.7542700
Vibrational harmonic frequencies (cm-1):
       30.1339                  61.3884                  79.9992
      100.0813                 114.8918                 148.6306
      185.3447                 199.5076                 212.5133
      341.2620                 367.1227                 416.6684
      450.4326                 470.8440                 544.3322
      556.1535                 589.8232                 641.8362
      650.7202                 722.1286                 853.5707
      945.4680                1226.7566                1258.8383
     1297.4994                1380.9804                1394.1516
     1436.4112                1929.2556                3726.7267
Zero-point correction (Hartree): 0.050879

CF2OCFCF2oxide
------------------------
E(UM062X/CC-pVDZ) (Hartree): -763.66994286
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.618728     -0.267317       0.055010
     C       0.342268      0.363359      -0.214158
     O      -0.739438     -0.369247      -0.607891
     F       0.264156      1.633928      -0.594234
     C      -1.811541     -0.308347       0.241818
     F      -2.214239      0.930430       0.486758
     F      -2.783941     -1.043499      -0.241506
     F       1.803889     -1.571341      -0.034415
     O       0.814851      0.166919       1.093429
     F       2.763465      0.371867      -0.103306
Rotational constants (GHz):    2.7697900    0.8727200    0.7390500
Vibrational harmonic frequencies (cm-1):
       31.0534                  61.5035                 127.8471
      177.1115                 243.9467                 296.4394
      381.8529                 502.1014                 515.8797
      550.5544                 557.1616                 596.5021
      685.2540                 755.5934                 825.7184
      887.6839                1079.7284                1186.0441
     1218.9193                1279.1284                1329.7550
     1361.9423                1368.8636                1684.8001
Zero-point correction (Hartree): 0.040336

CF3OCCF2oxide
------------------------
E(UM062X/CC-pVDZ) (Hartree): -763.68149156
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.914947      0.012978      -0.071451
     C      -0.551255     -0.383678      -0.291268
     O       0.483133      0.470455      -0.511606
     C       1.703853      0.031279      -0.056713
```

```
     F       2.059428     -1.097543      -0.658385
     F       2.582200      0.971735      -0.332870
     F      -2.287228      1.274355       0.057100
     O      -1.137969     -0.484820       0.969882
     F      -2.945167     -0.722478      -0.444706
     F       1.681075     -0.187020       1.251126
Rotational constants (GHz):    3.2482700    0.7258200    0.6986100
Vibrational harmonic frequencies (cm-1):
       20.4560                   65.3396                  113.2779
      201.2603                  265.6559                  358.6345
      442.2116                  502.3326                  528.4847
      549.4260                  622.1372                  632.4332
      675.5862                  734.2437                  809.1391
      925.7098                  966.1950                 1177.8388
     1224.4180                 1291.7392                 1311.4290
     1343.5575                 1381.0109                 1651.9387
Zero-point correction (Hartree): 0.040539

CF3OCOCF2OH
------------------------
E(RM062X/CC-pVDZ) (Hartree): -839.61717822
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.854914     -0.157632      -0.002875
     C       0.436579      0.445252      -0.004516
     O      -0.500059     -0.526803      -0.009251
     C      -1.829387     -0.130295      -0.001162
     F      -2.116372      0.589773      -1.071609
     F      -2.108393      0.571514       1.083410
     F      -2.548265     -1.232811      -0.007889
     F       1.975985     -0.988816      -1.054245
     O       2.787588      0.804982      -0.045269
     F       1.988208     -0.918359       1.102918
     H       2.332952      1.664197      -0.009814
     O       0.234212      1.621839       0.003002
Rotational constants (GHz):    2.2259100    0.6748200    0.6323600
Vibrational harmonic frequencies (cm-1):
        7.6795                   58.0155                  104.5933
      132.4288                  215.4772                  218.0114
      329.9825                  346.8529                  391.8969
      443.7729                  447.1603                  533.7401
      567.4955                  592.4113                  628.7016
      678.3863                  766.7280                  789.3800
      916.1523                  933.4619                 1128.1279
     1219.0141                 1230.7431                 1298.9084
     1339.9056                 1375.3228                 1380.2128
     1488.2195                 1936.3847                 3764.9931
Zero-point correction (Hartree): 0.057556

CFOHCF2
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -451.38638020
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.659810      0.013499      -0.011909
     C      -0.665037     -0.027700       0.009103
     O       1.440381     -1.071026      -0.106666
     F       1.290884      1.191847       0.007668
     F      -1.432303      1.042984      -0.004494
     F      -1.356974     -1.148147       0.016993
     H       1.993857     -1.126735       0.688658
Rotational constants (GHz):    5.4523500    3.2790500    2.0583800
Vibrational harmonic frequencies (cm-1):
      195.4942                  208.9100                  265.7097
      401.0679                  440.7599                  561.4975
      568.8550                  589.5642                  822.2124
     1181.7732                 1306.1006                 1387.9893
     1408.3588                 1971.4149                 3785.6745
Zero-point correction (Hartree): 0.034390

CFOCFOH
```

```
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -426.78665429
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.756121      0.121130       0.000383
     C       0.654128     -0.033315       0.000012
     F      -1.430369     -1.033527       0.000092
     O      -1.296256      1.203679      -0.000371
     F       1.257553     -1.192410      -0.000159
     O       1.457771      1.010350      -0.000048
     H       0.875186      1.794315       0.001579
Rotational constants (GHz):    5.6139100    3.5443500    2.1726500
Vibrational harmonic frequencies (cm-1):
      162.1495                226.0065                 335.7396
      409.8361                557.5674                 558.8438
      609.5359                648.9475                 845.0635
     1164.8958               1280.4961                1534.9799
     1639.6829               1808.3475                3723.5835
Zero-point correction (Hartree): 0.035325

CFOCF2O
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -525.96466685
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.321360     -0.881000       0.000000
     C      -0.045881      0.626598       0.000000
     F      -0.803099     -1.582466       0.000000
     O       1.399106     -1.350222       0.000000
     F      -0.803099      0.893056       1.079353
     F      -0.803099      0.893056      -1.079353
     O       1.104743      1.311921       0.000000
Rotational constants (GHz):    3.8873600    2.5794400    2.1288200
Vibrational harmonic frequencies (cm-1):
       33.3852 (  A")          216.2060 (  A')          223.9653 (  A")
      374.4052 (  A')          411.2589 (  A')          473.0212 (  A")
      591.2733 (  A')          682.6296 (  A')          768.5877 (  A")
      824.3158 (  A')         1069.0838 (  A')         1218.1761 (  A")
     1248.9357 (  A')         1336.0031 (  A')         2001.8490 (  A')
Zero-point correction (Hartree): 0.026138

OCCF2OH
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -426.76586253
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.039773     -0.603678      -0.369696
     C       0.373060      0.006150      -0.018933
     O      -2.033401     -0.058667      -0.061981
     F       1.244688     -0.286037      -0.979092
     F       0.764517     -0.632185       1.105392
     O       0.336131      1.343393       0.140207
     H      -0.504399      1.571367       0.569264
Rotational constants (GHz):    5.7016900    3.0407200    2.9893800
Vibrational harmonic frequencies (cm-1):
       90.8463                251.9533                 340.2675
      381.8375                421.9729                 539.0082
      563.0071                666.7879                 799.7310
     1097.2475               1195.4603                1313.7883
     1430.7454               2015.3724                3803.2641
Zero-point correction (Hartree): 0.033970

TS.CF3OCFCF2OH.CF3+HOCF2CFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.10683749
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.629197     -0.310862      -0.009215
     C       0.621532      0.725049      -0.487774
     O      -0.402939      0.472511      -1.099931
```

```
     F       0.824853      1.937740       0.054701
     C      -1.857238     -0.113453       0.023013
     F      -1.488521      0.259614       1.228762
     F      -1.969980     -1.412534      -0.067506
     F      -2.941701      0.502001      -0.368663
     F       1.942317     -1.128810      -1.017292
     O       2.770159      0.207774       0.489128
     F       0.982776     -1.075009       0.918540
     H       2.553609      1.006297       0.993404
Rotational constants (GHz):    1.8827000    0.7356500    0.6587200
Vibrational harmonic frequencies (cm-1):
     i551.1443                  26.3667                  41.6632
       59.9623                 103.3701                 146.1078
      197.2344                 251.8859                 265.8266
      303.6714                 400.6340                 444.0886
      510.6656                 527.5065                 539.5820
      599.7575                 639.9165                 679.3325
      720.7646                 820.8845                1042.6922
     1091.5365                1157.8104                1264.3768
     1365.8613                1379.6566                1391.7052
     1441.1681                1595.9698                3839.7409
Zero-point correction (Hartree): 0.052056

TS.CF3OCFCF2OH.CF3OCF2CFOH
--------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.08993652
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.657246     -0.363637      -0.273586
     C       0.597298      0.463397      -0.575642
     O      -0.592681      0.000751      -0.959725
     F       0.759773      1.760606      -0.599711
     C      -1.600205     -0.113743       0.001294
     F      -1.714495      0.990319       0.709831
     F      -1.378665     -1.140504       0.793635
     F      -2.712302     -0.320975      -0.678369
     F       1.520551     -1.645928      -0.440707
     O       2.845106      0.053490       0.083761
     F       0.790292      0.248350       1.463314
     H       2.668182      0.623154       0.863376
Rotational constants (GHz):    1.9178600    0.8277900    0.7541200
Vibrational harmonic frequencies (cm-1):
     i287.0679                  21.1511                  91.4147
      137.2784                 163.5648                 206.0898
      218.7353                 297.8701                 339.7178
      354.0187                 375.9234                 467.0722
      481.9111                 540.1653                 549.9658
      575.5125                 636.6884                 654.3041
      720.0576                 848.6219                 950.6233
     1194.6503                1206.7557                1291.6838
     1354.3349                1365.9412                1446.3046
     1520.8888                1773.4148                3648.3167
Zero-point correction (Hartree): 0.053384

TS.CF3OCFCF2OH.CF3OCFCF2+OH
---------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.06253826
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.407800     -0.377410      -0.336857
     C      -0.483199      0.544016      -0.029448
     O       0.588520      0.275364       0.748232
     F      -0.645469      1.813453      -0.369235
     C       1.721636     -0.086215       0.056132
     F       2.065339      0.848167      -0.823455
     F       1.532852     -1.221897      -0.606623
     F       2.684566     -0.243565       0.936059
     F      -1.268300     -1.639480      -0.058293
     O      -2.307203      0.158229       1.586709
     F      -2.436039     -0.112607      -1.097741
     H      -2.630899      1.052258       1.355102
```

Rotational constants (GHz): 1.8089000 0.7346200 0.6841400
Vibrational harmonic frequencies (cm-1):
i292.7795 37.9959 68.1747
79.6251 103.9954 140.7065
190.2716 199.6665 243.2688
342.3516 368.6890 411.5625
465.5586 507.0406 555.5844
558.1256 641.5671 649.4315
664.9366 719.6689 849.7104
946.4766 1228.5566 1262.8040
1304.6369 1384.9430 1398.6794
1452.5751 1846.1985 3726.2009
Zero-point correction (Hartree): 0.050915

TS.CF3OCFCF2OH.CF2O+CF2O+CF+HF

E(UM062X/CC-pVDZ) (Hartree): -864.04373107
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-1.659760	-0.423680	-0.038935
C	-1.064546	1.256439	0.572911
O	0.894282	0.465073	1.059965
F	-0.726443	1.990782	-0.391549
C	1.770485	0.316736	0.267872
F	1.727884	0.734706	-0.962318
F	1.220066	-1.782023	-0.583384
F	2.940241	-0.152963	0.545489
F	-1.510972	-1.136003	1.076006
O	-1.007207	-0.665198	-1.043958
F	-2.952916	-0.076374	-0.140271
H	0.345584	-1.499101	-0.834896

Rotational constants (GHz): 1.6736400 0.7458900 0.6414700
Vibrational harmonic frequencies (cm-1):
i121.2333 40.5500 50.4237
72.0061 101.7826 141.2068
156.0526 169.1996 203.6548
213.8516 232.6536 270.0908
369.4656 385.1384 560.4618
593.5700 617.0532 653.8522
716.5701 767.7607 795.0455
853.9754 959.6299 1040.6265
1252.6612 1387.9249 1431.3202
1708.7091 1942.5242 3455.6154
Zero-point correction (Hartree): 0.048168

TS.CF3OCFCF2OH.CF3OCFCFO+HF

E(UM062X/CC-pVDZ) (Hartree): -864.09142693
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.535440	-0.172146	-0.350612
C	0.485968	0.796778	-0.533397
O	-0.751730	0.481182	-0.925903
F	0.648998	1.987865	-0.026365
C	-1.581072	-0.117645	0.021875
F	-1.566644	0.571164	1.149995
F	-1.193118	-1.354356	0.265881
F	-2.791130	-0.123063	-0.489800
F	1.316057	-1.295749	-0.988405
O	2.721498	0.152674	-0.013472
F	1.273892	-0.662900	1.384220
H	2.407334	-0.219429	1.028059

Rotational constants (GHz): 1.8406000 0.8516200 0.7695600
Vibrational harmonic frequencies (cm-1):
i1442.1940 30.9921 62.5143
79.9027 104.8496 159.6607
206.6040 294.6185 346.2982
373.7423 449.7006 463.7451
538.5035 561.8552 620.8879
631.0149 664.3307 705.6063
790.7884 846.4672 926.3906

```
      946.2653                1201.8459                1246.3266
     1338.2892                1383.1716                1439.8977
     1521.3787                1671.2167                2151.7167
Zero-point correction (Hartree): 0.049570

TS.CF3OCFCF2OH.CF3OCFHCF2O
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.08853855
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.807480     -0.241396       0.005136
     C      -0.458082      0.427938       0.035456
     O       0.541447     -0.251413      -0.595244
     F      -2.814840      0.562866      -0.350202
     F      -0.440624      1.743397      -0.165095
     F      -1.891239     -1.354076      -0.728696
     O      -1.766299     -0.491366       1.353188
     H      -0.597301      0.114028       1.312167
     C       1.795591     -0.139531      -0.038174
     F       1.796741     -0.596210       1.210345
     F       2.207111      1.120209      -0.014545
     F       2.611288     -0.859949      -0.772942
Rotational constants (GHz):    2.1052600    0.6925300    0.6379300
Vibrational harmonic frequencies (cm-1):
    i1994.7735                  25.8416                  64.3534
       91.8140                 160.6811                 209.5000
      270.9146                 332.1101                 365.0041
      429.9808                 482.7567                 531.4378
      551.8734                 591.5122                 639.0407
      658.7853                 732.2696                 754.9359
      904.0860                 937.8266                1085.5425
     1182.7294                1216.6856                1247.4372
     1288.3268                1311.1927                1337.6063
     1390.5746                1488.5048                2032.7261
Zero-point correction (Hartree): 0.050840

TS.CF3OCFCFO.CFOCFO+CF3
-----------------------
E(UM062X/CC-pVDZ) (Hartree): -763.68593667
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.790748     -0.439115       0.009161
     C       0.914048      0.687222      -0.434052
     O      -0.123754      0.556627      -1.056845
     F       1.324932      1.863740       0.008022
     C      -1.639347     -0.055597       0.084879
     F      -2.533931      0.880655       0.253308
     F      -1.003871     -0.333381       1.202075
     F      -2.131731     -1.121514      -0.479623
     F       1.235963     -1.601515      -0.333068
     O       2.821885     -0.349993       0.579799
Rotational constants (GHz):    2.1866000    0.9042700    0.7559300
Vibrational harmonic frequencies (cm-1):
     i492.5493                  39.9501                  51.2726
       67.9916                 109.6130                 144.9495
      226.1791                 269.6194                 431.4772
      459.6702                 527.1826                 530.8548
      576.1467                 664.6601                 671.3077
      782.1377                 844.8291                1031.8328
     1184.2731                1341.5574                1377.1712
     1402.2187                1612.9540                1963.7628
Zero-point correction (Hartree): 0.037161

TS.CF3OCFCF2OH.CF3+HOCF2CFO.b
-----------------------
E(UM062X/CC-pVDZ) (Hartree): -864.10850576
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.578043     -0.338756       0.008103
     C       0.613740      0.745809      -0.442607
     O      -0.419402      0.511734      -1.071978
```

```
     F       0.870948      1.949370       0.040126
     C      -1.849126     -0.088973       0.026421
     F      -1.317030     -0.086511       1.226706
     F      -2.140226     -1.303625      -0.372583
     F      -2.876785      0.712454      -0.058010
     F       2.772789     -0.136441      -0.600710
     O       1.090308     -1.571962      -0.246713
     F       1.803807     -0.234887       1.325928
     H       0.555285     -1.529897      -1.055084
Rotational constants (GHz):    1.9127600    0.7309200    0.6589500
Vibrational harmonic frequencies (cm-1):
     i557.8708                35.1067                40.6900
       51.7458               102.0955               163.8409
      207.4582               242.0278               280.0163
      325.2953               421.7072               444.3114
      511.3547               528.5437               542.2412
      603.2652               638.0907               681.6789
      716.4092               824.9535              1040.8790
     1113.7136              1180.9823              1282.8568
     1366.0766              1372.0545              1387.8648
     1454.7492              1577.8987              3816.4843
Zero-point correction (Hartree): 0.052294

TS.CF3OCFOCF2OH.CF2OH+CF3OCFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -939.34915337
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.455216     -0.572011      -0.027808
     C       0.470431      0.989916       0.053244
     O      -0.737880      0.735443      -0.589470
     F       1.157256      1.719420      -0.845303
     C      -1.693806     -0.077919      -0.041016
     F      -1.715955     -0.054338       1.280807
     F      -1.510482     -1.336427      -0.434490
     F      -2.861251      0.335334      -0.503399
     F       1.378912     -0.978518      -1.271632
     O       2.699120     -0.276123       0.314632
     F       0.833343     -1.423385       0.777961
     H       2.664637      0.191275       1.168544
     O       0.589749      1.216932       1.261016
Rotational constants (GHz):    1.5427200    0.7666300    0.6939300
Vibrational harmonic frequencies (cm-1):
     i191.2982                19.9856                30.4818
      109.4788               161.5048               204.7069
      208.0590               273.6430               296.9906
      365.3265               408.5255               428.8971
      452.0698               457.4413               545.7483
      564.2543               568.3001               626.3329
      675.4160               735.3634               740.1965
      884.8728              1000.5867              1032.1709
     1192.9665              1218.8064              1290.5568
     1310.9766              1351.4774              1385.8185
     1459.2265              1593.8331              3769.0087
Zero-point correction (Hartree): 0.057781

TS.CF3OCFOCF2OH.CF3O+HOCF2CFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -939.31671301
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.435234     -0.519615      -0.006451
     C       0.880623      0.916880       0.112298
     O      -0.818989      0.800588      -0.557271
     F       1.367435      1.680865      -0.851310
     C      -1.756448     -0.071515      -0.050436
     F      -1.739164     -0.099099       1.269135
     F      -1.566590     -1.302670      -0.511871
     F      -2.941106      0.347191      -0.474978
     F       1.288057     -0.961528      -1.249797
     O       2.757825     -0.550947       0.296411
```

```
     F       0.725405     -1.299684       0.830517
     H       2.853600     -0.420001       1.252652
     O       0.509115      1.397838       1.174562
Rotational constants (GHz):    1.5575700    0.7348900    0.6657300
Vibrational harmonic frequencies (cm-1):
     i632.0476                 35.1574                 60.6623
      108.2176                131.7866                166.3456
      222.0512                245.5953                264.6131
      305.4907                379.7768                387.9266
      429.7950                450.5346                496.5667
      565.1058                590.3327                612.7000
      652.2858                673.2861                695.6424
      826.6604                930.9053               1139.2119
     1150.1990               1226.3768               1284.6814
     1316.3826               1330.8024               1367.2719
     1429.7164               1608.4539               3825.6804
Zero-point correction (Hartree): 0.056750

TS.CF3OCFOCF2OH.F+HOCF2COOCH3
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -939.30719846
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.800752     -0.345391      -0.024447
     C       0.391832      0.211881       0.262258
     O      -0.558815     -0.515209      -0.330466
     F       0.526627      1.747870      -0.758300
     C      -1.886715     -0.205650      -0.041757
     F      -2.153365      1.053392      -0.325325
     F      -2.152154     -0.435587       1.231722
     F      -2.618458     -0.997458      -0.794115
     F       1.947490     -0.586379      -1.328790
     O       2.763174      0.479078       0.410946
     F       1.850469     -1.545838       0.604193
     H       2.366151      1.119138       1.025012
     O       0.194786      1.010107       1.186294
Rotational constants (GHz):    1.6596700    0.6410100    0.5965800
Vibrational harmonic frequencies (cm-1):
     i635.6810                 49.9108                 63.5040
       89.2412                131.4915                147.6127
      201.9788                230.3687                236.8554
      320.1073                350.0361                380.2717
      434.6564                455.7166                519.3497
      567.1603                594.8585                612.6590
      652.4509                677.7699                767.8573
      907.6717                932.1051               1123.2011
     1202.6793               1222.4352               1308.9543
     1343.2433               1379.4643               1393.5740
     1479.7686               1629.2206               3784.3044
Zero-point correction (Hartree): 0.057388

TS.CF3OCFOCFO.CF3OCFO+CFO
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -838.91722482
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.857736     -0.559173      -0.111112
     C       0.577174      0.811581       0.163048
     O      -0.429416      0.412739      -0.706816
     F       1.216574      1.807261      -0.449126
     C      -1.559349     -0.126968      -0.134331
     F      -2.144419      0.736602       0.681322
     F      -1.294487     -1.236037       0.540724
     F      -2.379148     -0.412639      -1.127523
     F       1.334990     -1.702173       0.234743
     O       2.938802     -0.325927      -0.477604
     O       0.508743      0.726968       1.381059
Rotational constants (GHz):    1.8674600    0.8498000    0.7293900
Vibrational harmonic frequencies (cm-1):
     i378.6346                 34.3271                 66.4783
       98.7611                153.6847                192.4636
```

```
      199.2025                289.8169                378.8329
      390.5581                419.9109                481.6961
      556.2383                592.0313                630.2703
      675.3103                696.2131                747.8336
      901.5256               1011.6466               1153.2560
     1233.0026               1290.9599               1323.4873
     1365.6613               1631.5241               2036.5169
Zero-point correction (Hartree): 0.042263

TS.CF3OCFOCFO.CF3OCOCFO+F
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -838.87849309
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       2.048073      0.197450     -0.230674
     C       0.494052     -0.497121      0.004443
     O      -0.398463      0.516318      0.066026
     F       1.464165     -0.149493      1.386632
     C      -1.734904      0.146342     -0.052206
     F      -2.065960     -0.732044      0.875983
     F      -1.979592     -0.368719     -1.243820
     F      -2.432554      1.248802      0.105527
     F       1.931076      1.500903     -0.223702
     O       2.941697     -0.448144     -0.630835
     O       0.319573     -1.640057     -0.239560
Rotational constants (GHz):    2.2024900    0.7208000    0.6727100
Vibrational harmonic frequencies (cm-1):
     i445.3568                36.2862                 72.4269
      133.7687               160.7912                205.2082
      260.6222               324.3828                378.1907
      398.8609               435.3141                439.6874
      556.4235               591.1264                623.6830
      662.6422               678.8256                713.2768
      846.0060               915.1009               1124.8898
     1176.4417              1237.2151               1337.3931
     1384.0305              1854.7569               1952.4264
Zero-point correction (Hartree): 0.042146

TS.CF3OCFOCFO.FCOCFO+CF3O
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -838.88975913
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.624730     -0.622657     -0.153475
     C      -0.999610      0.778646     -0.228256
     O       0.503547      0.469536      0.749036
     F      -1.581848      1.616811      0.609912
     C       1.571019     -0.130350      0.123615
     F       2.258920      0.711472     -0.624845
     F       1.186232     -1.152732     -0.630164
     F       2.342162     -0.574479      1.106891
     F      -2.114718     -0.848576      1.055588
     O      -1.668080     -1.386040     -1.045651
     O      -0.397568      1.175716     -1.216853
Rotational constants (GHz):    1.7388500    0.8388600    0.7683600
Vibrational harmonic frequencies (cm-1):
     i669.6136                27.4940                 53.0315
       91.5743               135.8066                155.0051
      230.9810               259.8989                333.0859
      414.6621               432.7594                483.3394
      526.4895               614.4268                621.1924
      666.6544               679.1187                756.3493
      830.8795               934.3982               1177.1304
     1236.4302              1312.9719               1329.5020
     1352.8692              1595.5293               2011.9341
Zero-point correction (Hartree): 0.041607

TS.CF3OCFOHCF2.CF3OCFCF2+OH
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.06137899
Electronic state : 2-A
```

```
Cartesian coordinates (Angs):
     C       1.411821      0.563177      -0.210412
     C       0.578794     -0.487691      -0.125044
     O      -0.539000     -0.446809       0.646302
     F       0.702469     -1.532234      -0.911126
     C      -1.653741      0.072938       0.027938
     F      -1.931570     -0.578163      -1.093366
     F      -1.474679      1.355183      -0.275469
     F      -2.655376     -0.041820       0.871319
     F       1.259158      1.641698       0.511616
     F       2.481420      0.572933      -0.950557
     O       1.921931     -1.172309       1.396690
     H       1.482511     -0.695972       2.129420
Rotational constants (GHz):    1.7121400    0.7791000    0.7166000
Vibrational harmonic frequencies (cm-1):
     i318.5091                  40.9742                  70.4573
       96.9759                 111.7947                 127.9691
      196.7594                 209.0177                 264.8463
      339.5696                 359.0356                 406.5740
      466.5302                 515.3255                 546.4871
      558.0087                 639.1605                 651.5491
      702.0443                 712.5300                 846.8572
      947.1249                1228.1840                1265.8331
     1306.5812                1383.4519                1405.9371
     1452.6538                1844.6972                3731.8852
Zero-point correction (Hartree): 0.051097

TS.CF3OCFOHCF2.CF3OCFOCF2H
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.08151994
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.581099     -0.312717       0.167086
     C       1.967578      0.269312       0.087384
     F       2.858234     -0.406409      -0.613906
     O      -0.401920      0.611610      -0.155025
     F       2.081406      1.570169      -0.094982
     F       0.408299     -1.441083      -0.548552
     O       0.728547     -0.573196       1.514667
     H       1.934541     -0.075213       1.366350
     C      -1.700934      0.182881      -0.090145
     F      -2.465115      1.251190       0.036530
     F      -1.900612     -0.628154       0.945057
     F      -2.052657     -0.464486      -1.194085
Rotational constants (GHz):    2.0970700    0.7205500    0.6744300
Vibrational harmonic frequencies (cm-1):
    i2010.2961                  41.7103                  72.1776
      103.8572                 123.1684                 209.1708
      265.7493                 344.6287                 362.9963
      399.5847                 453.4509                 524.1736
      538.5823                 612.8344                 642.3207
      668.3162                 715.1296                 779.5455
      869.5129                 952.8196                1074.5215
     1169.6429                1193.1069                1227.3491
     1308.2535                1317.6407                1355.2006
     1368.4396                1504.2534                2038.0498
Zero-point correction (Hartree): 0.050658

TS.CF3OCFOHCF2.CF3OCOCF2+HF
--------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.08520329
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.325520      0.756909      -0.183472
     C      -0.766540     -0.536063      -0.455495
     O       0.547711     -0.664279      -0.735124
     F      -0.946929     -1.392721       1.177602
     C       1.533193      0.012793      -0.039883
     F       1.190624      0.237386       1.214762
     F       1.799318      1.172158      -0.629300
     F       2.611437     -0.739721      -0.080419
```

```
     F      -2.596050      0.864898       0.039534
     F      -0.634075      1.794226       0.185189
     O      -1.540689     -1.454542      -0.917887
     H      -1.521903     -1.877315       0.130875
Rotational constants (GHz):    1.7298600    0.9026100    0.7469200
Vibrational harmonic frequencies (cm-1):
    i1347.2893                43.4268                97.9282
      106.7756               123.7823               174.2174
      212.5826               255.7267               358.7171
      372.3259               389.3421               462.1516
      506.5857               546.5458               598.4069
      627.2798               655.1259               728.1086
      777.6425               830.7319               924.6459
      994.5221              1219.0501              1270.9563
     1326.4221              1378.8582              1471.8888
     1509.5827              1663.1788              2194.3313
Zero-point correction (Hartree): 0.049712

TS.CF3OCFOHCF2.CF3OCOHCF3
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -864.08396191
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.253229     -0.572603      -0.253868
     C       0.678312      0.678579      -0.340708
     O      -0.628427      0.983919      -0.273744
     C      -1.593110      0.032835      -0.024984
     F      -1.419917     -0.540690       1.150336
     F      -1.591166     -0.902234      -0.970049
     F      -2.746941      0.663542      -0.044571
     F       2.514386     -0.730557      -0.512213
     F       0.645663     -1.672134       0.059158
     O       1.434538      1.724489      -0.628642
     H       2.011243      1.803889       0.161878
     F       1.432341      0.481626       1.514513
Rotational constants (GHz):    1.8441400    0.8474900    0.7570000
Vibrational harmonic frequencies (cm-1):
     i344.4161                 30.2493                96.4331
      145.0258                158.9223               193.7578
      232.3611                277.2401               342.6229
      366.4745                381.7430               443.5963
      466.6893                511.6903               535.8137
      571.1586                628.5574               649.8572
      734.8371                815.8558               977.8304
     1216.1477               1262.7300              1284.4531
     1321.3611               1380.6372              1462.3312
     1486.7780               1774.3073              3635.8647
Zero-point correction (Hartree): 0.053276

TS.CFOCF2OH.CFOCFO+HF
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -526.58036479
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.523447      0.213250      -0.254719
     C       0.985572      0.077121      -0.043245
     O       1.727968      0.960271       0.190139
     F       1.344882     -1.188158      -0.181538
     F      -0.923618      1.433420      -0.031404
     O      -1.185264     -0.548049      -1.009632
     F      -1.050642     -0.687037       1.131659
     H      -1.449975     -1.064027       0.075273
Rotational constants (GHz):    3.6475200    2.5055800    1.9820300
Vibrational harmonic frequencies (cm-1):
    i1646.8304                63.8366               168.4411
      233.4023               324.1323               406.9839
      489.3905               637.5765               682.1138
      736.0815               829.3055               879.6634
      930.6562              1223.7996              1409.8650
     1683.6616              2009.6530              2039.5564
Zero-point correction (Hartree): 0.033599
```

TS.CF3+OCFCF2OH.CF4+OCFCFOH

E(UM062X/CC-pVDZ) (Hartree): -864.07045061
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-1.311918	0.684016	-0.012533
C	-1.982693	-0.629400	-0.170485
O	-2.288132	-1.182564	-1.168018
F	-2.140129	-1.182936	1.057406
C	2.102103	-0.141888	-0.004664
F	2.660478	0.932611	-0.500538
F	2.341103	-1.195030	-0.744156
F	2.461768	-0.338367	1.240927
F	-1.337908	1.447193	-1.074279
O	-1.466914	1.379967	1.105213
F	0.320776	0.135758	-0.002818
H	-1.559363	0.751358	1.839652

Rotational constants (GHz): 1.6336500 0.5942900 0.5647000
Vibrational harmonic frequencies (cm-1):

i1080.1972	12.3695	47.0225	
51.5692	97.6063	132.2606	
190.1267	196.8999	240.8138	
299.8201	333.9486	394.7373	
426.8272	512.1196	534.0525	
535.5335	552.1276	642.4711	
710.6455	760.0589	837.3126	
1058.0286	1110.2091	1242.3046	
1374.1614	1380.7016	1450.1824	
1502.3223	1959.9874	3814.8382	

Zero-point correction (Hartree): 0.051033

TS.CF3+OCFCF2OH.HCF3+OCFCF2O

E(UM062X/CC-pVDZ) (Hartree): -864.10213827
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.241590	0.903239	-0.111360
C	1.192367	-0.637745	-0.154407
F	2.324883	1.308292	0.534127
O	0.442537	1.636877	-0.574596
F	1.045777	-1.075743	1.111802
F	2.363231	-1.100336	-0.619552
O	0.233122	-1.121589	-0.978498
H	-0.944751	-0.457467	-0.640395
C	-1.871160	-0.039443	-0.023829
F	-2.430866	0.957557	-0.677499
F	-1.435730	0.375173	1.157683
F	-2.738106	-1.022847	0.138186

Rotational constants (GHz): 1.7577500 0.7239700 0.6307300
Vibrational harmonic frequencies (cm-1):

i810.9099	38.3740	49.5589	
65.5190	91.3804	121.1996	
164.9846	232.3184	241.8893	
352.5742	423.5195	438.6320	
518.5474	529.2110	610.4914	
656.2512	710.2377	779.9419	
808.7344	871.7337	1135.9724	
1149.6999	1214.6565	1247.8860	
1288.8744	1322.9989	1347.2995	
1378.2232	1510.3796	1998.9832	

Zero-point correction (Hartree): 0.048525

TS.CFOCF2OH+CF3.CF4+OCCF2OH

E(UM062X/CC-pVDZ) (Hartree): -864.05944840
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.054156	0.974810	-0.414156
C	1.726685	-0.352737	-0.011329
O	1.332864	2.041215	0.004675

```
     F       1.769688     -1.196173      -1.044795
     F       0.928366     -0.926892       0.926436
     O       2.976502     -0.151577       0.446968
     H       3.009299      0.733101       0.847017
     F      -0.494664      0.584715      -0.669886
     C      -1.992557     -0.062071       0.032026
     F      -2.995742      0.528642      -0.555928
     F      -1.970855     -1.344723      -0.192197
     F      -1.927229      0.219963       1.303103
Rotational constants (GHz):    1.9337200    0.6636600    0.6001200
Vibrational harmonic frequencies (cm-1):
    i1130.7500                  23.2924                  38.5311
       43.7886                  73.9340                 150.4409
      181.4332                 230.4892                 257.4333
      325.6407                 361.3560                 379.6501
      450.2445                 509.8560                 537.9792
      539.8998                 588.7911                 635.6631
      704.0672                 755.6148                 892.5297
     1050.6757                1144.2081                1193.8425
     1341.1067                1402.4700                1408.2008
     1425.7377                1945.1367                3789.1528
Zero-point correction (Hartree): 0.050988

TS.CFOCF2O.CFO+CF2O
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -525.95443095
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.039531      0.112075      -0.007761
     C       0.812832      0.189336      -0.008709
     F      -1.284151     -1.177678      -0.005331
     O      -1.797645      0.992345       0.002051
     F       1.073225     -0.646974      -1.026092
     F       1.051823     -0.494449       1.123204
     O       1.021661      1.390587      -0.092952
Rotational constants (GHz):    3.8794700    2.4342100    2.0242400
Vibrational harmonic frequencies (cm-1):
     i519.8411                  14.3781                 189.9886
      204.7994                 315.8166                 407.5797
      531.4701                 569.2972                 633.8294
      695.7399                 923.2170                1094.6740
     1208.9550                1588.8385                2053.2226
Zero-point correction (Hartree): 0.023765

TS.CFOCF2OH+H2O.CFOCFO+HF+H2O.a
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -603.03109006
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.327952      0.394170       0.009209
     C       0.009839     -0.185469      -0.450234
     F      -2.117850     -0.544527       0.520156
     O      -1.631129      1.531128      -0.057210
     O       0.792385      0.515628      -1.100269
     F      -0.079502     -1.489217      -0.720886
     F       0.635827     -0.347518       1.135423
     H       2.066310      0.426815      -0.531168
     O       2.720935      0.282662       0.311275
     H       1.869993     -0.051087       0.914456
     H       2.968572      1.168080       0.620260
Rotational constants (GHz):    3.1362200    1.3814200    1.2691300
Vibrational harmonic frequencies (cm-1):
     i684.6103                  33.6427                  55.5926
      179.2564                 230.1645                 339.2953
      369.5372                 433.1576                 463.9999
      529.4191                 541.7380                 589.0019
      641.9971                 704.7125                 736.6035
      837.3321                 895.7944                1166.1503
     1347.5157                1432.1526                1471.8233
     1651.6949                1754.7167                1963.3453
     2013.0355                2449.3264                3834.7792
```

Zero-point correction (Hartree): 0.060749

TS.CFOCF2OH+H2O.CFOCFO+HF+H2O.b

E(RM062X/CC-pVDZ) (Hartree): -603.03151100
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.382404	-0.239831	-0.026009
C	0.032950	0.417663	-0.299537
F	1.269490	-1.561553	-0.141192
O	2.395243	0.303317	0.232485
O	-0.699984	-0.001504	-1.206104
F	0.095745	1.723851	-0.062151
F	-0.666538	-0.046317	1.191343
H	-2.002863	-0.157911	-0.711296
O	-2.692705	-0.352250	0.089467
H	-1.874789	-0.256884	0.815081
H	-2.923183	-1.292524	0.030710

Rotational constants (GHz): 3.0718100 1.4535200 1.2498600
Vibrational harmonic frequencies (cm-1):

i682.0105	32.6504	61.0537
181.1320	227.0616	344.2053
367.5631	422.4128	455.7721
528.7839	539.5117	586.5739
641.5147	706.6372	745.9918
840.0502	902.1744	1175.3860
1352.0150	1428.0299	1472.1001
1648.0759	1753.6226	1957.0270
2010.7923	2458.0927	3833.2516

Zero-point correction (Hartree): 0.060762

```
*********************************************
CF3OCF=CF2 + OH : M06-2X/aug-cc-pVTZ geometry
*********************************************

CF3
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -336.91604862
E(CCSD/Aug-CC-pVDZ) (Hartree): -336.89690736
     T1 diagnostic:  0.016051
E(MP2/Aug-CC-pVDZ) (Hartree): -336.88703276
E(MP3/Aug-CC-pVDZ) (Hartree): -336.88631112
E(PMP2/Aug-CC-pVDZ) (Hartree): -336.88789619
E(PMP3/Aug-CC-pVDZ) (Hartree): -336.88682602
E(PUHF/Aug-CC-pVDZ) (Hartree): -336.17416151
E(UHF/Aug-CC-pVDZ) (Hartree): -336.17262351
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -336.93076910
     T1 diagnostic:  0.000481
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -337.20696132
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -337.18381127
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -337.18824773
     T1 diagnostic:  0.014568
     D1 diagnostic:  0.048241
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -337.16509769
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -337.20664407
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -337.18349403
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -337.20849049
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -337.18534045
E(ROHF/AUG-CC-PVDZ) (Hartree): -336.17041988
E(UM062X/Aug-CC-pVTZ) (Hartree): -337.59568155
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.000050     -0.000085       0.325037
     F      -1.197846     -0.359473      -0.072333
     F       0.910285     -0.857558      -0.072279
     F       0.287595      1.217087      -0.072080
Rotational constants (GHz):   10.9547500   10.9536700    5.6693500
Vibrational harmonic frequencies (cm-1):
      517.3827                 517.6520                 710.7345
     1119.4420                1310.0219                1310.3422
Zero-point correction (Hartree): 0.012497

CF3O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -411.98849576
E(CCSD/Aug-CC-pVDZ) (Hartree): -411.96407794
     T1 diagnostic:  0.015334
E(MP2/Aug-CC-pVDZ) (Hartree): -411.94476522
E(MP3/Aug-CC-pVDZ) (Hartree): -411.95241651
E(PMP2/Aug-CC-pVDZ) (Hartree): -411.94654256
E(PMP3/Aug-CC-pVDZ) (Hartree): -411.95345976
E(PUHF/Aug-CC-pVDZ) (Hartree): -411.06670151
E(UHF/Aug-CC-pVDZ) (Hartree): -411.06361863
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -412.33420441
E(CCSD/Aug-CC-pVTZ) (Hartree): -412.29586238
     T1 diagnostic:  0.014074
E(MP2/Aug-CC-pVTZ) (Hartree): -412.28571372
E(MP3/Aug-CC-pVTZ) (Hartree): -412.28768762
E(PMP2/Aug-CC-pVTZ) (Hartree): -412.28769056
E(PMP3/Aug-CC-pVTZ) (Hartree): -412.28880333
E(PUHF/Aug-CC-pVTZ) (Hartree): -411.18120075
E(UHF/Aug-CC-pVTZ) (Hartree): -411.17773468
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -411.99440504
     T1 diagnostic:  0.000215
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -412.34303404
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -412.31374557
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -412.31930684
     T1 diagnostic:  0.013568
     D1 diagnostic:  0.044179
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -412.29001836
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -412.34260727
```

```
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -412.31331880
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -412.34474919
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -412.31546072
E(ROHF/AUG-CC-PVDZ) (Hartree): -411.05905363
E(UM062X/Aug-CC-pVTZ) (Hartree): -412.82107529
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.006571      0.000343       0.033248
     F      -0.772785     -1.069473      -0.014373
     F       0.843088     -0.010899      -0.994138
     F      -0.770794      1.070309      -0.035049
     O       0.783124      0.011063       1.149069
Rotational constants (GHz):    6.0660100    5.8857900    5.6437400
Vibrational harmonic frequencies (cm-1):
      267.1286                 417.7304                 588.9537
      606.4694                 629.1854                 926.4697
     1254.4370                1273.1352                1310.9422
Zero-point correction (Hartree): 0.016572

CFOCF2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -449.99813181
E(CCSD/Aug-CC-pVDZ) (Hartree): -449.96486152
     T1 diagnostic:  0.021485
E(MP2/Aug-CC-pVDZ) (Hartree): -449.94576231
E(MP3/Aug-CC-pVDZ) (Hartree): -449.94619591
E(PMP2/Aug-CC-pVDZ) (Hartree): -449.95357447
E(PMP3/Aug-CC-pVDZ) (Hartree): -449.95125759
E(PUHF/Aug-CC-pVDZ) (Hartree): -448.93111686
E(UHF/Aug-CC-pVDZ) (Hartree): -448.92124577
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -450.00806528
     T1 diagnostic:  0.000468
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -450.38991069
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -450.35663922
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -450.35709843
     T1 diagnostic:  0.017211
     D1 diagnostic:  0.063304
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -450.32382695
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -450.38926694
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -450.35599546
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -450.39278884
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -450.35951736
E(ROHF/AUG-CC-PVDZ) (Hartree): -448.91221652
E(UM062X/Aug-CC-pVTZ) (Hartree): -450.93515226
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):
     C      -0.155605     -0.774946       0.000000
     C       0.000000      0.642754       0.000000
     F       1.035812     -1.385601       0.000000
     O      -1.190350     -1.362945       0.000000
     F       1.146662      1.248069       0.000000
     F      -1.020648      1.437167       0.000000
Rotational constants (GHz):    5.7371300    3.4339200    2.1481500
Vibrational harmonic frequencies (cm-1):
      128.0493 (  A")           205.8804 (  A")           227.2438 (  A')
      415.7058 (  A')           539.2289 (  A')           615.8811 (  A')
      645.1764 (  A")           827.1702 (  A')          1156.3462 (  A')
     1447.0106 (  A')          1565.4192 (  A')          1828.4957 (  A')
Zero-point correction (Hartree): 0.021874

CFOCF2OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -525.74929926
E(CCSD/Aug-CC-pVDZ) (Hartree): -525.70880050
     T1 diagnostic:  0.015331
E(MP2/Aug-CC-pVDZ) (Hartree): -525.69623314
E(MP3/Aug-CC-pVDZ) (Hartree): -525.69243515
E(RHF/Aug-CC-pVDZ) (Hartree): -524.44082680
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -526.21072651
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -526.17054324
```

```
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -526.17163048
     T1 diagnostic:  0.013498
     D1 diagnostic:  0.048046
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -526.13144721
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -526.20995940
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -526.16977613
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -526.21358603
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -526.17340276
E(RHF/AUG-CC-PVDZ) (Hartree): -524.44082679
E(RM062X/Aug-CC-pVTZ) (Hartree): -526.84003187
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.929047      0.134498      -0.000171
     C      -0.607494      0.021071      -0.000078
     F       1.509983     -1.046438      -0.000278
     O       1.519779      1.153804       0.000040
     F      -0.978647     -0.691862       1.078483
     F      -0.979141     -0.694302      -1.076682
     O      -1.192509      1.226434      -0.001584
     H      -0.517234      1.918099       0.000146
Rotational constants (GHz):    3.8203600    2.5446700    2.0827900
Vibrational harmonic frequencies (cm-1):
       33.3716                  210.5089                  241.1353
      305.5466                  397.5701                  441.0268
      529.8981                  613.8764                  702.6013
      787.4974                  836.8157                 1102.3224
     1187.8995                 1248.4435                 1341.6037
     1456.1852                 1962.9970                 3803.7008
Zero-point correction (Hartree): 0.039191

CFOCFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -425.47323729
E(CCSD/Aug-CC-pVDZ) (Hartree): -425.43606739
     T1 diagnostic:  0.016755
E(MP2/Aug-CC-pVDZ) (Hartree): -425.43116557
E(MP3/Aug-CC-pVDZ) (Hartree): -425.42066496
E(RHF/Aug-CC-pVDZ) (Hartree): -424.39234723
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -425.84644472
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -425.81388459
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -425.81073389
     T1 diagnostic:  0.015542
     D1 diagnostic:  0.046093
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -425.77817376
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -425.84556309
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -425.81300296
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -425.84950321
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -425.81694308
E(RHF/AUG-CC-PVDZ) (Hartree): -424.39234723
E(RM062X/Aug-CC-pVTZ) (Hartree): -426.36655918
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       0.000000      0.766517       0.000000
     C      -0.000005     -0.766518       0.000000
     O      -0.950757      1.452662       0.000000
     O       0.950759     -1.452655       0.000000
     F       1.239417      1.218915       0.000000
     F      -1.239416     -1.218919       0.000000
Rotational constants (GHz):    6.0128900    3.5767100    2.2426700
Vibrational harmonic frequencies (cm-1):
       52.2591 (  A")           250.5281 (  A')           422.5548 (  A')
      458.8021 (  A")           536.7023 (  A')           693.7135 (  A')
      835.7030 (  A")           839.3270 (  A')          1173.8611 (  A')
     1335.5356 (  A')          1976.6718 (  A')          1977.9391 (  A')
Zero-point correction (Hartree): 0.024043

CFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -212.66782019
E(CCSD/Aug-CC-pVDZ) (Hartree): -212.64990301
```

```
     T1 diagnostic:  0.022821
E(MP2/Aug-CC-pVDZ) (Hartree): -212.64389186
E(MP3/Aug-CC-pVDZ) (Hartree): -212.63876694
E(PMP2/Aug-CC-pVDZ) (Hartree): -212.64672252
E(PMP3/Aug-CC-pVDZ) (Hartree): -212.64064141
E(PUHF/Aug-CC-pVDZ) (Hartree): -212.14496698
E(UHF/Aug-CC-pVDZ) (Hartree): -212.14114534
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -212.67245338
     T1 diagnostic:  0.000793
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -212.85268665
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -212.83667697
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -212.83520252
     T1 diagnostic:  0.023178
     D1 diagnostic:  0.068730
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -212.81919284
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -212.85218889
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -212.83617920
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -212.85482458
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -212.83881490
E(ROHF/AUG-CC-PVDZ) (Hartree): -212.13632136
E(UM062X/Aug-CC-pVTZ) (Hartree): -213.11139379
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.000000      0.418366       0.000000
     F      -1.008812     -0.433873       0.000000
     O       1.134913      0.174333       0.000000
Rotational constants (GHz):  192.1730700   11.6329400   10.9689500
Vibrational harmonic frequencies (cm-1):
      650.9356 (  A')          1091.2606 (  A')          1982.8252 (  A')
Zero-point correction (Hartree): 0.008486

F
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree):  -99.55006944
E(CCSD/Aug-CC-pVDZ) (Hartree):  -99.54774893
     T1 diagnostic:  0.009722
E(MP2/Aug-CC-pVDZ) (Hartree):  -99.53569906
E(MP3/Aug-CC-pVDZ) (Hartree):  -99.54577504
E(PMP2/Aug-CC-pVDZ) (Hartree):  -99.53706645
E(PMP3/Aug-CC-pVDZ) (Hartree):  -99.54652791
E(PUHF/Aug-CC-pVDZ) (Hartree):  -99.38373494
E(UHF/Aug-CC-pVDZ) (Hartree):  -99.38109179
E(UM062X/Aug-CC-pVTZ) (Hartree):  -99.73232189
Point group : OH
Cartesian coordinates (Angs):
     F       0.000000      0.000000       0.000000
Zero-point correction (Hartree): 0.000000

HF
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -100.26362258
E(CCSD/Aug-CC-pVDZ) (Hartree): -100.25947091
     T1 diagnostic:  0.012484
E(MP2/Aug-CC-pVDZ) (Hartree): -100.25577890
E(MP3/Aug-CC-pVDZ) (Hartree): -100.25644635
E(RHF/Aug-CC-pVDZ) (Hartree): -100.03333500
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -100.34962473
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -100.34247742
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -100.34547449
     T1 diagnostic:  0.008822
     D1 diagnostic:  0.014652
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -100.33832718
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -100.34965408
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -100.34250677
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -100.34978276
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -100.34263545
E(RHF/AUG-CC-PVDZ) (Hartree): -100.03333500
E(RM062X/Aug-CC-pVTZ) (Hartree): -100.45301335
Point group : C*V
Electronic state : 1-SG
```

```
Cartesian coordinates (Angs):
     F       0.000000      0.000000       0.091997
     H       0.000000      0.000000      -0.827973
Rotational constants (GHz):    0.0000000  623.9250717  623.9250717
Vibrational harmonic frequencies (cm-1):
     4159.7924 (  SG)
Zero-point correction (Hartree): 0.009477

O2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -150.01974010
E(CCSD/Aug-CC-pVDZ) (Hartree): -150.00798598
     T1 diagnostic:  0.017237
E(MP2/Aug-CC-pVDZ) (Hartree): -150.00187910
E(MP3/Aug-CC-pVDZ) (Hartree): -149.99995982
E(PMP2/Aug-CC-pVDZ) (Hartree): -150.00860413
E(PMP3/Aug-CC-pVDZ) (Hartree): -150.00309231
E(PUHF/Aug-CC-pVDZ) (Hartree): -149.65562822
E(UHF/Aug-CC-pVDZ) (Hartree): -149.64482689
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -150.03256052
     T1 diagnostic:  0.001007
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -150.14485938
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -150.13379610
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -150.13259123
     T1 diagnostic:  0.009707
     D1 diagnostic:  0.016332
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -150.12152796
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -150.14458503
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -150.13352175
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -150.14450572
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -150.13344245
E(ROHF/AUG-CC-PVDZ) (Hartree): -149.62284252
E(UM062X/Aug-CC-pVTZ) (Hartree): -150.32479538
Point group : D*H
Electronic state : 3-SGG
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.594925
     O       0.000000      0.000000      -0.594925
Rotational constants (GHz):    0.0000000   44.6355313   44.6355313
Vibrational harmonic frequencies (cm-1):
     1754.4580 ( SGG)
Zero-point correction (Hartree): 0.003997

OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree):  -75.58403081
E(CCSD/Aug-CC-pVDZ) (Hartree):  -75.58066519
     T1 diagnostic:  0.012131
E(MP2/Aug-CC-pVDZ) (Hartree):  -75.56556372
E(MP3/Aug-CC-pVDZ) (Hartree):  -75.57786120
E(PMP2/Aug-CC-pVDZ) (Hartree):  -75.56732589
E(PMP3/Aug-CC-pVDZ) (Hartree):  -75.57892392
E(PUHF/Aug-CC-pVDZ) (Hartree):  -75.40650427
E(UHF/Aug-CC-pVDZ) (Hartree):  -75.40357810
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree):  -75.57183096
     T1 diagnostic:  0.000130
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree):  -75.64685987
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree):  -75.64057201
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree):  -75.64358240
     T1 diagnostic:  0.008897
     D1 diagnostic:  0.015262
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree):  -75.63729455
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree):  -75.64687263
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree):  -75.64058478
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree):  -75.64693076
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree):  -75.64064291
E(ROHF/AUG-CC-PVDZ) (Hartree):  -75.39925405
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

FO2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -249.57802139
E(CCSD/Aug-CC-pVDZ) (Hartree): -249.55129982
     T1 diagnostic:  0.040624
E(MP2/Aug-CC-pVDZ) (Hartree): -249.53506491
E(MP3/Aug-CC-pVDZ) (Hartree): -249.52903895
E(PMP2/Aug-CC-pVDZ) (Hartree): -249.53879473
E(PMP3/Aug-CC-pVDZ) (Hartree): -249.53124506
E(PUHF/Aug-CC-pVDZ) (Hartree): -248.94171267
E(UHF/Aug-CC-pVDZ) (Hartree): -248.93634014
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -249.56305878
     T1 diagnostic:  0.000845
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -249.78791795
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -249.76938471
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -249.76217378
     T1 diagnostic:  0.042129
     D1 diagnostic:  0.138980
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -249.74364053
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -249.78758819
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -249.76905495
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -249.79135691
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -249.77282367
E(ROHF/AUG-CC-PVDZ) (Hartree): -248.92908639
E(UM062X/Aug-CC-pVTZ) (Hartree): -250.06141196
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):
     F      -0.990182     -0.605894       0.000000
     O       0.000000      0.548845       0.000000
     O       1.113954      0.132785       0.000000
Rotational constants (GHz):   81.4651100   11.4030800   10.0029200
Vibrational harmonic frequencies (cm-1):
      436.8240 (  A')           671.6464 (  A')          1523.0971 (  A')
Zero-point correction (Hartree): 0.005995

CF4
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -436.66486364
E(CCSD/Aug-CC-pVDZ) (Hartree): -436.64021317
     T1 diagnostic:  0.013058
E(MP2/Aug-CC-pVDZ) (Hartree): -436.63214204
E(MP3/Aug-CC-pVDZ) (Hartree): -436.62942215
E(RHF/Aug-CC-pVDZ) (Hartree): -435.69485173
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -437.04452276
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -437.01456001
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -437.02052419
     T1 diagnostic:  0.010845
     D1 diagnostic:  0.027692
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -436.99056143
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -437.04412895
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -437.01416620
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -437.04602440
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -437.01606165
E(RHF/AUG-CC-PVDZ) (Hartree): -435.69485172
E(RM062X/Aug-CC-pVTZ) (Hartree): -437.53902683
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C      -0.000011      0.000013       0.000000
     F      -1.075299      0.760407       0.000000
     F       1.075327      0.760333       0.000000
     F      -0.000011     -0.760374       1.075325
     F      -0.000011     -0.760374      -1.075325
Rotational constants (GHz):    5.7513200    5.7512700    5.7511800
```

```
Vibrational harmonic frequencies (cm-1):
      438.8158 (  A')           439.1734 (  A")           636.8057 (  A')
      637.0667 (  A")           637.0717 (  A')           941.5475 (  A')
     1320.6264 (  A")          1320.7493 (  A')          1321.2840 (  A')
Zero-point correction (Hartree): 0.017526

HCF3
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -337.59215799
E(CCSD/Aug-CC-pVDZ) (Hartree): -337.57256318
     T1 diagnostic:  0.013587
E(MP2/Aug-CC-pVDZ) (Hartree): -337.56049378
E(MP3/Aug-CC-pVDZ) (Hartree): -337.56277752
E(RHF/Aug-CC-pVDZ) (Hartree): -336.81510309
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -337.88713544
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -337.86291101
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -337.86802468
     T1 diagnostic:  0.011165
     D1 diagnostic:  0.027248
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -337.84380025
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -337.88684220
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -337.86261776
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -337.88837738
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -337.86415295
E(RHF/AUG-CC-PVDZ) (Hartree): -336.81510309
E(RM062X/Aug-CC-pVTZ) (Hartree): -338.27266965
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.000087     -0.000124       0.340583
     F      -0.798904     -0.956222      -0.128595
     F       1.227729     -0.213570      -0.128578
     F      -0.428866      1.169883      -0.128547
     H      -0.000157     -0.000077       1.427986
Rotational constants (GHz):   10.4024900   10.3988600    5.7107400
Vibrational harmonic frequencies (cm-1):
      515.0152                  515.2700                  712.2913
     1172.3039                 1200.9083                 1201.6049
     1414.1147                 1414.2983                 3178.9846
Zero-point correction (Hartree): 0.025800

FNO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -229.26335692
E(CCSD/Aug-CC-pVDZ) (Hartree): -229.23913560
     T1 diagnostic:  0.022157
E(MP2/Aug-CC-pVDZ) (Hartree): -229.23987876
E(MP3/Aug-CC-pVDZ) (Hartree): -229.22602153
E(RHF/Aug-CC-pVDZ) (Hartree): -228.65800609
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -229.45853503
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -229.44115566
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -229.43538718
     T1 diagnostic:  0.021528
     D1 diagnostic:  0.060852
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -229.41800781
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -229.45773443
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -229.44035505
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -229.46128411
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -229.44390474
E(RHF/AUG-CC-PVDZ) (Hartree): -228.65800609
E(RM062X/Aug-CC-pVTZ) (Hartree): -229.72011450
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     F      -0.940989     -0.579405       0.000000
     N       0.000000      0.551202       0.000000
     O       1.058613      0.169529       0.000000
Rotational constants (GHz):   97.6744100   12.4354500   11.0310300
Vibrational harmonic frequencies (cm-1):
      580.8086 (  A')           827.3994 (  A')          1981.8837 (  A')
Zero-point correction (Hartree): 0.007723
```

```
NO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -129.62340013
E(CCSD/Aug-CC-pVDZ) (Hartree): -129.61043015
     T1 diagnostic:  0.022643
E(MP2/Aug-CC-pVDZ) (Hartree): -129.60198234
E(MP3/Aug-CC-pVDZ) (Hartree): -129.60094805
E(PMP2/Aug-CC-pVDZ) (Hartree): -129.60591473
E(PMP3/Aug-CC-pVDZ) (Hartree): -129.60340171
E(PUHF/Aug-CC-pVDZ) (Hartree): -129.27660045
E(UHF/Aug-CC-pVDZ) (Hartree): -129.27121024
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -129.61991150
     T1 diagnostic:  0.000669
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -129.73304160
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -129.72263170
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -129.72039356
     T1 diagnostic:  0.020809
     D1 diagnostic:  0.045520
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -129.70998366
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -129.73269619
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -129.72228629
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -129.73424813
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -129.72383822
E(ROHF/AUG-CC-PVDZ) (Hartree): -129.26419668
E(UM062X/Aug-CC-pVTZ) (Hartree): -129.89335138
Point group : C*V
Cartesian coordinates (Angs):
     N       0.000000      0.000000      -0.606410
     O       0.000000      0.000000       0.530609
Rotational constants (GHz):    0.0000000   52.3561998   52.3561998
Vibrational harmonic frequencies (cm-1):
     2066.0391 (  SG)
Zero-point correction (Hartree): 0.004707

CF2O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -312.40224471
E(CCSD/Aug-CC-pVDZ) (Hartree): -312.37961809
     T1 diagnostic:  0.015319
E(MP2/Aug-CC-pVDZ) (Hartree): -312.37639437
E(MP3/Aug-CC-pVDZ) (Hartree): -312.36978218
E(RHF/Aug-CC-pVDZ) (Hartree): -311.65523696
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -312.67659354
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -312.65401106
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -312.65478245
     T1 diagnostic:  0.014042
     D1 diagnostic:  0.045636
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -312.63219997
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -312.67611355
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -312.65353107
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -312.67831177
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -312.65572929
E(RHF/AUG-CC-PVDZ) (Hartree): -311.65523696
E(RM062X/Aug-CC-pVTZ) (Hartree): -313.04496676
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     C       0.000000      0.000000       0.141685
     O       0.000000      0.000000       1.308682
     F       0.000000      1.057949      -0.628865
     F       0.000000     -1.057949      -0.628865
Rotational constants (GHz):   11.8834000   11.8530400    5.9341000
Vibrational harmonic frequencies (cm-1):
      589.8658                631.4124                 797.9617
     1010.4306               1300.3034                2020.6839
Zero-point correction (Hartree): 0.014468

H2O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree):  -76.27377604
E(CCSD/Aug-CC-pVDZ) (Hartree):  -76.26855934
```

```
     T1 diagnostic:  0.012284
E(MP2/Aug-CC-pVDZ) (Hartree):  -76.26079349
E(MP3/Aug-CC-pVDZ) (Hartree):  -76.26553289
E(RHF/Aug-CC-pVDZ) (Hartree):  -76.04133056
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree):  -76.34547905
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree):  -76.33832353
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree):  -76.34048177
     T1 diagnostic:  0.009595
     D1 diagnostic:  0.017559
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree):  -76.33332624
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree):  -76.34547247
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree):  -76.33831694
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree):  -76.34566631
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree):  -76.33851078
E(RHF/AUG-CC-PVDZ) (Hartree):  -76.04133056
E(RM062X/Aug-CC-pVTZ) (Hartree):  -76.43010673
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
     O       0.000000      0.000000       0.116390
     H       0.000000      0.762470      -0.465561
     H       0.000000     -0.762470      -0.465561
Rotational constants (GHz):  833.6308100  431.2772300  284.2309300
Vibrational harmonic frequencies (cm-1):
     1619.5204                3869.6600                3972.6125
Zero-point correction (Hartree): 0.021556

CF3OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -412.68034333
E(CCSD/Aug-CC-pVDZ) (Hartree): -412.65448293
     T1 diagnostic:  0.013152
E(MP2/Aug-CC-pVDZ) (Hartree): -412.64325767
E(MP3/Aug-CC-pVDZ) (Hartree): -412.64377238
E(RHF/Aug-CC-pVDZ) (Hartree): -411.70621449
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -413.04287317
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -413.01274678
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -413.01779508
     T1 diagnostic:  0.010914
     D1 diagnostic:  0.029502
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -412.98766869
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -413.04249503
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -413.01236864
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -413.04432387
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -413.01419748
E(RHF/AUG-CC-PVDZ) (Hartree): -411.70621449
E(RM062X/Aug-CC-pVTZ) (Hartree): -413.51933257
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.004770      0.022374       0.000027
     F       0.264983     -0.731883      -1.071617
     F       0.269124     -0.728063       1.073263
     F       0.807798      1.062014      -0.003307
     O      -1.271624      0.466482       0.001623
     H      -1.875528     -0.284719       0.001796
Rotational constants (GHz):    5.7367500    5.6817300    5.6378500
Vibrational harmonic frequencies (cm-1):
      251.7883                 445.3654                 455.5775
      608.3323                 630.1886                 642.8287
      931.0605                1132.7543                1223.7762
     1326.0300                1432.5993                3857.2159
Zero-point correction (Hartree): 0.029474

CF3OCFCF2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -787.00837175
E(CCSD/Aug-CC-pVDZ) (Hartree): -786.95343314
     T1 diagnostic:  0.013967
E(MP2/Aug-CC-pVDZ) (Hartree): -786.93380512
E(MP3/Aug-CC-pVDZ) (Hartree): -786.93357391
E(RHF/Aug-CC-pVDZ) (Hartree): -785.14914490
```

```
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -787.69440603
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -787.63710232
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -787.64116203
     T1 diagnostic:  0.012171
     D1 diagnostic:  0.036034
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -787.58385832
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -787.69354502
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -787.63624131
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -787.69767868
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -787.64037497
E(RHF/AUG-CC-PVDZ) (Hartree): -785.14914490
E(RM062X/Aug-CC-pVTZ) (Hartree): -788.62828972
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.688942     -0.285791      -0.062739
     C       0.700416      0.547437      -0.322426
     O      -0.480816      0.152285      -0.855667
     F       0.829571      1.851845      -0.147668
     C      -1.486193     -0.110863       0.040109
     F      -1.715822      0.926726       0.833412
     F      -1.185912     -1.150646       0.807160
     F      -2.568138     -0.380648      -0.654268
     F       1.609467     -1.579624      -0.233086
     F       2.856115      0.096460       0.385080
Rotational constants (GHz):    2.3722300    0.9247100    0.7685300
Vibrational harmonic frequencies (cm-1):
       37.5078                74.7467               120.8240
      198.0165               213.2699               344.4227
      369.4525               445.6470               470.1532
      544.6117               557.0763               614.0070
      643.3737               651.5821               727.8200
      849.3273               945.4895              1219.7324
     1240.0152              1268.3436              1345.5522
     1364.9966              1401.8671              1937.4241
Zero-point correction (Hartree): 0.040062

CF3OCFCF2OH.b
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.67940195
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.61985276
     T1 diagnostic:  0.015011
E(MP2/Aug-CC-pVDZ) (Hartree): -862.59333768
E(MP3/Aug-CC-pVDZ) (Hartree): -862.59527210
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.59481043
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.59616170
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.62487051
E(UHF/Aug-CC-pVDZ) (Hartree): -860.62247052
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.45363994
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.518734     -0.252099      -0.020518
     C       0.533475      0.767904      -0.565023
     O      -0.712525      0.387214      -0.947776
     F       0.570982      1.928007       0.060637
     C      -1.599449     -0.095831      -0.027759
     F      -1.644657      0.650552       1.064778
     F      -1.267976     -1.337953       0.353610
     F      -2.783372     -0.136948      -0.589199
     F       1.450197     -1.344777      -0.808124
     O       1.345658     -0.587610       1.287134
     F       2.740312      0.275692      -0.126404
     H       0.629000     -1.227850       1.367257
Rotational constants (GHz):    1.9736900    0.8326600    0.7393400
Vibrational harmonic frequencies (cm-1):
       30.0127                73.9088               118.6704
      161.3775               201.9144               217.8709
      249.0447               325.6431               356.8960
      430.3517               479.6864               510.7112
      554.5476               586.4402               630.1259
      638.1139               688.3116               756.0145
      820.2984               918.7688              1113.7329
```

```
     1133.7301                1201.5724                1230.6017
     1244.8910                1331.3237                1348.5507
     1380.4784                1422.2351                3850.6365
Zero-point correction (Hartree): 0.054691

CF3OCFCF2OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.67938565
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.61998113
     T1 diagnostic:  0.014933
E(MP2/Aug-CC-pVDZ) (Hartree): -862.59347533
E(MP3/Aug-CC-pVDZ) (Hartree): -862.59540270
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.59495995
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.59629719
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.62565487
E(UHF/Aug-CC-pVDZ) (Hartree): -860.62324094
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.45383120
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.510545     -0.281409      -0.045150
     C       0.536932      0.730124      -0.609555
     O      -0.721333      0.397795      -0.950609
     F       0.651089      1.923102      -0.032890
     C      -1.599479     -0.095959      -0.008830
     F      -1.529678      0.589442       1.122669
     F      -1.353475     -1.368017       0.254568
     F      -2.808913      0.011401      -0.513900
     F       1.456386     -1.392563      -0.775455
     O       2.787224      0.167227      -0.049836
     F       1.132515     -0.608677       1.223468
     H       2.853567      0.971113       0.478627
Rotational constants (GHz):    1.9671300    0.8517200    0.7523600
Vibrational harmonic frequencies (cm-1):
       56.1864                  64.2653                 100.0778
      145.6761                 195.6141                 217.2406
      231.8838                 333.9885                 355.5384
      430.3594                 473.7716                 518.6328
      551.6080                 588.2199                 631.7813
      635.5767                 688.9757                 756.4629
      817.0888                 919.8916                1076.6466
     1115.4015                1195.0133                1252.5595
     1279.5839                1324.2073                1334.9484
     1380.0539                1445.4786                3851.2739
Zero-point correction (Hartree): 0.054603

CF3OCFCFOH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -763.03065280
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.97447156
     T1 diagnostic:  0.014030
E(MP2/Aug-CC-pVDZ) (Hartree): -762.95275856
E(MP3/Aug-CC-pVDZ) (Hartree): -762.95492937
E(RHF/Aug-CC-pVDZ) (Hartree): -761.16788487
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.70066848
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -763.64327573
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -763.64634146
     T1 diagnostic:  0.012242
     D1 diagnostic:  0.039870
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -763.58894871
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.69982780
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -763.64243505
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.70385615
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -763.64646340
E(RHF/AUG-CC-PVDZ) (Hartree): -761.16788486
E(RM062X/Aug-CC-pVTZ) (Hartree): -764.61669024
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.697303     -0.314127      -0.065234
     C       0.696456      0.508023      -0.332742
     O      -0.498166      0.147337      -0.860605
     F       0.864571      1.827593      -0.167327
```

```
     C      -1.498558     -0.097117       0.042375
     F      -1.698955      0.942592       0.843706
     F      -1.218999     -1.146717       0.803783
     F      -2.595628     -0.337827      -0.641731
     F       1.582652     -1.611350      -0.229121
     O       2.906087      0.023870       0.381457
     H       2.962662      0.981061       0.483004
Rotational constants (GHz):    2.3678000    0.9378600    0.7770100
Vibrational harmonic frequencies (cm-1):
       39.3526                  75.9167                 113.6979
      196.8963                 210.8595                 333.3735
      343.3296                 369.5487                 430.9537
      470.1321                 546.0914                 561.8221
      633.2306                 642.1482                 653.3715
      718.7025                 848.4312                 945.1177
     1141.9258                1241.8175                1261.1224
     1275.7995                1340.5050                1347.0802
     1453.5124                1912.3119                3852.1868
Zero-point correction (Hartree): 0.052305

CF3OCFCFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -762.41668276
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.36085840
     T1 diagnostic:  0.018660
E(MP2/Aug-CC-pVDZ) (Hartree): -762.33613262
E(MP3/Aug-CC-pVDZ) (Hartree): -762.33453882
E(PMP2/Aug-CC-pVDZ) (Hartree): -762.34370037
E(PMP3/Aug-CC-pVDZ) (Hartree): -762.33949247
E(PUHF/Aug-CC-pVDZ) (Hartree): -760.59888672
E(UHF/Aug-CC-pVDZ) (Hartree): -760.58936602
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -762.43563794
     T1 diagnostic:  0.000371
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.08010394
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -763.02364568
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -763.02552988
     T1 diagnostic:  0.015132
     D1 diagnostic:  0.062102
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -762.96907162
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.07905991
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -763.02260164
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.08425775
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -763.02779948
E(ROHF/AUG-CC-PVDZ) (Hartree): -760.58090571
E(UM062X/Aug-CC-pVTZ) (Hartree): -763.99861019
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.873488     -0.283003      -0.005999
     C       0.732139      0.553543      -0.268754
     O      -0.410369      0.124131      -0.815363
     F       0.856461      1.843711      -0.142807
     C      -1.471029     -0.111747       0.038604
     F      -1.800357      0.988057       0.697154
     F      -1.163206     -1.046276       0.922696
     F      -2.479154     -0.508567      -0.697243
     F       1.582952     -1.570207      -0.221660
     O       2.938138      0.086718       0.364567
Rotational constants (GHz):    2.4015400    0.9527600    0.7876000
Vibrational harmonic frequencies (cm-1):
       30.8096                  54.9156                  79.5883
      148.8373                 212.8933                 327.6208
      357.1783                 380.5919                 465.8821
      530.7936                 567.1727                 638.9214
      665.2909                 669.9304                 703.4067
      832.0471                 943.3547                1149.2375
     1208.2625                1280.0836                1354.9931
     1409.3401                1503.0235                1845.4521
Zero-point correction (Hartree): 0.039548

CF3OCFOCF2OH
-------------------------
```

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -937.74545787
E(CCSD/Aug-CC-pVDZ) (Hartree): -937.67914431
T1 diagnostic: 0.017289
E(MP2/Aug-CC-pVDZ) (Hartree): -937.64401159
E(MP3/Aug-CC-pVDZ) (Hartree): -937.65164978
E(PMP2/Aug-CC-pVDZ) (Hartree): -937.64616276
E(PMP3/Aug-CC-pVDZ) (Hartree): -937.65300845
E(PUHF/Aug-CC-pVDZ) (Hartree): -935.50218141
E(UHF/Aug-CC-pVDZ) (Hartree): -935.49864713
E(UM062X/Aug-CC-pVTZ) (Hartree): -939.67178872
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.380403	-0.521443	-0.023440
C	0.565405	0.857434	-0.000780
O	-0.721756	0.778985	-0.534941
F	1.203447	1.683136	-0.848147
C	-1.680708	-0.058606	-0.042483
F	-1.699462	-0.104059	1.281207
F	-1.527345	-1.295254	-0.497423
F	-2.840391	0.401564	-0.471954
F	1.241341	-1.033102	-1.236549
O	2.689990	-0.343433	0.214143
F	0.811390	-1.355972	0.863406
H	2.823771	0.113820	1.053303
O	0.642367	1.258830	1.262304

Rotational constants (GHz): 1.5690500 0.7777300 0.7075900
Vibrational harmonic frequencies (cm-1):

41.5964	65.2281	117.6917
158.8565	197.5291	220.4649
248.5576	317.1541	337.4952
349.6156	373.1564	432.1009
467.0354	521.1334	536.1744
585.5829	625.3223	668.9336
692.3582	731.0070	778.8964
867.7167	974.3913	1091.4635
1149.4329	1203.4483	1255.8633
1272.0385	1277.2491	1300.5400
1342.0130	1413.1134	3840.4384

Zero-point correction (Hartree): 0.057988

CF3OCFOCFO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -837.47280392
E(CCSD/Aug-CC-pVDZ) (Hartree): -837.41044764
T1 diagnostic: 0.016370
E(MP2/Aug-CC-pVDZ) (Hartree): -837.38394495
E(MP3/Aug-CC-pVDZ) (Hartree): -837.38469304
E(PMP2/Aug-CC-pVDZ) (Hartree): -837.38594288
E(PMP3/Aug-CC-pVDZ) (Hartree): -837.38592337
E(PUHF/Aug-CC-pVDZ) (Hartree): -835.46096970
E(UHF/Aug-CC-pVDZ) (Hartree): -835.45766747
E(UM062X/Aug-CC-pVTZ) (Hartree): -839.20080563
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.555107	-0.553596	0.169987
C	0.720907	0.725950	-0.137611
O	-0.504024	0.459298	-0.754731
F	1.405239	1.422662	-1.063895
C	-1.483177	-0.139469	-0.013081
F	-2.090763	0.717269	0.789941
F	-0.985749	-1.126159	0.734756
F	-2.363411	-0.636134	-0.852945
F	1.519219	-1.354387	-0.881463
O	2.157596	-0.771354	1.148906
O	0.581698	1.386236	1.024160

Rotational constants (GHz): 1.7520800 0.9117100 0.8377000
Vibrational harmonic frequencies (cm-1):

48.7130	56.8937	87.6194
161.1413	214.2614	231.8856
327.8106	357.1793	375.8044
435.9079	486.7333	516.3118

```
      621.8567                 643.5234                 679.5603
      716.0841                 791.8045                 817.8198
      940.6982                1073.4457                1169.4076
     1200.0343                1262.6999                1276.5884
     1285.8286                1351.7603                1977.0995
Zero-point correction (Hartree): 0.043532

CF3OCFOHCF2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.67823901
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.61849154
     T1 diagnostic:  0.015042
E(MP2/Aug-CC-pVDZ) (Hartree): -862.59266732
E(MP3/Aug-CC-pVDZ) (Hartree): -862.59369205
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.59389342
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.59443402
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.62203596
E(UHF/Aug-CC-pVDZ) (Hartree): -860.61996547
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.45173426
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.489195      0.654573       0.099178
     C      -0.883855     -0.731683      -0.002240
     O       0.415719     -0.800292      -0.558508
     F      -0.816477     -1.234597       1.254094
     C       1.417062      0.008786      -0.116461
     F       1.555906     -0.016787       1.201120
     F       1.216253      1.272691      -0.480181
     F       2.533853     -0.416748      -0.674872
     F      -1.564058      1.306421      -1.037024
     F      -1.022788      1.406063       1.070653
     O      -1.686380     -1.470557      -0.795468
     H      -1.222976     -2.276653      -1.055168
Rotational constants (GHz):    1.5627000    0.9837300    0.8717900
Vibrational harmonic frequencies (cm-1):
       56.5679                  85.7806                 130.8114
      157.6260                 206.2864                 223.6211
      296.7746                 350.1205                 367.4183
      400.5865                 449.6121                 503.7303
      552.3728                 582.8158                 612.7878
      659.3554                 682.7016                 751.8294
      822.5844                 930.1136                1073.3260
     1123.2349                1239.6282                1270.2941
     1275.8182                1327.0924                1334.4584
     1349.5862                1490.0589                3828.4442
Zero-point correction (Hartree): 0.054985

CF3OCOHCF2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -763.02985823
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.97351005
     T1 diagnostic:  0.013960
E(MP2/Aug-CC-pVDZ) (Hartree): -762.95168113
E(MP3/Aug-CC-pVDZ) (Hartree): -762.95394099
E(RHF/Aug-CC-pVDZ) (Hartree): -761.16563384
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.69972079
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -763.64233447
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -763.64523972
     T1 diagnostic:  0.012156
     D1 diagnostic:  0.035790
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -763.58785340
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.69887598
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -763.64148966
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.70287446
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -763.64548814
E(RHF/AUG-CC-PVDZ) (Hartree): -761.16563383
E(RM062X/Aug-CC-pVTZ) (Hartree): -764.61538532
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.678096     -0.291577      -0.055468
     C       0.710327      0.567035      -0.323176
```

```
     O      -0.473649      0.100157      -0.866355
     C      -1.465067     -0.130761       0.028176
     F      -1.678083      0.942631       0.807627
     F      -1.188354     -1.146419       0.836749
     F      -2.568124     -0.396081      -0.635380
     F       2.850439      0.057041       0.409667
     F       1.589966     -1.582927      -0.254277
     O       0.869225      1.899256      -0.231098
     H       0.242670      2.268319       0.402951
Rotational constants (GHz):    2.3772400    0.9333700    0.7776800
Vibrational harmonic frequencies (cm-1):
       47.4401                  76.4699                 127.1506
      204.4254                 216.0984                 297.9877
      355.5515                 370.6517                 444.6534
      479.0097                 541.0661                 562.9832
      625.1109                 646.9510                 653.3066
      720.3848                 844.9401                 939.5104
     1171.1641                1212.0809                1262.7407
     1294.9651                1346.2558                1350.8466
     1391.3225                1919.8654                3817.5206
Zero-point correction (Hartree): 0.052217

complex.CF3OCFCF2.OH.a
------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.59807137
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.53797614
     T1 diagnostic:  0.016079
E(MP2/Aug-CC-pVDZ) (Hartree): -862.50298195
E(MP3/Aug-CC-pVDZ) (Hartree): -862.51390028
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.50576865
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.51582359
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.55092244
E(UHF/Aug-CC-pVDZ) (Hartree): -860.54721272
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.36843635
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.418486      0.500640      -0.330002
     C       0.517285     -0.464442      -0.227240
     O      -0.541192     -0.389634       0.618146
     F       0.637440     -1.600055      -0.883083
     C      -1.717468      0.068731       0.075703
     F      -2.083036     -0.655524      -0.971429
     F      -1.602458      1.329406      -0.318686
     F      -2.635448     -0.013519       1.011633
     F       1.324506      1.637659       0.304185
     F       2.478816      0.415204      -1.078209
     H       1.606075     -0.612321       2.277499
     O       2.291909     -0.864840       1.635857
Rotational constants (GHz):    1.6907800    0.7131500    0.6825900
Vibrational harmonic frequencies (cm-1):
       34.2782                  45.7880                  63.8957
       78.2298                 121.4535                 135.6739
      164.3050                 200.6411                 216.1293
      344.2503                 368.2670                 453.0312
      464.7562                 473.9792                 544.9255
      558.4325                 602.9293                 644.2961
      652.0892                 725.0745                 848.4207
      946.5575                1221.9930                1237.9249
     1272.8852                1344.6454                1371.4613
     1417.4671                1893.5131                3758.5733
Zero-point correction (Hartree): 0.050589

complex.CF3OCFCF2.OH.b
------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.59820785
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.53817586
     T1 diagnostic:  0.015977
E(MP2/Aug-CC-pVDZ) (Hartree): -862.50282845
E(MP3/Aug-CC-pVDZ) (Hartree): -862.51411269
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.50592076
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.51628754
```

```
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.55195866
E(UHF/Aug-CC-pVDZ) (Hartree): -860.54803000
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.36919563
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.586220     -0.171660      -0.488051
     C       0.565543      0.670581      -0.459746
     O      -0.655646      0.365890      -0.966548
     F       0.701298      1.910311      -0.033530
     C      -1.596676     -0.082121      -0.081446
     F      -1.739527      0.735201       0.949257
     F      -1.267410     -1.284038       0.399233
     F      -2.733310     -0.182973      -0.729610
     F       1.486623     -1.400739      -0.920015
     F       2.793714      0.149499      -0.127497
     H       0.313624     -1.090926       2.008692
     O       1.053567     -0.460292       2.007326
Rotational constants (GHz):    1.6995100    0.7728000    0.7418400
Vibrational harmonic frequencies (cm-1):
       48.0406                   53.7971                   75.4763
      105.9341                  124.4629                  141.9200
      195.7721                  211.7467                  218.5406
      344.4485                  368.4928                  411.6841
      446.6154                  472.3467                  545.1325
      558.7250                  604.8006                  643.6548
      651.1163                  722.6584                  848.4529
      945.5485                 1220.0265                 1235.1844
     1262.6165                 1347.5944                 1368.8487
     1414.4823                 1899.8467                 3769.7304
Zero-point correction (Hartree): 0.050707

CF2OCFCF2oxide
--------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -762.34736815
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.29155883
     T1 diagnostic:  0.015476
E(MP2/Aug-CC-pVDZ) (Hartree): -762.27324443
E(MP3/Aug-CC-pVDZ) (Hartree): -762.26916913
E(PMP2/Aug-CC-pVDZ) (Hartree): -762.27414350
E(PMP3/Aug-CC-pVDZ) (Hartree): -762.26971430
E(PUHF/Aug-CC-pVDZ) (Hartree): -760.51813262
E(UHF/Aug-CC-pVDZ) (Hartree): -760.51652241
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -762.36705355
     T1 diagnostic:  0.000342
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.01222617
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -762.95573571
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -762.95816991
     T1 diagnostic:  0.013927
     D1 diagnostic:  0.051838
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -762.90167945
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.01121960
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -762.95472914
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.01597650
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -762.95948604
E(ROHF/AUG-CC-PVDZ) (Hartree): -760.51420455
E(UM062X/Aug-CC-pVTZ) (Hartree): -763.93270461
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.665535     -0.235154      -0.001502
     C       0.355397      0.375006      -0.062484
     O      -0.721466     -0.316469      -0.520953
     F       0.211460      1.688877      -0.179776
     C      -1.865512     -0.170195       0.208155
     F      -2.557483      0.904881      -0.110769
     F      -2.602517     -1.245800       0.102795
     F       1.890295     -1.485551      -0.349794
     O       0.928535     -0.039089       1.148952
     F       2.770572      0.473874      -0.116791
Rotational constants (GHz):    2.8170800    0.8481800    0.7059000
Vibrational harmonic frequencies (cm-1):
       23.4862                   54.7258                  120.8768
```

```
      189.3076                 247.9181                 291.8713
      399.6678                 464.2976                 524.7385
      557.1793                 580.4822                 591.7129
      676.9716                 754.6718                 818.6343
      889.2836                1073.3178                1168.9634
     1223.0893                1243.9420                1310.3014
     1330.9024                1335.4954                1659.4276
Zero-point correction (Hartree): 0.039939

CF3OCCF2oxide
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -762.35692294
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.30086983
     T1 diagnostic:  0.016113
E(MP2/Aug-CC-pVDZ) (Hartree): -762.28211803
E(MP3/Aug-CC-pVDZ) (Hartree): -762.27828136
E(PMP2/Aug-CC-pVDZ) (Hartree): -762.28366849
E(PMP3/Aug-CC-pVDZ) (Hartree): -762.27925679
E(PUHF/Aug-CC-pVDZ) (Hartree): -760.52736845
E(UHF/Aug-CC-pVDZ) (Hartree): -760.52492002
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -762.37617071
     T1 diagnostic:  0.000424
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.02262505
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -762.96612639
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -762.96833382
     T1 diagnostic:  0.015178
     D1 diagnostic:  0.070706
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -762.91183515
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.02160517
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -762.96510650
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.02651683
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -762.97001817
E(ROHF/AUG-CC-PVDZ) (Hartree): -760.52154358
E(UM062X/Aug-CC-pVTZ) (Hartree): -763.94181699
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.929430      0.011476      -0.068472
     C      -0.548650     -0.339502      -0.197303
     O       0.479595      0.522828      -0.370075
     C       1.723486      0.031340      -0.061111
     F       2.052733     -0.972269      -0.861393
     F       2.581219      1.013707      -0.218257
     F      -2.352541      1.257836       0.024335
     O      -1.201452     -0.452380       1.023170
     F      -2.909313     -0.758319      -0.495813
     F       1.772616     -0.405785       1.188523
Rotational constants (GHz):    3.2260600    0.7128200    0.6888800
Vibrational harmonic frequencies (cm-1):
       29.5396                  59.8188                 110.7674
      205.4997                 262.9486                 360.7505
      440.7598                 500.5218                 527.3636
      542.8031                 622.4714                 631.4558
      673.4118                 733.0941                 805.9305
      921.0847                 957.7983                1170.2819
     1211.1854                1265.9956                1276.5725
     1309.1788                1346.3577                1630.7166
Zero-point correction (Hartree): 0.040087

CF3OCOCF2OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -838.16777797
E(CCSD/Aug-CC-pVDZ) (Hartree): -838.10449444
     T1 diagnostic:  0.014858
E(MP2/Aug-CC-pVDZ) (Hartree): -838.08658535
E(MP3/Aug-CC-pVDZ) (Hartree): -838.08037577
E(RHF/Aug-CC-pVDZ) (Hartree): -836.10817264
E(RM062X/Aug-CC-pVTZ) (Hartree): -839.90423913
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.854856     -0.159767      -0.000011
     C      -0.438818      0.455911       0.000000
```

```
     O       0.500736     -0.509017       0.000034
     C       1.831717     -0.128909       0.000000
     F       2.125130      0.576524       1.075987
     F       2.125026      0.576573      -1.075978
     F       2.538438     -1.237262      -0.000079
     F      -1.977278     -0.955777       1.077806
     O      -2.796308      0.792654      -0.000322
     F      -1.977171     -0.956220      -1.077485
     H      -2.374405      1.663323       0.000029
     O      -0.249572      1.628704       0.000010
Rotational constants (GHz):    2.2283300    0.6736300    0.6310900
Vibrational harmonic frequencies (cm-1):
       32.8480                61.5489                110.0044
      134.2569               219.0461                226.7349
      343.4511               353.8895                390.5974
      443.1185               445.6198                535.5075
      566.9201               593.4068                630.0337
      678.5275               767.6590                794.5522
      906.4158               932.3305               1117.0631
     1186.4887              1205.3410               1275.5785
     1303.3657              1337.7853               1349.8449
     1463.0118              1915.2829               3788.5830
Zero-point correction (Hartree): 0.057202

CFOHCF2
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -450.60736301
E(CCSD/Aug-CC-pVDZ) (Hartree): -450.57401707
     T1 diagnostic:  0.014209
E(MP2/Aug-CC-pVDZ) (Hartree): -450.55676005
E(MP3/Aug-CC-pVDZ) (Hartree): -450.56202051
E(RHF/Aug-CC-pVDZ) (Hartree): -449.49611634
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -451.00406231
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -450.96988970
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -450.97185401
     T1 diagnostic:  0.012657
     D1 diagnostic:  0.036188
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -450.93768139
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -451.00362064
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -450.96944803
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -451.00594509
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -450.97177247
E(RHF/AUG-CC-PVDZ) (Hartree): -449.49611633
E(RM062X/Aug-CC-pVTZ) (Hartree): -451.54768494
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.656130      0.013701      -0.006502
     C      -0.661490     -0.030323       0.009164
     O       1.446122     -1.060012      -0.107734
     F       1.280076      1.192610       0.007123
     F      -1.429429      1.035357      -0.004390
     F      -1.353870     -1.146394       0.015487
     H       1.992182     -1.154327       0.681922
Rotational constants (GHz):    5.4919500    3.2940600    2.0698000
Vibrational harmonic frequencies (cm-1):
      194.0972               216.8521                264.6386
      400.8565               431.6542                564.5436
      571.4981               602.0626                820.2360
     1172.3342              1287.8268               1362.9885
     1380.5251              1948.8876               3814.8780
Zero-point correction (Hartree): 0.034250

CFOCFOH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -426.02904005
E(CCSD/Aug-CC-pVDZ) (Hartree): -425.99420552
     T1 diagnostic:  0.020264
E(MP2/Aug-CC-pVDZ) (Hartree): -425.97529967
E(MP3/Aug-CC-pVDZ) (Hartree): -425.97757400
E(PMP2/Aug-CC-pVDZ) (Hartree): -425.98123547
E(PMP3/Aug-CC-pVDZ) (Hartree): -425.98126355
```

```
E(PUHF/Aug-CC-pVDZ) (Hartree): -424.95311725
E(UHF/Aug-CC-pVDZ) (Hartree): -424.94538756
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -426.03132137
     T1 diagnostic:  0.000396
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -426.40556281
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -426.37222904
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -426.37143085
     T1 diagnostic:  0.017109
     D1 diagnostic:  0.064312
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -426.33809709
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -426.40494249
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -426.37160872
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -426.40829172
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -426.37495795
E(ROHF/AUG-CC-PVDZ) (Hartree): -424.93771413
E(UM062X/Aug-CC-pVTZ) (Hartree): -426.93307043
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.754553      0.128359       0.000367
     C      -0.651790     -0.033475       0.000070
     F       1.430825     -1.023298      -0.000033
     O       1.293598      1.205334      -0.000041
     F      -1.240602     -1.195519      -0.000078
     O      -1.468606      0.994490      -0.000164
     H      -0.928519      1.801454       0.000004
Rotational constants (GHz):    5.6555000    3.5529700    2.1821000
Vibrational harmonic frequencies (cm-1):
      157.5606                 225.7205                 328.2947
      408.4199                 535.6237                 557.3604
      612.8479                 653.8507                 841.1988
     1148.6338                1250.4243                1508.4537
     1610.2012                1790.5511                3755.1269
Zero-point correction (Hartree): 0.035048

CFOCF2O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -525.05836483
E(CCSD/Aug-CC-pVDZ) (Hartree): -525.01929689
     T1 diagnostic:  0.017057
E(MP2/Aug-CC-pVDZ) (Hartree): -524.99814725
E(MP3/Aug-CC-pVDZ) (Hartree): -525.00159692
E(PMP2/Aug-CC-pVDZ) (Hartree): -525.00012655
E(PMP3/Aug-CC-pVDZ) (Hartree): -525.00281169
E(PUHF/Aug-CC-pVDZ) (Hartree): -523.80160897
E(UHF/Aug-CC-pVDZ) (Hartree): -523.79834834
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -525.05863601
     T1 diagnostic:  0.000285
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -525.51096034
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -525.47167219
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -525.47318757
     T1 diagnostic:  0.015868
     D1 diagnostic:  0.051619
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -525.43389942
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -525.51016783
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -525.47087968
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -525.51399971
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -525.47471156
E(ROHF/AUG-CC-PVDZ) (Hartree): -523.79361420
E(UM062X/Aug-CC-pVTZ) (Hartree): -526.14217031
Point group : CS
Electronic state : 2-A'
Cartesian coordinates (Angs):
     C       0.318830     -0.884516       0.000000
     C      -0.047256      0.625293       0.000000
     F      -0.800310     -1.588483       0.000000
     O       1.393234     -1.348090       0.000000
     F      -0.800310      0.896921       1.077851
     F      -0.800310      0.896921      -1.077851
     O       1.104130      1.311478       0.000000
Rotational constants (GHz):    3.9044600    2.5750200    2.1287000
Vibrational harmonic frequencies (cm-1):
```

```
       43.6510 (  A")           223.1176 (  A')           227.8454 (  A")
      376.3144 (  A')           412.0765 (  A')           471.7187 (  A")
      591.1972 (  A')           685.9632 (  A')           772.8299 (  A")
      824.5014 (  A')          1064.9203 (  A')          1188.8857 (  A")
     1229.0920 (  A')          1309.9565 (  A')          1979.7835 (  A')
Zero-point correction (Hartree): 0.025975

OCCF2OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -426.01734478
E(CCSD/Aug-CC-pVDZ) (Hartree): -425.98232323
     T1 diagnostic:  0.018175
E(MP2/Aug-CC-pVDZ) (Hartree): -425.96617013
E(MP3/Aug-CC-pVDZ) (Hartree): -425.96587666
E(PMP2/Aug-CC-pVDZ) (Hartree): -425.96865245
E(PMP3/Aug-CC-pVDZ) (Hartree): -425.96733430
E(PUHF/Aug-CC-pVDZ) (Hartree): -424.93616796
E(UHF/Aug-CC-pVDZ) (Hartree): -424.93238472
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -426.01665548
     T1 diagnostic:  0.000562
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -426.39048335
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -426.35695254
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -426.35645981
     T1 diagnostic:  0.017714
     D1 diagnostic:  0.066500
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -426.32292900
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -426.38977793
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -426.35624712
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -426.39343365
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -426.35990284
E(ROHF/AUG-CC-PVDZ) (Hartree): -424.92717822
E(UM062X/Aug-CC-pVTZ) (Hartree): -426.91125170
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.049838     -0.584821      -0.365029
     C       0.372313      0.004091      -0.021205
     O      -2.039488     -0.048544      -0.059200
     F       1.245081     -0.355275      -0.953054
     F       0.729001     -0.593934       1.134673
     O       0.379505      1.346198       0.078770
     H      -0.421722      1.646023       0.526285
Rotational constants (GHz):    5.7013100    3.0374700    2.9896300
Vibrational harmonic frequencies (cm-1):
       84.2093                  234.1835                  322.9303
      377.1291                  422.6526                  537.6628
      560.6715                  667.3818                  799.1284
     1088.4371                 1156.8923                 1272.6315
     1401.8200                 2009.1179                 3826.4575
Zero-point correction (Hartree): 0.033629

TS.CF3OCFCF2OH.CF3+HOCF2CFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.64053884
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.57751906
     T1 diagnostic:  0.021698
E(MP2/Aug-CC-pVDZ) (Hartree): -862.54113787
E(MP3/Aug-CC-pVDZ) (Hartree): -862.54154177
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.55622720
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.55218426
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.58615424
E(UHF/Aug-CC-pVDZ) (Hartree): -860.56834725
E(ROHF/CC-PVDZ) (Hartree): -860.48484834
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.41078610
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.675179     -0.301957      -0.020319
     C       0.601874      0.679554      -0.466645
     O      -0.427502      0.409188      -1.057597
     F       0.791182      1.893652       0.066706
     C      -1.902316     -0.114266       0.024439
     F      -1.567591      0.212967       1.247567
```

```
     F      -2.066878     -1.401137      -0.102985
     F      -2.937743      0.554336      -0.395947
     F       1.712072     -1.327230      -0.865208
     O       2.913542      0.232442       0.052739
     F       1.288419     -0.795856       1.190007
     H       2.888084      1.056401       0.552753
Rotational constants (GHz):    1.9154300    0.7076500    0.6410400
Vibrational harmonic frequencies (cm-1):
     i554.3051                  17.6969                  29.9469
       60.0456                 106.4047                 159.4376
      193.3809                 228.9851                 253.3864
      303.7389                 398.2146                 441.5904
      509.4854                 529.9397                 542.0100
      588.3353                 640.8728                 684.9633
      720.1813                 821.6012                1037.7657
     1087.9941                1114.6423                1230.4715
     1337.5576                1354.5967                1363.3952
     1415.4877                1566.2214                3853.5012
Zero-point correction (Hartree): 0.051468

TS.CF3OCFCF2OH.CF3OCF2CFOH
--------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.62089616
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.55628508
     T1 diagnostic:  0.017062
E(MP2/Aug-CC-pVDZ) (Hartree): -862.53597953
E(MP3/Aug-CC-pVDZ) (Hartree): -862.53031313
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.53927138
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.53214927
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.54326571
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53815295
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.39472005
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.711898     -0.336597      -0.266718
     C       0.594830      0.423750      -0.531622
     O      -0.564049     -0.101718      -0.902386
     F       0.693846      1.724209      -0.560208
     C      -1.638371     -0.119125      -0.010078
     F      -1.747004      1.022736       0.632788
     F      -1.519375     -1.107347       0.844149
     F      -2.710604     -0.313017      -0.750733
     F       1.645994     -1.620026      -0.414891
     O       2.891437      0.135433       0.017250
     F       0.813663      0.192743       1.497945
     H       2.782080      0.828425       0.690152
Rotational constants (GHz):    1.9562300    0.7969100    0.7328400
Vibrational harmonic frequencies (cm-1):
     i288.5897                  39.9094                  71.1590
      122.4052                 141.5482                 198.9146
      220.6904                 293.9334                 310.8448
      352.1449                 374.8366                 453.0971
      468.9650                 534.7445                 558.8619
      576.5838                 635.7790                 656.6258
      719.1082                 845.1584                 949.7707
     1175.1196                1178.4222                1277.9653
     1322.9519                1331.8935                1430.5431
     1516.0337                1744.2349                3734.9404
Zero-point correction (Hartree): 0.052938

TS.CF3OCFCF2OH.CF3OCFCF2+OH
---------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.59765570
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.53604781
     T1 diagnostic:  0.022139
E(MP2/Aug-CC-pVDZ) (Hartree): -862.49515544
E(MP3/Aug-CC-pVDZ) (Hartree): -862.50566040
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.50376341
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.51202356
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.54923808
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53923177
```

```
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.36729051
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.430017     -0.389354      -0.342970
     C      -0.493943      0.520273      -0.057218
     O       0.577187      0.264575       0.716942
     F      -0.639776      1.777369      -0.433494
     C       1.730628     -0.086846       0.056047
     F       2.087416      0.843581      -0.819237
     F       1.576661     -1.227432      -0.602013
     F       2.670646     -0.225187       0.959978
     F      -1.320795     -1.642314      -0.031017
     O      -2.256083      0.235902       1.631870
     F      -2.462013     -0.123902      -1.090793
     H      -2.618092      1.112699       1.423514
Rotational constants (GHz):    1.8013900    0.7260600    0.6812700
Vibrational harmonic frequencies (cm-1):
     i269.7903                  35.5640                  75.2433
       80.9655                  96.5386                 143.5073
      193.0727                 205.3903                 234.8082
      345.5931                 368.7527                 416.3289
      467.0634                 514.0674                 558.6978
      559.9480                 630.7137                 644.3130
      652.2667                 720.9117                 843.0935
      946.2057                1223.8594                1231.1164
     1269.6484                1348.6497                1377.9124
     1431.2420                1803.7253                3772.7118
Zero-point correction (Hartree): 0.050557

TS.CF3OCFCF2OH.CF2O+CF2O+CF+HF
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.58433156
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.51846768
     T1 diagnostic:  0.018586
E(MP2/Aug-CC-pVDZ) (Hartree): -862.49719885
E(MP3/Aug-CC-pVDZ) (Hartree): -862.48651034
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.50060635
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.48867594
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.51216120
E(UHF/Aug-CC-pVDZ) (Hartree): -860.50737212
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.34864816
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.679507     -0.400523      -0.016743
     C      -1.046212      1.204728       0.536700
     O       0.889177      0.463150       1.010832
     F      -0.762172      1.959309      -0.416475
     C       1.814145      0.335115       0.278699
     F       1.857814      0.773474      -0.938003
     F       1.235130     -1.818077      -0.644830
     F       2.950707     -0.161798       0.619384
     F      -1.642567     -1.104947       1.114722
     O      -1.018363     -0.738867      -0.988259
     F      -2.953887      0.008852      -0.196581
     H       0.337709     -1.541497      -0.816473
Rotational constants (GHz):    1.6701500    0.7216100    0.6239500
Vibrational harmonic frequencies (cm-1):
     i115.4814                  32.1340                  54.5247
       88.8987                 101.8802                 131.4933
      158.8324                 171.8931                 187.1125
      222.4105                 234.4065                 290.6940
      383.1021                 418.6631                 563.0746
      597.7023                 620.3676                 657.7788
      734.7096                 777.5463                 830.7555
      877.2384                 952.7793                1043.5024
     1190.9469                1384.0759                1427.6633
     1640.0739                1905.8151                3367.2170
Zero-point correction (Hartree): 0.047949

TS.CF3OCFCF2OH.CF3OCFCFO+HF
-------------------------
```

```
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.62002013
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.55533439
     T1 diagnostic:  0.017866
E(MP2/Aug-CC-pVDZ) (Hartree): -862.53576873
E(MP3/Aug-CC-pVDZ) (Hartree): -862.52686098
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.53782573
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.52814138
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.54313662
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53989298
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.39324575
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.556082     -0.175304      -0.376269
     C       0.479334      0.755273      -0.514002
     O      -0.745688      0.430512      -0.912185
     F       0.642071      1.959233      -0.057421
     C      -1.619128     -0.119969       0.026731
     F      -1.621320      0.598691       1.132480
     F      -1.272191     -1.355312       0.315304
     F      -2.810145     -0.108620      -0.521387
     F       1.339248     -1.318588      -0.962025
     O       2.745198      0.171731      -0.081777
     F       1.387507     -0.602490       1.444578
     H       2.519656     -0.134170       0.969177
Rotational constants (GHz):    1.8474200    0.8202600    0.7500100
Vibrational harmonic frequencies (cm-1):
    i1374.2634                  38.9989                  61.4906
       83.4007                 110.1025                 157.3347
      211.8273                 278.0787                 349.3974
      370.1721                 451.4480                 463.6846
      524.6076                 554.5607                 579.1052
      632.8354                 656.9980                 699.8217
      796.6602                 842.8946                 913.8695
      943.2971                1170.9947                1241.5041
     1309.4966                1350.2878                1432.0946
     1492.3127                1648.5753                2223.0076
Zero-point correction (Hartree): 0.049183

TS.CF3OCFCF2OH.CF3OCFHCF2O
--------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.61672615
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.55411607
     T1 diagnostic:  0.019024
E(MP2/Aug-CC-pVDZ) (Hartree): -862.52060322
E(MP3/Aug-CC-pVDZ) (Hartree): -862.52494024
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.52743790
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.52909278
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.55284052
E(UHF/Aug-CC-pVDZ) (Hartree): -860.54339114
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.38698276
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.804584     -0.246054       0.005822
     C      -0.462313      0.445265       0.028629
     O       0.545804     -0.210806      -0.603969
     F      -2.827331      0.537295      -0.340948
     F      -0.468615      1.757231      -0.168416
     F      -1.878282     -1.356963      -0.726917
     O      -1.746009     -0.494039       1.353106
     H      -0.586774      0.133735       1.306255
     C       1.796478     -0.137223      -0.038498
     F       1.798170     -0.682814       1.170723
     F       2.207568      1.115582       0.077505
     F       2.614148     -0.799987      -0.820287
Rotational constants (GHz):    2.1031100    0.6925800    0.6373700
Vibrational harmonic frequencies (cm-1):
    i1996.4691                  22.5775                  63.9986
       86.7921                 162.5658                 208.0786
      276.0575                 332.5992                 365.4500
      429.7050                 481.7408                 531.8349
      551.9575                 591.4560                 638.1031
```

```
      657.9074                  728.9378                  758.0103
      899.1180                  935.4871                 1089.4735
     1173.2517                 1189.6807                 1222.2583
     1258.2395                 1277.8000                 1317.2779
     1353.5748                 1463.1174                 2014.8314
Zero-point correction (Hartree): 0.050306

TS.CF3OCFCFO.CFOCFO+CF3
------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -762.37291173
E(CCSD/Aug-CC-pVDZ) (Hartree): -762.31353776
     T1 diagnostic:  0.024691
E(MP2/Aug-CC-pVDZ) (Hartree): -762.28306046
E(MP3/Aug-CC-pVDZ) (Hartree): -762.27742277
E(PMP2/Aug-CC-pVDZ) (Hartree): -762.29903778
E(PMP3/Aug-CC-pVDZ) (Hartree): -762.28901160
E(PUHF/Aug-CC-pVDZ) (Hartree): -760.55094787
E(UHF/Aug-CC-pVDZ) (Hartree): -760.53247703
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -762.39039281
     T1 diagnostic:  0.000789
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -763.03266543
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -762.97609684
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -762.97438622
     T1 diagnostic:  0.021568
     D1 diagnostic:  0.119084
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -762.91781763
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -763.03175773
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -762.97518913
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -763.03792702
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -762.98135842
E(ROHF/AUG-CC-PVDZ) (Hartree): -760.51923147
E(UM062X/Aug-CC-pVTZ) (Hartree): -763.94798878
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.882104     -0.383208       0.020853
     C       0.890233      0.639866      -0.434929
     O      -0.125158      0.408804      -1.054218
     F       1.189742      1.856701      -0.021705
     C      -1.681629     -0.085399       0.087392
     F      -2.544698      0.887351       0.128964
     F      -1.113469     -0.290508       1.249035
     F      -2.180694     -1.173108      -0.417159
     F       1.454279     -1.602365      -0.291486
     O       2.901323     -0.175078       0.570625
Rotational constants (GHz):    2.2250000    0.8638900    0.7306400
Vibrational harmonic frequencies (cm-1):
     i469.8749                  29.9762                  40.4820
       60.0664                  98.7742                 147.1805
      218.5968                 269.6410                 432.5613
      460.9035                 527.0947                 531.1295
      576.9237                 672.4402                 678.7719
      782.1003                 844.4182                1030.0366
     1169.8016                1316.6842                1353.2941
     1375.1597                1591.0766                1938.2571
Zero-point correction (Hartree): 0.036782

TS.CF3OCFCF2OH.CF3+HOCF2CFO.b
------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.64143690
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.57833043
     T1 diagnostic:  0.021296
E(MP2/Aug-CC-pVDZ) (Hartree): -862.54305868
E(MP3/Aug-CC-pVDZ) (Hartree): -862.54315242
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.55766115
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.55337565
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.58559720
E(UHF/Aug-CC-pVDZ) (Hartree): -860.56828990
E(ROHF/AUG-CC-PVDZ) (Hartree): -860.53719978
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.41264558
Electronic state : 2-A
Cartesian coordinates (Angs):
```

```
     C       1.643618     -0.317813       0.007686
     C       0.592362      0.686344      -0.435467
     O      -0.428319      0.391852      -1.050652
     F       0.786050      1.907760       0.024192
     C      -1.895640     -0.104331       0.032360
     F      -1.403107     -0.125308       1.243888
     F      -2.269831     -1.290869      -0.362798
     F      -2.847050      0.774481      -0.096808
     F       2.827480      0.037615      -0.545708
     O       1.306590     -1.581765      -0.315238
     F       1.818142     -0.245982       1.335655
     H       0.726653     -1.585167      -1.086147
Rotational constants (GHz):    1.9442600    0.7014200    0.6381900
Vibrational harmonic frequencies (cm-1):
     i554.9889                  30.7411                  40.2811
       52.2054                 102.6362                 170.8503
      203.8192                 224.4021                 252.8621
      287.5366                 416.7374                 441.2303
      510.9703                 530.2345                 543.7918
      603.1876                 643.0244                 686.5523
      716.5144                 825.8487                1036.4248
     1097.3670                1150.3383                1251.7802
     1339.0225                1351.7626                1361.6419
     1430.9888                1552.9938                3834.9776
Zero-point correction (Hartree): 0.051693

TS.CF3OCFOCF2OH.CF2OH+CF3OCFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -937.74202802
E(CCSD/Aug-CC-pVDZ) (Hartree): -937.67388820
     T1 diagnostic:  0.021478
E(MP2/Aug-CC-pVDZ) (Hartree): -937.63715236
E(MP3/Aug-CC-pVDZ) (Hartree): -937.64267252
E(PMP2/Aug-CC-pVDZ) (Hartree): -937.64083195
E(PMP3/Aug-CC-pVDZ) (Hartree): -937.64508852
E(PUHF/Aug-CC-pVDZ) (Hartree): -935.48985728
E(UHF/Aug-CC-pVDZ) (Hartree): -935.48447937
E(UM062X/Aug-CC-pVTZ) (Hartree): -939.67113747
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.423577     -0.537545      -0.032357
     C       0.524255      0.910984       0.047453
     O      -0.730656      0.759311      -0.543005
     F       1.174813      1.719825      -0.809178
     C      -1.695078     -0.065255      -0.040411
     F      -1.726008     -0.092379       1.281715
     F      -1.536173     -1.309415      -0.477289
     F      -2.852315      0.385085      -0.488265
     F       1.293460     -0.958347      -1.272796
     O       2.707097     -0.309166       0.234017
     F       0.848204     -1.409986       0.792731
     H       2.794963      0.114579       1.098074
     O       0.632395      1.177764       1.285430
Rotational constants (GHz):    1.5704300    0.7679200    0.6989100
Vibrational harmonic frequencies (cm-1):
     i332.3175                  43.4372                  75.3512
      118.8831                 167.9631                 196.3794
      227.2453                 275.4721                 332.6196
      340.9035                 361.0959                 389.5071
      429.9941                 461.1038                 544.2182
      559.9386                 579.3278                 627.3729
      675.8678                 732.9627                 741.3972
      863.7859                 970.7471                1053.9986
     1159.9015                1187.5700                1263.0971
     1277.1348                1308.8452                1316.7117
     1391.0107                1438.9925                3823.7297
Zero-point correction (Hartree): 0.056810

TS.CF3OCFOCF2OH.CF3O+HOCF2CFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -937.71943602
```

```
E(CCSD/Aug-CC-pVDZ) (Hartree): -937.64922839
     T1 diagnostic:  0.021029
E(MP2/Aug-CC-pVDZ) (Hartree): -937.60911516
E(MP3/Aug-CC-pVDZ) (Hartree): -937.61365277
E(PMP2/Aug-CC-pVDZ) (Hartree): -937.62395586
E(PMP3/Aug-CC-pVDZ) (Hartree): -937.62379711
E(PUHF/Aug-CC-pVDZ) (Hartree): -935.47239880
E(UHF/Aug-CC-pVDZ) (Hartree): -935.45430877
E(UM062X/Aug-CC-pVTZ) (Hartree): -939.63900777
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.466486     -0.510372      -0.011660
     C       0.866124      0.911549       0.115324
     O      -0.831182      0.791376      -0.533606
     F       1.337547      1.693055      -0.836794
     C      -1.778961     -0.080304      -0.047648
     F      -1.817105     -0.089910       1.268798
     F      -1.570140     -1.315568      -0.481429
     F      -2.944991      0.328536      -0.525151
     F       1.323347     -0.953977      -1.252681
     O       2.790918     -0.488665       0.280771
     F       0.799006     -1.318774       0.826258
     H       2.912051     -0.421763       1.235664
     O       0.492400      1.373073       1.182489
Rotational constants (GHz):    1.5631000    0.7213300    0.6548900
Vibrational harmonic frequencies (cm-1):
     i628.7103                  40.6591                  62.2319
      115.2759                 129.0157                 161.0747
      216.4083                 244.9752                 250.9064
      294.7989                 379.6499                 386.5131
      431.6183                 450.4395                 496.0167
      565.1062                 591.5541                 613.9707
      652.3146                 675.3761                 698.8486
      826.7784                 929.1785                1123.6266
     1135.5794                1195.3604                1253.2480
     1283.2263                1297.8371                1341.1639
     1401.9115                1574.4071                3844.1724
Zero-point correction (Hartree): 0.056187

TS.CF3OCFOCF2OH.F+HOCF2COOCH3
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -937.71185877
E(CCSD/Aug-CC-pVDZ) (Hartree): -937.64208949
     T1 diagnostic:  0.021073
E(MP2/Aug-CC-pVDZ) (Hartree): -937.60199907
E(MP3/Aug-CC-pVDZ) (Hartree): -937.60717835
E(PMP2/Aug-CC-pVDZ) (Hartree): -937.61411966
E(PMP3/Aug-CC-pVDZ) (Hartree): -937.61552018
E(PUHF/Aug-CC-pVDZ) (Hartree): -935.46831054
E(UHF/Aug-CC-pVDZ) (Hartree): -935.45360121
E(UM062X/Aug-CC-pVTZ) (Hartree): -939.62871153
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.797299     -0.357837      -0.024446
     C       0.394143      0.223616       0.263938
     O      -0.559790     -0.484117      -0.334062
     F       0.557327      1.791532      -0.747198
     C      -1.891841     -0.204733      -0.041423
     F      -2.187932      1.047922      -0.310492
     F      -2.151156     -0.455370       1.227252
     F      -2.607134     -1.002080      -0.800031
     F       1.941340     -0.596897      -1.327946
     O       2.776898      0.436665       0.421449
     F       1.821497     -1.560892       0.596334
     H       2.414389      1.132145       0.986166
     O       0.210707      1.032907       1.173131
Rotational constants (GHz):    1.6432800    0.6407200    0.5926400
Vibrational harmonic frequencies (cm-1):
     i580.4901                  51.2225                  64.6886
       87.4923                 128.4582                 153.5557
      194.8202                 228.0485                 234.7415
```

```
      321.3706                343.3728                377.8342
      435.4696                452.3041                522.0948
      566.7010                594.7533                617.1754
      657.0881                678.1758                768.1261
      898.6162                930.4179               1108.0816
     1177.1383               1192.6682               1283.9011
     1310.2182               1344.4806               1367.1172
     1453.0168               1608.3332               3809.0531
Zero-point correction (Hartree): 0.056864

TS.CF3OCFOCFO.CF3OCFO+CFO
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -837.46524178
E(CCSD/Aug-CC-pVDZ) (Hartree): -837.39834265
     T1 diagnostic:  0.023844
E(MP2/Aug-CC-pVDZ) (Hartree): -837.37162475
E(MP3/Aug-CC-pVDZ) (Hartree): -837.36400140
E(PMP2/Aug-CC-pVDZ) (Hartree): -837.38168932
E(PMP3/Aug-CC-pVDZ) (Hartree): -837.37073540
E(PUHF/Aug-CC-pVDZ) (Hartree): -835.43430294
E(UHF/Aug-CC-pVDZ) (Hartree): -835.42138532
E(UM062X/Aug-CC-pVTZ) (Hartree): -839.19865386
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.879207      0.546995      -0.115421
     C      -0.591487     -0.779432       0.150928
     O       0.431770     -0.382353      -0.695201
     F      -1.191844     -1.801725      -0.454384
     C       1.574872      0.123791      -0.124111
     F       2.132703     -0.751298       0.695389
     F       1.347212      1.242918       0.543153
     F       2.404375      0.378072      -1.115463
     F      -1.357463      1.699910       0.174938
     O      -2.963318      0.289452      -0.434282
     O      -0.548442     -0.689476       1.371849
Rotational constants (GHz):    1.8991800    0.8400000    0.7230500
Vibrational harmonic frequencies (cm-1):
     i370.8262                 42.7355                 64.9691
       89.2924                159.4585                186.9478
      208.2233                297.4666                376.8775
      390.2583                418.8619                481.9112
      555.8845                607.3861                631.3872
      679.9620                696.7828                747.4453
      889.4183               1007.4192               1136.9004
     1203.0303               1263.4581               1287.5968
     1329.2013               1571.1631               2022.8479
Zero-point correction (Hartree): 0.041797

TS.CF3OCFOCFO.CF3OCOCFO+F
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -837.43219275
E(CCSD/Aug-CC-pVDZ) (Hartree): -837.36003044
     T1 diagnostic:  0.021182
E(MP2/Aug-CC-pVDZ) (Hartree): -837.35010221
E(MP3/Aug-CC-pVDZ) (Hartree): -837.32777222
E(PMP2/Aug-CC-pVDZ) (Hartree): -837.35888663
E(PMP3/Aug-CC-pVDZ) (Hartree): -837.33323747
E(PUHF/Aug-CC-pVDZ) (Hartree): -835.37222406
E(UHF/Aug-CC-pVDZ) (Hartree): -835.36068024
E(UM062X/Aug-CC-pVTZ) (Hartree): -839.16044089
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       2.065619      0.204204      -0.230711
     C       0.486934     -0.505151      -0.000707
     O      -0.403153      0.500511       0.059028
     F       1.460745     -0.157452       1.379908
     C      -1.743650      0.146473      -0.051731
     F      -2.081639     -0.721503       0.880000
     F      -2.001338     -0.367288      -1.238136
     F      -2.426088      1.256074       0.105014
     F       1.944933      1.501271      -0.219434
```

```
     O       2.954348     -0.441787      -0.619895
     O       0.333439     -1.642858      -0.247542
Rotational constants (GHz):    2.2089000    0.7157400    0.6676600
Vibrational harmonic frequencies (cm-1):
     i441.4778                  36.9800                  71.6160
      129.2402                 159.6948                 198.1710
      256.6988                 322.1329                 377.8939
      396.1222                 430.4005                 437.5991
      557.0824                 590.6606                 622.6895
      660.1061                 678.0296                 706.8826
      838.5195                 907.3406                1110.8786
     1159.1472                1211.7602                1304.6640
     1348.7953                1853.4532                1948.1994
Zero-point correction (Hartree): 0.041724

TS.CF3OCFOCFO.FCOCFO+CF3O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -837.44812455
E(CCSD/Aug-CC-pVDZ) (Hartree): -837.38134344
     T1 diagnostic:  0.022634
E(MP2/Aug-CC-pVDZ) (Hartree): -837.34757892
E(MP3/Aug-CC-pVDZ) (Hartree): -837.34565704
E(PMP2/Aug-CC-pVDZ) (Hartree): -837.36389217
E(PMP3/Aug-CC-pVDZ) (Hartree): -837.35697153
E(PUHF/Aug-CC-pVDZ) (Hartree): -835.43202413
E(UHF/Aug-CC-pVDZ) (Hartree): -835.41233663
E(UM062X/Aug-CC-pVTZ) (Hartree): -839.17012119
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.615557     -0.611459       0.167332
     C       1.010145      0.802606       0.143083
     O      -0.557765      0.531430      -0.734433
     F       1.596647      1.548703      -0.773627
     C      -1.563351     -0.131506      -0.075447
     F      -2.257598      0.657755       0.717746
     F      -1.095564     -1.145694       0.641700
     F      -2.353915     -0.600421      -1.027964
     F       1.822958     -1.054577      -1.060247
     O       1.879264     -1.206063       1.139665
     O       0.455144      1.298416       1.108733
Rotational constants (GHz):    1.7192600    0.8504700    0.7798900
Vibrational harmonic frequencies (cm-1):
     i648.6765                  23.7542                  53.6856
       92.7687                 132.3501                 160.0546
      231.5583                 264.8513                 335.0105
      408.8784                 432.9679                 469.9908
      531.8542                 617.6893                 632.7302
      665.5211                 682.2925                 764.5716
      829.1010                 931.1272                1156.2570
     1209.1234                1274.5178                1295.0814
     1323.6037                1581.3031                1988.3552
Zero-point correction (Hartree): 0.041210

TS.CF3OCFOHCF2.CF3OCFCF2+OH
---------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.59673149
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.53431566
     T1 diagnostic:  0.023363
E(MP2/Aug-CC-pVDZ) (Hartree): -862.49349129
E(MP3/Aug-CC-pVDZ) (Hartree): -862.50288816
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.50215836
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.50924109
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.54255594
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53245923
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.36683411
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.436578      0.525811      -0.240306
     C       0.563514     -0.483445      -0.106182
     O      -0.547336     -0.386869       0.658071
     F       0.685200     -1.578384      -0.812154
```

```
     C      -1.682096      0.076497       0.032129
     F      -1.998175     -0.670863      -1.013818
     F      -1.518767      1.323532      -0.390273
     F      -2.652741      0.037621       0.913973
     F       1.315673      1.656418       0.390785
     F       2.496295      0.450046      -0.979172
     O       1.994672     -1.004276       1.432824
     H       1.565972     -0.549355       2.174937
Rotational constants (GHz):    1.7590800    0.7611000    0.7045100
Vibrational harmonic frequencies (cm-1):
     i208.6375                  34.5023                  79.1320
      105.1782                 118.6201                 143.5370
      202.4421                 213.5280                 277.9692
      344.0591                 363.3976                 422.4983
      467.5007                 512.1654                 545.7766
      562.7722                 641.5639                 651.2857
      705.1343                 713.5189                 841.3200
      946.9926                1221.2347                1237.4507
     1273.2712                1348.5922                1389.0336
     1438.6167                1803.3672                3784.1755
Zero-point correction (Hartree): 0.051005

TS.CF3OCFOHCF2.CF3OCFOCF2H
--------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.60971245
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.54705959
     T1 diagnostic:  0.019146
E(MP2/Aug-CC-pVDZ) (Hartree): -862.51333376
E(MP3/Aug-CC-pVDZ) (Hartree): -862.51764804
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.52035324
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.52192476
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.54543759
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53576565
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.37996583
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       0.584079     -0.319081       0.166980
     C       1.971163      0.269459       0.084270
     F       2.860488     -0.390354      -0.626697
     O      -0.405099      0.596571      -0.142219
     F       2.079851      1.569393      -0.082849
     F       0.414327     -1.443539      -0.549266
     O       0.749695     -0.585351       1.512433
     H       1.955479     -0.084164       1.358693
     C      -1.706731      0.182334      -0.087925
     F      -2.457953      1.254972       0.060719
     F      -1.920645     -0.647007       0.925947
     F      -2.065325     -0.432560      -1.205672
Rotational constants (GHz):    2.0980500    0.7174500    0.6717500
Vibrational harmonic frequencies (cm-1):
    i2015.9899                  42.6400                  69.2004
       99.6316                 121.9042                 207.3065
      270.9150                 346.1038                 362.3987
      400.5431                 453.6452                 524.0217
      536.6286                 613.4970                 641.1175
      669.4857                 713.1116                 781.4713
      861.0625                 951.0369                1083.7002
     1143.3029                1179.7979                1211.4550
     1272.3321                1292.3885                1330.0886
     1331.9661                1480.4397                2022.9537
Zero-point correction (Hartree): 0.050152

TS.CF3OCFOHCF2.CF3OCOCF2+HF
---------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.61401792
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.54899858
     T1 diagnostic:  0.018543
E(MP2/Aug-CC-pVDZ) (Hartree): -862.52915280
E(MP3/Aug-CC-pVDZ) (Hartree): -862.52017158
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.53110680
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.52140711
```

E(PUHF/Aug-CC-pVDZ) (Hartree): -860.53479003
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53171880
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.38724771
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-1.312258	0.760795	-0.164717
C	-0.758554	-0.511710	-0.477459
O	0.549150	-0.672335	-0.702377
F	-1.070041	-1.392942	1.206577
C	1.554121	0.000751	-0.031792
F	1.243507	0.226919	1.226136
F	1.816906	1.153574	-0.630045
F	2.620940	-0.761173	-0.097674
F	-2.582001	0.885309	-0.003054
F	-0.630389	1.793135	0.206504
O	-1.533504	-1.426639	-0.946334
H	-1.615323	-1.850619	0.057490

Rotational constants (GHz): 1.7230700 0.8863000 0.7393900
Vibrational harmonic frequencies (cm-1):

i1223.2278	37.9054	86.3594
112.7170	126.5213	163.5551
210.2271	250.8651	360.5204
375.2722	393.6866	459.4113
504.3533	510.2285	566.2184
627.0775	648.9168	723.6016
788.0626	836.9924	911.0038
986.5642	1201.7558	1260.3519
1293.3931	1350.2492	1465.4356
1474.7543	1661.4034	2314.2668

Zero-point correction (Hartree): 0.049440

TS.CF3OCFOHCF2.CF3OCOHCF3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.61664555
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.55182261
T1 diagnostic: 0.017516
E(MP2/Aug-CC-pVDZ) (Hartree): -862.53166476
E(MP3/Aug-CC-pVDZ) (Hartree): -862.52541472
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.53497081
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.52736079
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.53732842
E(UHF/Aug-CC-pVDZ) (Hartree): -860.53233584
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.39021090
Electronic state : 2-A
Cartesian coordinates (Angs):

C	1.248349	-0.568850	-0.260649
C	0.673860	0.686173	-0.264747
O	-0.614678	0.975595	-0.075765
C	-1.613908	0.031073	-0.018360
F	-1.563172	-0.666071	1.097302
F	-1.547144	-0.797425	-1.052973
F	-2.747865	0.691339	-0.067818
F	2.473231	-0.728017	-0.638377
F	0.670858	-1.658911	0.108418
O	1.380495	1.739705	-0.610560
H	2.125039	1.787772	0.014780
F	1.591715	0.447913	1.524377

Rotational constants (GHz): 1.8324500 0.8303900 0.7467900
Vibrational harmonic frequencies (cm-1):

i325.1781	33.4947	89.7242
146.9702	152.1645	192.9073
235.0765	268.2588	320.7191
366.9892	385.8086	433.2069
463.7913	508.6374	547.4901
575.3980	628.2495	652.0262
733.9534	813.0123	974.4926
1206.6632	1230.8965	1274.7873
1289.2789	1345.0598	1459.0618
1477.1835	1737.7700	3705.4499

Zero-point correction (Hartree): 0.052964

TS.CFOCF2OH.CFOCFO+HF

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -525.67501740
E(CCSD/Aug-CC-pVDZ) (Hartree): -525.62938469
T1 diagnostic: 0.017762
E(MP2/Aug-CC-pVDZ) (Hartree): -525.62524209
E(MP3/Aug-CC-pVDZ) (Hartree): -525.60970230
E(RHF/Aug-CC-pVDZ) (Hartree): -524.34365141
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -526.13420652
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -526.09368003
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -526.09008279
T1 diagnostic: 0.015939
D1 diagnostic: 0.062387
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -526.04955631
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -526.13317517
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -526.09264868
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -526.13823069
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -526.09770420
E(RHF/AUG-CC-PVDZ) (Hartree): -524.34365140
E(RM062X/Aug-CC-pVTZ) (Hartree): -526.76180267
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.521730	0.218288	-0.256601
C	0.990286	0.073453	-0.038949
O	1.727696	0.951575	0.200869
F	1.350120	-1.185959	-0.187213
F	-0.913873	1.432775	-0.028416
O	-1.186420	-0.532654	-1.012257
F	-1.067457	-0.695876	1.127884
H	-1.460660	-1.060285	0.054098

Rotational constants (GHz): 3.6577100 2.4959500 1.9794400
Vibrational harmonic frequencies (cm-1):

i1718.0616	59.8729	169.9897	
239.4132	315.8077	407.4263	
491.5837	637.4505	659.1799	
723.6792	823.8337	873.0426	
917.9924	1210.9887	1386.1750	
1642.7519	1987.6056	2033.5102	

Zero-point correction (Hartree): 0.033216

TS.CF3+OCFCF2OH.CF4+OCFCFOH

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.60928919
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.54248391
T1 diagnostic: 0.021610
E(MP2/Aug-CC-pVDZ) (Hartree): -862.51465178
E(MP3/Aug-CC-pVDZ) (Hartree): -862.50636818
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.52848288
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.51602616
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.53522157
E(UHF/Aug-CC-pVDZ) (Hartree): -860.51870478
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.37462523
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-1.320575	0.685812	-0.015120
C	-1.977503	-0.634834	-0.163911
O	-2.272130	-1.192534	-1.155896
F	-2.130870	-1.185508	1.060254
C	2.105478	-0.141260	-0.003165
F	2.518447	0.051810	1.220336
F	2.618760	0.725365	-0.829737
F	2.309447	-1.368058	-0.394799
F	-1.340311	1.431340	-1.083131
O	-1.470709	1.396218	1.088526
F	0.318605	0.134282	0.002727
H	-1.548391	0.809139	1.851308

Rotational constants (GHz): 1.6359200 0.5969900 0.5664500
Vibrational harmonic frequencies (cm-1):

i1064.4289	10.2986	47.6263	
51.4001	98.9299	133.4582	
187.5836	199.2136	236.2362	

```
      300.6501                330.2411                388.8668
      418.1217                513.5960                534.6885
      536.8198                552.7081                648.2857
      714.4174                761.1712                832.7928
     1043.2207               1101.4942               1207.7526
     1351.6877               1358.7800               1424.5491
     1479.7072               1935.0598               3835.1276
Zero-point correction (Hartree): 0.050654

TS.CF3+OCFCF2OH.HCF3+OCFCF2O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.63813342
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.57501365
     T1 diagnostic:  0.020325
E(MP2/Aug-CC-pVDZ) (Hartree): -862.54160471
E(MP3/Aug-CC-pVDZ) (Hartree): -862.54336663
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.54575705
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.54595130
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.57613376
E(UHF/Aug-CC-pVDZ) (Hartree): -860.56986068
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.40226723
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.287707      0.902589      -0.109434
     C       1.228456     -0.641211      -0.133815
     F       2.407610      1.306273       0.464526
     O       0.465996      1.631851      -0.522222
     F       1.156978     -1.056976       1.145321
     F       2.363450     -1.118368      -0.660409
     O       0.219075     -1.130316      -0.888205
     H      -0.941948     -0.458569      -0.524408
     C      -1.922161     -0.033622      -0.011129
     F      -2.767482     -1.037070       0.128362
     F      -1.610751      0.458920       1.174133
     F      -2.450098      0.900528      -0.770368
Rotational constants (GHz):    1.7554700    0.6916500    0.6065400
Vibrational harmonic frequencies (cm-1):
     i944.6941                33.9637                 45.9322
       52.0862                91.1267                108.0265
      160.6220               235.8734                245.2956
      345.5741               421.3763                438.1111
      518.0687               526.0069                609.1327
      646.6749               709.9752                783.4166
      806.4170               870.0984               1128.1046
     1142.4991              1192.5069               1232.1537
     1265.9506              1289.3734               1332.7500
     1358.0416              1422.5710               1979.9759
Zero-point correction (Hartree): 0.047823

TS.CFOCF2OH+CF3.CF4+OCCF2OH
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -862.59903132
E(CCSD/Aug-CC-pVDZ) (Hartree): -862.53181085
     T1 diagnostic:  0.021581
E(MP2/Aug-CC-pVDZ) (Hartree): -862.50284981
E(MP3/Aug-CC-pVDZ) (Hartree): -862.49495069
E(PMP2/Aug-CC-pVDZ) (Hartree): -862.51698383
E(PMP3/Aug-CC-pVDZ) (Hartree): -862.50465381
E(PUHF/Aug-CC-pVDZ) (Hartree): -860.52186956
E(UHF/Aug-CC-pVDZ) (Hartree): -860.50486614
E(UM062X/Aug-CC-pVTZ) (Hartree): -864.36185024
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.073557      0.938723      -0.302073
     C       1.893291     -0.339558      -0.013227
     O       1.356232      2.029302      -0.004132
     F       1.690322     -1.243401      -0.966721
     F       1.403048     -0.850408       1.138355
     O       3.212563     -0.084822       0.068536
     H       3.356729      0.777952       0.477902
     F      -0.533755      0.472006      -0.409471
```

```
     C      -2.163997     -0.066748       0.016449
     F      -2.667357     -0.629599      -1.044343
     F      -2.026939     -0.910107       0.998941
     F      -2.834675      0.991698       0.372124
Rotational constants (GHz):    1.9659000    0.5803500    0.5323400
Vibrational harmonic frequencies (cm-1):
    i1098.4268                  12.9482                  34.1881
       43.2479                  70.8067                 141.9630
      172.2737                 215.5960                 241.4977
      307.6501                 318.4633                 360.9121
      445.1286                 500.1687                 538.5659
      538.9492                 581.7717                 618.6026
      690.1078                 750.0476                 880.8564
     1049.3430                1125.4035                1169.2282
     1294.2123                1363.7877                1365.5017
     1394.2881                1985.0453                3821.2553
Zero-point correction (Hartree): 0.050192

TS.CFOCF2O.CFO+CF2O
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -525.04961433
E(CCSD/Aug-CC-pVDZ) (Hartree): -525.00575542
     T1 diagnostic:  0.027180
E(MP2/Aug-CC-pVDZ) (Hartree): -524.98542696
E(MP3/Aug-CC-pVDZ) (Hartree): -524.97941667
E(PMP2/Aug-CC-pVDZ) (Hartree): -524.99602995
E(PMP3/Aug-CC-pVDZ) (Hartree): -524.98651874
E(PUHF/Aug-CC-pVDZ) (Hartree): -523.77194651
E(UHF/Aug-CC-pVDZ) (Hartree): -523.75842729
E(RHF-RMP2/AUG-CC-PVDZ) (Hartree): -525.06953066
     T1 diagnostic:  0.000268
E(RHF-UCCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -525.50712744
E(RHF-UCCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -525.46790236
E(RHF-UCCSD-F12a/AUG-CC-PVDZ) (Hartree): -525.46349363
     T1 diagnostic:  0.016960
     D1 diagnostic:  0.056838
E(RHF-UCCSD-F12b/AUG-CC-PVDZ) (Hartree): -525.42426856
E(RHF-UCCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -525.50610936
E(RHF-UCCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -525.46688428
E(RHF-UCCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -525.51085236
E(RHF-UCCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -525.47162728
E(ROHF/AUG-CC-PVDZ) (Hartree): -523.73968032
E(UM062X/Aug-CC-pVTZ) (Hartree): -526.13876657
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.034634      0.162510      -0.045069
     C      -0.835679     -0.057742       0.137164
     F       1.577481     -1.016995      -0.049748
     O       1.536504      1.207259      -0.069259
     F      -1.077515     -0.874796      -0.892121
     F      -1.270166      1.148662      -0.201935
     O      -0.819245     -0.449815       1.286967
Rotational constants (GHz):    3.9225000    2.3782900    1.9750900
Vibrational harmonic frequencies (cm-1):
     i391.6888                 55.5061                 168.5440
      191.1711                303.7387                 425.2446
      536.0196                599.4151                 643.9384
      697.6817                928.6932                1147.5914
     1224.1061               1622.1894                2020.4906
Zero-point correction (Hartree): 0.024067

TS.CFOCF2OH+H2O.CFOCFO+HF+H2O.a
-------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -602.00307406
E(CCSD/Aug-CC-pVDZ) (Hartree): -601.95060972
     T1 diagnostic:  0.016785
E(MP2/Aug-CC-pVDZ) (Hartree): -601.94110899
E(MP3/Aug-CC-pVDZ) (Hartree): -601.92921718
E(RHF/Aug-CC-pVDZ) (Hartree): -600.43006680
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -602.53227995
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -602.48427164
```

```
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -602.48159532
     T1 diagnostic:  0.014827
     D1 diagnostic:  0.059287
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -602.43358701
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -602.53127136
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -602.48326305
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -602.53641579
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -602.48840748
E(RHF/AUG-CC-PVDZ) (Hartree): -600.43006678
E(RM062X/Aug-CC-pVTZ) (Hartree): -603.24766211
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.814999      0.738943      -0.154037
     C      -0.171044     -0.648419      -0.301181
     F      -2.058281      0.697710       0.282002
     O      -0.248261      1.747395      -0.384948
     O       0.740999     -0.808852      -1.109902
     F      -1.018641     -1.630518      -0.075016
     F       0.531945     -0.515102       1.262377
     H       1.831870     -0.029684      -0.641654
     O       2.385765      0.440331       0.146763
     H       1.703336      0.091561       0.879984
     H       2.257823      1.395189       0.053410
Rotational constants (GHz):    2.5596500    1.7880700    1.3795400
Vibrational harmonic frequencies (cm-1):
     i634.5895                  58.6533                  99.6759
      201.9683                 246.3559                 318.5067
      359.3176                 404.6756                 502.9935
      536.6809                 551.2843                 570.4571
      641.3512                 714.4591                 737.5793
      823.1345                 860.3918                1186.6084
     1344.6038                1453.5953                1526.9168
     1615.6893                1726.2058                1952.4157
     2077.5790                2525.7216                3816.3529
Zero-point correction (Hartree): 0.061176

TS.CFOCF2OH+H2O.CFOCFO+HF+H2O.b
------------------------
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -602.00221312
E(CCSD/Aug-CC-pVDZ) (Hartree): -601.94998022
     T1 diagnostic:  0.016664
E(MP2/Aug-CC-pVDZ) (Hartree): -601.94016463
E(MP3/Aug-CC-pVDZ) (Hartree): -601.92849928
E(RHF/Aug-CC-pVDZ) (Hartree): -600.42936206
E(CCSD(T)-F12a/AUG-CC-PVDZ) (Hartree): -602.53116844
E(CCSD(T)-F12b/AUG-CC-PVDZ) (Hartree): -602.48317884
E(CCSD-F12a/AUG-CC-PVDZ) (Hartree): -602.48071017
     T1 diagnostic:  0.014746
     D1 diagnostic:  0.058358
E(CCSD-F12b/AUG-CC-PVDZ) (Hartree): -602.43272056
E(CCSD-T-F12a/AUG-CC-PVDZ) (Hartree): -602.53016264
E(CCSD-T-F12b/AUG-CC-PVDZ) (Hartree): -602.48217303
E(CCSD[T]-F12a/AUG-CC-PVDZ) (Hartree): -602.53522266
E(CCSD[T]-F12b/AUG-CC-PVDZ) (Hartree): -602.48723305
E(RHF/AUG-CC-PVDZ) (Hartree): -600.42936204
E(RM062X/Aug-CC-pVTZ) (Hartree): -603.24685084
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.073937     -0.599170      -0.058424
     C       0.204028      0.645199      -0.258120
     F       0.302512     -1.693366      -0.184836
     O       2.224301     -0.659527       0.143898
     O      -0.647909      0.678940      -1.150882
     F       0.885128      1.735323       0.019541
     F      -0.606116      0.436021       1.233275
     H      -1.791649     -0.016085      -0.728148
     O      -2.438286     -0.405476       0.036256
     H      -1.753059     -0.104516       0.801414
     H      -2.461642     -1.368882      -0.020004
Rotational constants (GHz):    2.5726800    1.7783000    1.3496700
Vibrational harmonic frequencies (cm-1):
```

```
     i680.6466                70.7687                74.8132
      205.3512               239.9946               329.6123
      353.3892               401.9789               500.4400
      519.0699               540.4093               578.2923
      659.1031               702.6761               733.0959
      827.7661               856.6118              1131.0343
     1324.0065              1411.1517              1459.8003
     1608.1318              1714.7500              1999.3620
     2035.1924              2480.1621              3849.2532
Zero-point correction (Hartree): 0.060613
```

```
*********************************************
CF3CF=CF2 + OH : M06-2X/cc-pVDZ geometry
*********************************************

CF3CFCF2
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -713.14454132
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.402535     -0.157078      -0.000002
     C       0.241372      0.488409      -0.000029
     C      -1.119024     -0.134950      -0.000001
     F       0.223975      1.823237      -0.000021
     F       2.553768      0.463613       0.000017
     F       1.543737     -1.455671      -0.000006
     F      -1.046686     -1.464353      -0.000102
     F      -1.812307      0.251056       1.074853
     F      -1.812409      0.251196      -1.074720
Rotational constants (GHz):    2.5537100    1.2667000    0.9927100
Vibrational harmonic frequencies (cm-1):
       37.6737                129.4577                175.5998
      247.7172                248.0135                367.1500
      373.9281                474.5601                518.7231
      586.9552                612.2294                669.6819
      684.1958                790.8516               1075.6346
     1260.1232               1271.3807               1295.6839
     1408.1577               1472.8593               1912.1661
Zero-point correction (Hartree): 0.035568

CF2CFCF2OH
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -689.13327169
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.130387     -0.155677      -0.013341
     C      -0.237318      0.471407       0.012577
     C      -1.411410     -0.144718      -0.006079
     F      -0.194039      1.815783       0.032421
     F       1.667032     -0.092489       1.234137
     F       1.050162     -1.447904      -0.344061
     F      -1.572666     -1.441633      -0.024193
     F      -2.554524      0.495258      -0.004832
     O       1.955663      0.450639      -0.905135
     H       1.901059      1.407668      -0.759111
Rotational constants (GHz):    2.5271100    1.2794000    1.0000900
Vibrational harmonic frequencies (cm-1):
       39.3905                129.6122                163.7252
      237.8446                260.9031                293.8011
      372.3207                380.1755                478.6689
      514.6170                583.7531                609.4401
      666.6879                686.9422                786.5067
     1058.5628               1153.0456               1218.6495
     1289.1613               1373.2415               1403.4459
     1477.1091               1919.5303               3830.8603
Zero-point correction (Hartree): 0.047677

CF3CFCF2OH
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -788.93888163
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.303451     -0.125659      -0.031349
     C      -0.012458      0.591152      -0.341223
     C       1.286070     -0.107464      -0.053253
     F      -0.017123      1.886270      -0.079736
     F      -2.313601      0.450548      -0.687155
     F      -1.164890     -1.396558      -0.483118
     F       1.227696     -0.716933       1.160464
     F       1.545173     -1.055425      -0.945956
     F       2.293452      0.753572      -0.023522
```

```
     O      -1.631398     -0.113679       1.288385
     H      -0.906144     -0.532003       1.779079
Rotational constants (GHz):    2.0845200    1.0701800    0.9353500
Vibrational harmonic frequencies (cm-1):
       48.3876                  68.2928                 150.0408
      172.5356                 253.2285                 295.2930
      326.2258                 347.4436                 364.4615
      460.5885                 514.9848                 540.8673
      554.7354                 619.6182                 691.2520
      710.6764                 801.7906                1006.1738
     1160.7549                1173.7163                1224.9472
     1264.1820                1315.2839                1390.6640
     1434.8583                1480.1216                3820.5567
Zero-point correction (Hartree): 0.050556

CF3CFOHCF2
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -788.92967318
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.492087      0.117492      -0.010636
     C       0.093616      0.696578      -0.072352
     C      -0.996979     -0.381197       0.052457
     F      -0.042576      1.250952      -1.315383
     F       1.828803     -0.668544      -1.012126
     F       1.818916     -0.409933       1.155231
     F      -0.879622     -1.016590       1.216775
     F      -2.205770      0.161420      -0.022284
     F      -0.865974     -1.271564      -0.930083
     O      -0.129021      1.596847       0.924706
     H       0.615840      2.216318       0.956367
Rotational constants (GHz):    1.7887100    1.1952500    1.1640100
Vibrational harmonic frequencies (cm-1):
       29.8252                  88.1596                 147.0810
      211.2630                 228.0769                 278.2800
      323.2286                 348.1811                 379.4977
      400.5734                 514.3736                 524.6588
      557.5784                 613.5478                 642.0341
      700.0667                 792.8711                1007.5044
     1164.5180                1264.7544                1279.1357
     1298.8124                1306.6746                1359.8392
     1430.6224                1453.2474                3814.6291
Zero-point correction (Hartree): 0.050482

CF2CFCF2OH
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -689.13327169
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.130387     -0.155677      -0.013341
     C      -0.237318      0.471407       0.012577
     C      -1.411410     -0.144718      -0.006079
     F      -0.194039      1.815783       0.032421
     F       1.667032     -0.092489       1.234137
     F       1.050162     -1.447904      -0.344061
     F      -1.572666     -1.441633      -0.024193
     F      -2.554524      0.495258      -0.004832
     O       1.955663      0.450639      -0.905135
     H       1.901059      1.407668      -0.759111
Rotational constants (GHz):    2.5271100    1.2794000    1.0000900
Vibrational harmonic frequencies (cm-1):
       39.3905                 129.6122                 163.7252
      237.8446                 260.9031                 293.8011
      372.3207                 380.1755                 478.6689
      514.6170                 583.7531                 609.4401
      666.6879                 686.9422                 786.5067
     1058.5628                1153.0456                1218.6495
     1289.1613                1373.2415                1403.4459
     1477.1091                1919.5303                3830.8603
Zero-point correction (Hartree): 0.047677
```

```
*********************************************
CF3OCF=CF2 + Cl : M06-2X/cc-pVDZ geometry
*********************************************

CF3OCFCF2
-------------------------
E(RM062X/CC-pVDZ) (Hartree): -788.35463805
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.672616     -0.287932      -0.068459
     C       0.694091      0.564996      -0.335089
     O      -0.488561      0.168681      -0.874721
     F       0.823924      1.869870      -0.148821
     C      -1.471733     -0.111240       0.043085
     F      -1.683853      0.918544       0.854497
     F      -1.141887     -1.159607       0.790339
     F      -2.570402     -0.380072      -0.628547
     F       1.566372     -1.581829      -0.246295
     F       2.843472      0.072607       0.396666
Rotational constants (GHz):    2.3475600    0.9395300    0.7772000
Vibrational harmonic frequencies (cm-1):
       42.7445                  67.2912                 118.5448
      192.6827                 210.7831                 341.5436
      369.1534                 452.4712                 469.3770
      546.3894                 554.7824                 607.0276
      641.9512                 652.4408                 726.3140
      856.0562                 946.8563                1225.8433
     1270.7324                1303.7518                1382.7947
     1388.7653                1429.0729                1961.5734
Zero-point correction (Hartree): 0.040458

Cl
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -460.12141082
Point group : OH
Cartesian coordinates (Angs):
    Cl       0.000000      0.000000       0.000000
Zero-point correction (Hartree): 0.000000


CF3OCFCF2Cl
-------------------------
E(UM062X/CC-pVDZ) (Hartree): -1248.52010876
Electronic state : 2-A
Cartesian coordinates (Angs):
     C       1.169693     -0.358406      -0.014712
     C       0.279604      0.718444      -0.580233
     O      -0.976187      0.397586      -0.970858
     F       0.385550      1.889082       0.023170
     C      -1.870659     -0.059709      -0.021859
     F      -1.799266      0.657819       1.091094
     F      -1.627993     -1.327747       0.283720
     F      -3.074623      0.038479      -0.541604
     F       1.012173     -1.471282      -0.730603
     F       0.841879     -0.638347       1.260388
    Cl       2.864600      0.157959      -0.059281
Rotational constants (GHz):    1.9522300    0.6495700    0.5887900
Vibrational harmonic frequencies (cm-1):
       41.2676                  60.3426                 100.3693
      154.3055                 177.1877                 209.7793
      272.9062                 339.4980                 367.3236
      436.4009                 456.5008                 499.3195
      557.3173                 602.5320                 627.1769
      646.2689                 733.0174                 766.8344
      907.1656                1010.7153                1129.5933
     1227.7668                1244.5698                1313.5165
     1360.0125                1381.4091                1421.3548
Zero-point correction (Hartree): 0.041108
```