

Supporting Information: Kinetics and mechanism of the reaction of perfluoro propyl vinyl ether (PPVE, C₃F₇OCF=CF₂) with OH: Assessment of its fate in the atmosphere

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Table SI 1. Results of the UV absorption cross section of PPVE

λ (nm)	σ (10 ⁻²⁰ cm ² molecule ⁻¹)	λ (nm)	σ (10 ⁻²⁰ cm ² molecule ⁻¹)
195.0	32.27	205.2	0.80
195.2	31.03	205.4	0.75
195.4	29.58	205.6	0.67
195.6	28.34	205.8	0.60
195.8	26.42	206.0	0.56
196.0	25.32	206.2	0.52
196.2	24.11	206.4	0.48
196.4	23.04	206.6	0.44
196.6	21.38	206.8	0.39
196.8	20.23	207.0	0.38
197.0	18.79	207.2	0.34
197.2	17.97	207.4	0.31
197.4	16.32	207.6	0.28
197.6	15.19	207.8	0.27
197.8	14.26	208.0	0.24
198.0	13.70	208.2	0.22
198.2	12.85	208.4	0.20
198.4	11.85	208.6	0.18
198.6	10.62	208.8	0.17
198.8	10.23	209.0	0.17
199.0	9.54	209.2	0.15
199.2	9.02	209.4	0.14
199.4	8.28	209.6	0.12
199.6	7.49	209.8	0.12
199.8	7.10	210.0	0.10
200.0	6.64	210.2	0.10
200.2	6.01	210.4	0.08
200.4	5.44	210.6	0.08
200.6	5.11	210.8	0.08
200.8	4.75	211.0	0.07
201.0	4.51	211.2	0.06
201.2	4.16	211.4	0.05
201.4	3.81	211.6	0.06
201.6	3.47	211.8	0.06
201.8	3.23	212.0	0.05
202.0	3.06	212.2	0.05
202.2	2.79	212.4	0.04
202.4	2.48	212.6	0.04
202.6	2.37	212.8	0.04
202.8	2.21	213.0	0.04
203.0	2.04	213.2	0.03
203.2	1.87	213.4	0.03
203.4	1.70	213.6	0.04
203.6	1.60	213.8	0.03
203.8	1.50	214.0	0.03
204.0	1.36	214.2	0.03
204.2	1.21	214.4	0.03
204.4	1.12	214.6	0.02
204.6	1.07	214.8	0.02
204.8	1.00	215.0	0.02
205.0	0.90		

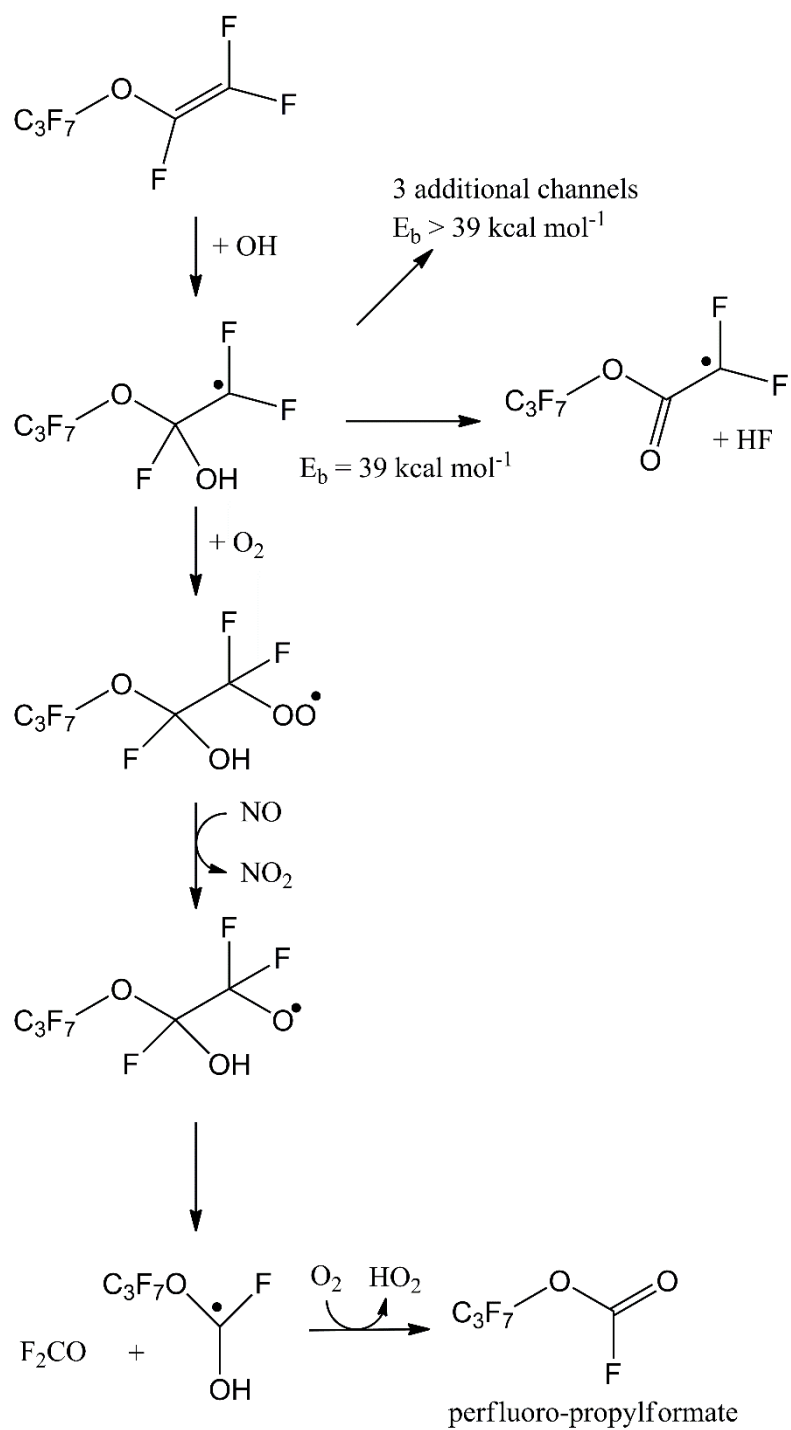


Figure SI 1. OH-initiated oxidation pathways for $\text{C}_3\text{F}_7\text{OCF}=\text{CF}_2$, at the M06-2X/aug-cc-pVTZ level of theory, following OH-addition on the inner carbon atom. The 3 additional pathways for the adduct can be found in figure SI 2.

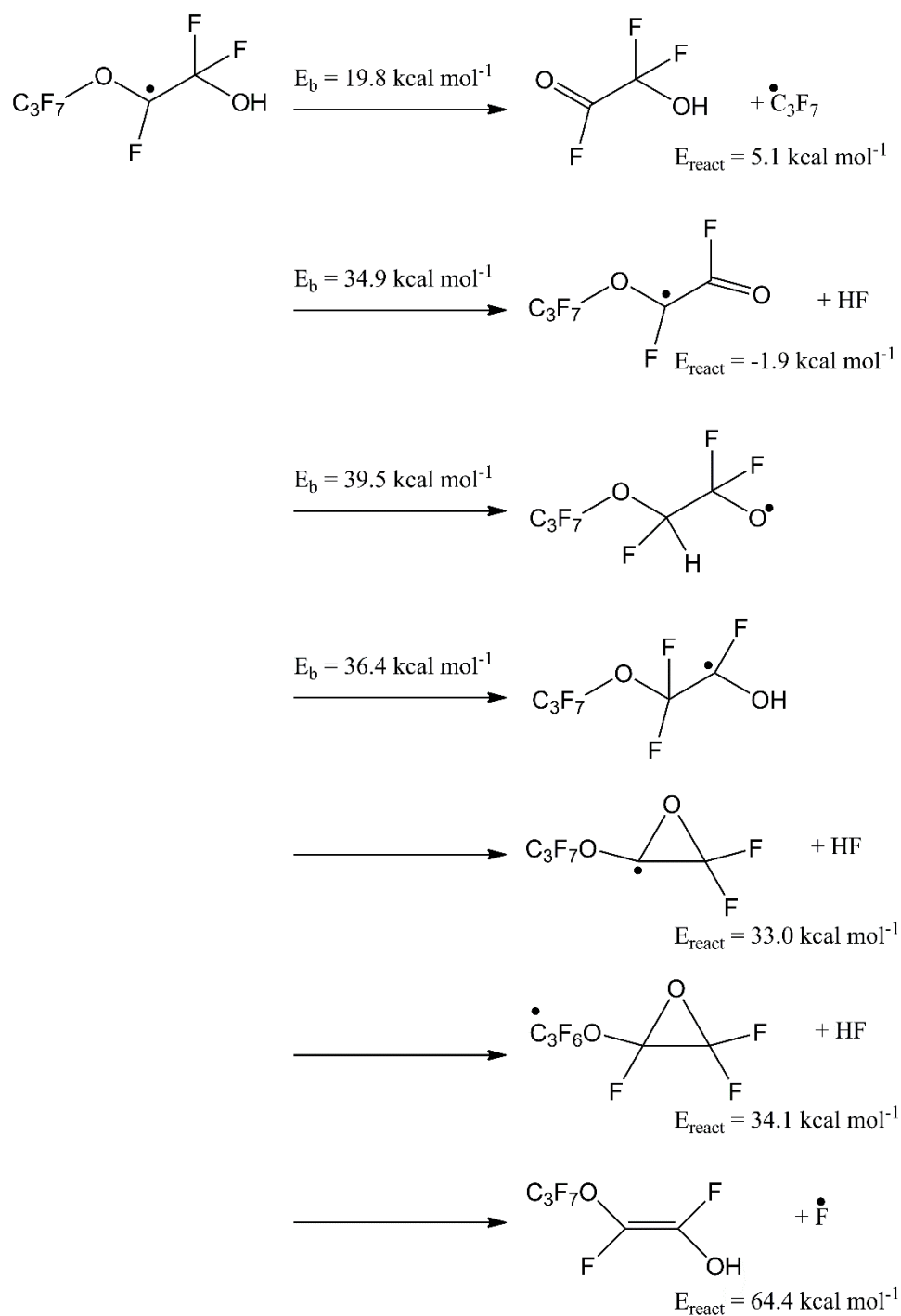


Figure SI 2. Unimolecular pathways for the most stable adduct formed in the OH + C₃F₇OCF=CF₂ reaction. Energies and barrier heights obtained at the M06-2X/aug-cc-pVTZ level of theory.

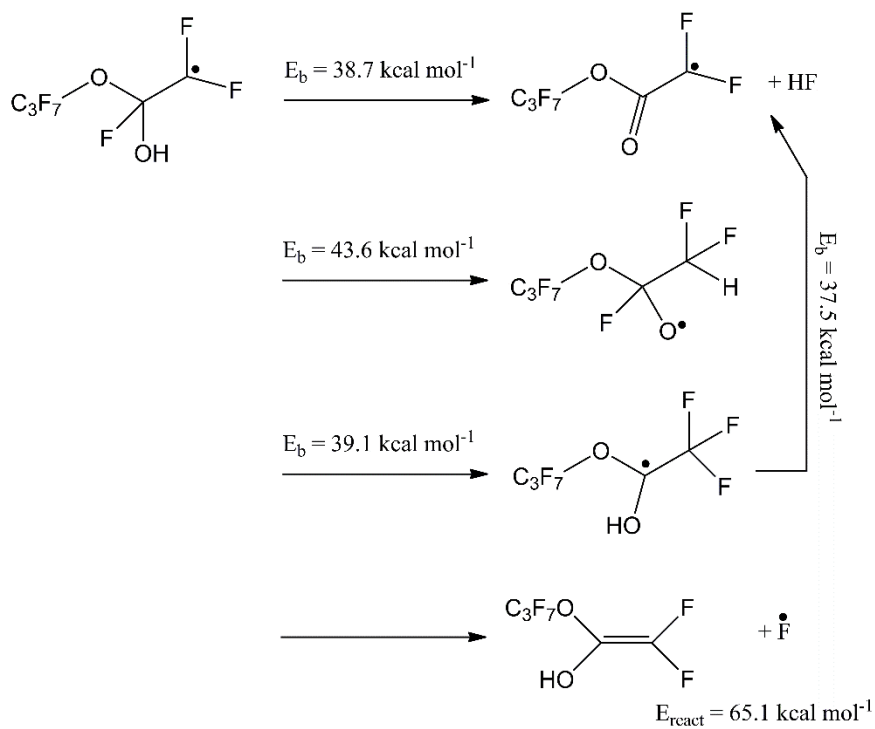


Figure SI 3. Unimolecular pathways for the least stable adduct formed in the OH + C₃F₇OCF=CF₂ reaction; this isomer is predicted to be 1.4 kcal mol⁻¹ above the more stable adduct. Energies and barrier heights obtained at the M06-2X/aug-cc-pVTZ level of theory.

Selected quantum chemical properties for reactants, intermediates, products, and TS studied in this work.

 C3F7OCF=CF2 + OH : M06-2X/aug-cc-pVTZ geometry

C3F7OCFCF2

 E (RM062X/Aug-CC-pVTZ) (Hartree): -1264.25066580

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-3.102207	-0.447351	0.044024
C	-2.235625	0.528537	0.231765
O	-0.989898	0.329002	0.732043
F	-2.554887	1.792393	0.013339
F	-2.833293	-1.707633	0.263575
F	-4.326272	-0.254150	-0.371851
C	0.008786	0.155677	-0.193376
C	1.339408	0.089068	0.587974
C	2.591378	-0.181471	-0.279211
F	-0.174479	-0.972091	-0.886798
F	0.036230	1.164082	-1.068407
F	1.517425	1.257742	1.212268
F	1.251988	-0.890569	1.493547
F	2.721408	0.747055	-1.215919
F	2.514000	-1.371703	-0.855455
F	3.659963	-0.153878	0.504210

Rotational constants (GHz): 1.1644300 0.2995400 0.2845100

Vibrational harmonic frequencies (cm-1):

15.6037	26.2446	60.9535
77.2590	96.8434	155.6351
176.4783	216.8574	225.2384
232.1689	239.9667	297.5304
327.3632	340.4896	383.7597
388.0563	444.1678	481.6395
538.1716	542.6142	564.8442
588.1473	603.7076	632.2368
645.4812	686.1023	763.4425
826.8864	849.8500	1032.3416
1191.4441	1210.3508	1216.0612
1232.6037	1268.7656	1292.0210
1300.1737	1344.5447	1391.0446
1401.7278	1421.6771	1935.3064

Zero-point correction (Hartree): 0.065306

OH

 E (UM062X/Aug-CC-pVTZ) (Hartree): -75.73381016

Point group : C_v

Cartesian coordinates (Angs):

O	0.000000	0.000000	0.107984
H	0.000000	0.000000	-0.863871

Rotational constants (GHz): 0.0000000 564.3727589 564.3727589

Vibrational harmonic frequencies (cm-1):

3770.5842 (SG)

Zero-point correction (Hartree): 0.008590

C3F7OCFCF2OH

 E (UM062X/Aug-CC-pVTZ) (Hartree): -1340.07631630

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.918346	-0.373133	-0.089803
C	2.022747	0.811911	-0.379275
O	0.740682	0.659701	-0.766619
F	2.222952	1.823050	0.459350
C	-0.170908	0.017063	0.046229
F	2.793569	-1.262240	-1.072073
O	4.222695	-0.026229	0.005133
F	2.507203	-0.977899	1.060823
H	4.340384	0.616229	0.714614
C	-1.575639	0.426446	-0.451780
C	-2.746358	-0.318041	0.232540
F	-0.013376	0.376011	1.320538
F	-0.029950	-1.306213	-0.033771
F	-1.730776	1.735523	-0.227533
F	-1.652587	0.188502	-1.764545
F	-2.668815	-0.195755	1.550680
F	-2.734184	-1.603105	-0.085564
F	-3.886984	0.214405	-0.182370

Rotational constants (GHz): 1.0591700 0.2775000 0.2667300

Vibrational harmonic frequencies (cm-1):

22.6482	33.6208	57.0005
70.1107	80.3144	113.7833
146.2515	193.2194	197.5303

224.1660	227.3574	237.6552
252.3670	298.2786	323.6596
342.1079	378.5191	384.9736
440.0225	475.2645	509.9351
539.5613	549.9889	559.9036
595.6286	616.1559	662.2152
669.7273	696.3220	770.8679
805.7168	840.9004	1010.3115
1073.3120	1114.3750	1180.0615
1197.2897	1239.6226	1251.8617
1269.7168	1283.6199	1300.3367
1308.0560	1377.4052	1383.9355
1416.6924	1442.0542	3850.6640

Zero-point correction (Hartree): 0.079770

C3F7OCFOHCF2

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.07439811

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.849975	-0.718367	-0.117458
C	2.263250	0.664302	0.081829
O	0.901960	0.816233	-0.292445
F	2.354518	0.958962	1.399930
C	-0.056655	-0.051380	0.128702
F	2.783329	-1.171974	-1.346506
F	2.482900	-1.620853	0.763516
O	2.972786	1.523649	-0.676134
H	2.499174	2.362799	-0.737088
C	-1.418857	0.574701	-0.254374
C	-2.654374	-0.307914	0.041593
F	0.069654	-1.243902	-0.473761
F	-0.015800	-0.263377	1.446707
F	-1.416264	0.840475	-1.565272
F	-1.559743	1.717635	0.427389
F	-2.701000	-0.637236	1.324227
F	-2.629678	-1.411522	-0.690025
F	-3.745382	0.381803	-0.263542

Rotational constants (GHz): 0.9311100 0.3063600 0.2919900

Vibrational harmonic frequencies (cm-1):

17.0637	41.7092	62.8512
81.0711	95.9043	123.8631
150.9156	194.2363	221.4734
226.7848	242.3990	250.8941
291.1059	300.2997	336.7432
350.7687	374.3428	385.0837
398.2916	461.2741	506.1970
531.4424	547.0798	570.6197
598.5494	613.5602	650.4812
686.2749	695.1250	766.9047
807.4114	861.4649	968.3982
1072.9160	1120.8654	1190.4655
1212.2118	1238.7941	1263.6854
1277.5990	1293.6167	1301.5094
1324.7091	1346.7708	1386.6016
1412.0187	1491.7016	3828.0051

Zero-point correction (Hartree): 0.080128

C3F7OCFCFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1239.62089461

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-3.260565	-0.495727	-0.032188
C	-2.270677	0.517938	0.221143
O	-1.042611	0.273787	0.696512
F	-2.621022	1.770073	0.161582
C	-0.003392	0.247410	-0.214562
F	0.108866	1.423684	-0.831601
F	-0.222312	-0.680956	-1.144478
C	1.279090	-0.073644	0.583404
F	-2.740798	-1.718824	0.112707
O	-4.390031	-0.304427	-0.340726
C	2.573233	-0.122213	-0.262813
F	1.121380	-1.264979	1.166304
F	1.435979	0.865798	1.520980
F	2.807407	1.055059	-0.823172
F	2.475997	-1.043311	-1.209902
F	3.585058	-0.428484	0.534671

Rotational constants (GHz): 1.1668700 0.3096200 0.2930300

Vibrational harmonic frequencies (cm-1):

5.2814	22.9733	45.8238
62.7857	86.1587	117.1482
173.2589	185.9717	224.5231
229.7033	237.4305	296.7296
335.8130	338.8072	341.5481
383.9848	393.9296	479.4916
531.4612	544.0250	563.0303
586.8833	622.2073	649.5544

668.3888	684.5357	761.8180
817.4179	832.3817	1025.2784
1145.2893	1184.8043	1200.9258
1241.2633	1272.0242	1292.0254
1303.0936	1378.6245	1392.5851
1428.3020	1502.9335	1846.1755

Zero-point correction (Hartree): 0.064783

CFOCF2OH

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

C3F7

E(UM062X/Aug-CC-pVTZ) (Hartree): -813.22558951

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-1.168781	0.197943	-0.099725
C	0.190215	-0.495567	0.123033
C	1.360270	0.328411	-0.364566
F	-1.301967	0.521398	-1.381066
F	-1.257164	1.298285	0.633779
F	-2.147227	-0.626100	0.241326
F	0.308258	-0.762322	1.439395
F	0.183327	-1.656139	-0.544493
F	1.457493	1.520861	0.177651
F	2.502810	-0.316508	-0.339086

Rotational constants (GHz): 1.9976200 1.1348900 0.9928700

Vibrational harmonic frequencies (cm-1):

29.7152	74.8226	148.6521
216.1888	223.5978	268.4289
330.8045	354.0293	388.8335
461.9374	539.5340	582.3851
621.4316	648.6424	748.5743
812.4711	1051.1668	1168.4453
1238.0746	1277.8694	1284.2630
1348.2035	1409.9481	1417.1331

Zero-point correction (Hartree): 0.037920

C3F7OCFOCF2OH

E(UM062X/Aug-CC-pVTZ) (Hartree): -1415.29426113

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.750346	-0.570370	-0.140210
C	1.964699	0.794949	0.149515
O	0.642936	0.808562	-0.308454
F	2.561806	1.737829	-0.598686
C	-0.305071	-0.082543	0.102895
F	-0.235694	-0.348247	1.408596
F	-0.201693	-1.242332	-0.556638
C	-1.673788	0.566165	-0.220621
F	2.530999	-0.880632	-1.408258
O	4.074571	-0.444340	0.042688
F	2.217932	-1.529308	0.636144
H	4.266685	-0.134581	0.936165
O	2.123494	0.993811	1.451418
C	-2.904000	-0.331687	0.051560
F	-1.798776	1.668246	0.527739
F	-1.696897	0.903066	-1.513641
F	-2.918540	-0.739338	1.312959
F	-2.901545	-1.388771	-0.746050
F	-4.000682	0.376292	-0.182190

Rotational constants (GHz): 0.9388900 0.2598500 0.2487800

Vibrational harmonic frequencies (cm-1):

15.1029	31.9507	54.1734
77.6590	84.1563	123.6738
152.4776	192.9443	208.7284
227.2179	229.6829	241.7742
257.3545	298.4176	311.4832

333.3640	346.6107	356.6467
381.5685	384.5612	441.2600
476.0917	518.4603	533.6256
548.7051	571.5892	594.6191
619.2219	647.3754	672.9100
698.8385	765.5391	779.5384
839.5522	887.6267	1029.5695
1088.2764	1141.5134	1189.1648
1192.6139	1223.7766	1242.7180
1263.9882	1268.1156	1299.8110
1300.5189	1321.1989	1381.6029
1408.5844	1416.6307	3841.4124

Zero-point correction (Hartree): 0.083185

C3F7OCFOCFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1314.82361732

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.723564	0.815766	-0.231419
C	2.232197	-0.599273	0.194970
O	0.913300	-0.614548	0.663424
F	2.961579	-0.955608	1.268479
C	-0.095633	-0.401329	-0.232140
F	-0.377963	-1.503690	-0.927665
F	0.234267	0.561655	-1.108074
C	-1.334474	0.039075	0.583677
F	2.305376	1.703796	0.654362
O	3.392307	1.066618	-1.157904
O	2.407102	-1.411657	-0.859520
C	-2.637015	0.175007	-0.240280
F	-1.063770	1.227140	1.132884
F	-1.552029	-0.859229	1.548207
F	-3.039271	-1.008030	-0.677416
F	-2.449491	0.981001	-1.276350
F	-3.577974	0.686434	0.539257

Rotational constants (GHz): 0.9688200 0.3053100 0.2979200

Vibrational harmonic frequencies (cm-1):

21.3625	41.6542	57.1180
61.3271	84.5708	100.8250
188.1077	196.2132	213.9200
229.8280	233.2284	244.0706
297.5392	335.0310	343.5287
353.7411	376.6552	384.6137
447.3309	487.0651	519.5773
549.9565	580.9858	595.2566
633.2924	669.3554	698.7990
753.9589	783.1786	810.0941
855.3655	998.9394	1082.9234
1148.1262	1187.9252	1196.4268
1230.0356	1250.3650	1270.8254
1287.2968	1299.4977	1306.7468
1387.5441	1413.4754	1978.4922

Zero-point correction (Hartree): 0.068769

complex.C3F7OCFCF2.OH.b

E(UM062X/Aug-CC-pVTZ) (Hartree): -1339.99146149

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.949426	-0.141597	0.564582
C	2.040119	-0.743658	-0.185238
O	0.762745	-0.952318	0.229339
F	2.344376	-1.282362	-1.348318
C	-0.172629	-0.034998	-0.164521
F	-0.138748	0.169316	-1.480680
F	0.046569	1.152197	0.428703
C	-1.552587	-0.583271	0.262082
F	2.680241	0.385823	1.729238
F	4.204580	-0.050006	0.236969
H	1.730262	2.269912	-0.633936
O	2.526717	1.852337	-1.003453
C	-2.745537	0.360660	-0.019323
F	-1.525850	-0.825415	1.576311
F	-1.767812	-1.725158	-0.397874
F	-2.808113	0.664290	-1.307741
F	-2.634082	1.478043	0.684468
F	-3.863239	-0.257046	0.332409

Rotational constants (GHz): 0.9689600 0.2677500 0.2655900

Vibrational harmonic frequencies (cm-1):

7.5981	34.9268	47.2881
60.5152	74.2005	92.6895
110.4392	125.4216	160.4679
175.3234	191.6414	218.9911
226.1331	234.3025	242.7093
298.5752	327.5547	341.4762
381.3717	387.0624	390.1138
448.6005	481.8092	538.4065
542.9656	563.6575	586.3451

603.3637	624.1335	644.4313
685.3353	762.9734	828.2956
845.8461	1033.2475	1185.8255
1202.5509	1219.5346	1232.4612
1270.1162	1293.8103	1298.3866
1348.3462	1390.0806	1414.2651
1421.0250	1897.3474	3768.3200

Zero-point correction (Hartree): 0.075772

C3F6OCFCF2oxide

E(UM062X/Aug-CC-pVTZ) (Hartree): -1239.56573178

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-3.042411	-0.510558	-0.171230
C	-2.042609	0.471923	0.188424
O	-0.835570	0.107837	0.719288
F	-2.378579	1.706602	0.528164
C	0.254025	0.353694	-0.041853
F	0.361458	1.603015	-0.467167
C	1.512563	-0.226695	0.545878
F	-2.847277	-1.806178	-0.042880
O	-2.293617	0.129260	-1.143426
F	-4.330283	-0.237915	-0.154063
C	2.720025	-0.132016	-0.411102
F	1.301741	-1.519575	0.822443
F	1.848723	0.403574	1.690763
F	3.062709	1.132490	-0.610478
F	2.412571	-0.686021	-1.578188
F	3.749376	-0.777644	0.115008

Rotational constants (GHz): 1.1621200 0.2786000 0.2640200

Vibrational harmonic frequencies (cm-1):

14.7945	23.6659	43.4229
63.6524	81.8983	151.8611
178.8888	200.9785	222.6329
225.5843	251.3281	297.8141
306.8526	355.9146	388.5834
459.3786	511.4441	522.4432
531.2790	548.2107	584.7481
589.8199	632.9620	653.8904
722.3901	765.4707	806.2464
821.2237	896.4627	1046.3072
1153.5401	1166.0911	1206.8097
1234.9445	1260.8355	1279.2158
1285.2141	1331.4271	1335.8804
1408.9022	1422.0860	1649.0031

Zero-point correction (Hartree): 0.065233

C3F7OCCF2oxide

E(UM062X/Aug-CC-pVTZ) (Hartree): -1239.56413237

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-3.444434	0.112732	-0.053601
C	-2.132129	-0.436515	-0.206413
O	-0.977193	0.268792	-0.291779
C	0.173662	-0.446506	-0.079493
F	0.357768	-1.348101	-1.048214
C	1.340049	0.567010	-0.069228
F	-3.671064	1.396143	0.150755
O	-2.815479	-0.554642	0.994282
F	-4.523393	-0.454581	-0.552225
F	0.122233	-1.103312	1.080886
C	2.747484	-0.065863	0.039978
F	1.173000	1.385233	0.974279
F	1.298548	1.275980	-1.201874
F	3.019117	-0.791013	-1.034458
F	2.831274	-0.834946	1.116085
F	3.640693	0.908112	0.136156

Rotational constants (GHz): 1.3348500 0.2672100 0.2583800

Vibrational harmonic frequencies (cm-1):

14.5791	30.3433	36.4902
62.8185	92.1055	149.8196
204.2028	219.5295	226.0623
230.5867	274.7001	299.2569
340.7517	358.4546	383.5478
460.6431	499.6167	523.6661
532.8372	547.2583	564.2846
604.8328	639.0931	670.3345
696.8797	764.0175	802.2119
839.3663	928.2693	1032.9952
1166.2065	1186.0932	1202.9367
1227.1700	1240.7683	1269.7316
1297.8720	1301.8863	1310.6335
1390.1648	1418.6670	1627.5271

Zero-point correction (Hartree): 0.065313

F

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(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): 0.000000 623.9250717 623.9250717
 Vibrational harmonic frequencies (cm-1):
 4159.7924 (SG)
 Zero-point correction (Hartree): 0.009477

C3F7OCOHC2

 E(RM062X/Aug-CC-pVTZ) (Hartree): -1240.23795680
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -3.083041 -0.467600 0.038820
 C -2.252185 0.542207 0.225719
 O -0.993217 0.292667 0.749460
 C -0.004650 0.145519 -0.166951
 F -0.003356 1.172282 -1.045273
 F -0.151483 -0.972723 -0.887522
 C 1.341046 0.113042 0.590845
 F -4.307576 -0.328007 -0.400141
 F -2.792483 -1.716746 0.302625
 O -2.615202 1.827647 0.073360
 H -2.084984 2.247102 -0.614909
 C 2.576264 -0.200748 -0.285848
 F 1.273613 -0.820343 1.544777
 F 1.530716 1.311504 1.154266
 F 3.666287 -0.072919 0.457461
 F 2.651555 0.643344 -1.306515
 F 2.520254 -1.439074 -0.751140
 Rotational constants (GHz): 1.1603800 0.3034300 0.2882300
 Vibrational harmonic frequencies (cm-1):
 16.1998 33.8154 62.6230
 77.1697 101.3164 155.8828
 180.1103 216.1329 226.9612
 237.1513 247.7312 295.8240
 299.4947 335.5073 340.7186
 382.8654 390.8184 446.8589
 486.5985 540.0467 545.2777
 565.2707 589.1274 605.6997
 638.6409 647.0719 686.6724
 762.5537 825.8099 845.6603
 1030.0157 1155.0230 1184.9829
 1199.3465 1228.2606 1267.5134
 1280.7704 1293.3589 1303.1104
 1338.9938 1389.2378 1395.5585
 1417.1671 1919.2491 3817.5526
 Zero-point correction (Hartree): 0.077471

C3F7OCFCFOH

 E(RM062X/Aug-CC-pVTZ) (Hartree): -1240.23912999
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -3.122921 -0.458006 0.045771
 C -2.228458 0.496444 0.241286
 O -0.979686 0.314814 0.741284
 F -2.566743 1.774474 0.024933
 C 0.013985 0.140843 -0.186140
 F 0.031407 1.142510 -1.071841
 F -0.159631 -0.994092 -0.870569
 C 1.350144 0.093269 0.586751
 F -2.837905 -1.720521 0.263958
 O -4.377312 -0.297865 -0.372570
 H -4.559091 0.638114 -0.517122
 C 2.600146 -0.172041 -0.284563
 F 1.279564 -0.879350 1.501547
 F 1.522414 1.268987 1.200695
 F 2.718879 0.751294 -1.228285
 F 2.532180 -1.366682 -0.852858
 F 3.672912 -0.129594 0.493396
 Rotational constants (GHz): 1.1659900 0.3032100 0.2879000
 Vibrational harmonic frequencies (cm-1):
 15.6277 27.9181 61.6967
 75.4421 97.4427 150.7555
 176.4478 215.1164 225.2439
 232.4947 239.5975 297.7652
 325.9159 329.3940 340.9049

383.4591	386.6714	428.4128
482.3873	538.8497	545.2317
569.1199	593.0685	604.2811
638.8680	649.4644	684.0203
762.0894	827.0340	845.9714
1031.8612	1140.4856	1192.9891
1213.3417	1226.3633	1266.8858
1271.6066	1289.4426	1299.4517
1324.7094	1391.3567	1419.9633
1453.5367	1908.7675	3849.0696

Zero-point correction (Hartree): 0.077527

C3F7OCOHC3

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.08823226

Electronic state : 2-A

Cartesian coordinates (Angs):

C	3.032950	-0.431900	-0.029588
C	1.970442	0.632316	-0.057193
O	0.791751	0.232201	0.509332
C	-0.312896	0.314047	-0.289981
F	-0.205103	-0.498090	-1.347942
F	-0.485030	1.554920	-0.755318
C	-1.526724	-0.100907	0.570806
F	4.153356	0.061610	-0.579655
F	2.657735	-1.505268	-0.709374
O	2.325073	1.872924	0.297988
H	3.206236	2.074970	-0.040960
F	3.340085	-0.819404	1.212972
C	-2.874872	-0.157031	-0.185376
F	-1.654251	0.779333	1.569378
F	-1.295651	-1.316712	1.077369
F	-3.832699	-0.452208	0.682683
F	-3.149168	1.013399	-0.744007
F	-2.848634	-1.090371	-1.124952

Rotational constants (GHz): 1.0545600 0.2540600 0.2473000

Vibrational harmonic frequencies (cm-1):

9.4935	28.2394	34.5601
45.7617	84.7651	94.2800
165.3933	188.2774	220.9204
231.2300	233.7744	245.9556
297.5661	320.0832	340.4827
372.2520	382.9360	393.5089
442.4926	467.1515	504.8872
543.7426	556.0485	568.2027
603.0720	614.2005	643.0544
684.5332	699.0448	764.7525
825.3325	864.1371	1012.0118
1118.3340	1185.4166	1195.3119
1218.1225	1224.9224	1235.5584
1266.0455	1273.7079	1294.7574
1301.6188	1377.6709	1395.8334
1421.6975	1466.8260	3833.2539

Zero-point correction (Hartree): 0.080399

TS.C3F7OCFCF2OH.C3F7+HOCF2CFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.04160831

Electronic state : 2-A

Cartesian coordinates (Angs):

C	3.066708	-0.201586	0.145565
C	1.927995	0.623184	-0.428935
O	1.014291	0.234425	-1.147938
F	1.944978	1.871103	0.043632
C	-0.410155	-0.586379	-0.306076
F	0.067261	-0.861935	0.882775
F	-0.614177	-1.654551	-1.023953
C	-1.542938	0.420793	-0.314885
F	3.006796	-1.429271	-0.357825
O	4.292500	0.309670	-0.135349
F	2.897215	-0.291628	1.490364
H	4.379942	1.181194	0.268297
C	-2.845203	-0.063197	0.364176
F	-1.130630	1.519511	0.331801
F	-1.831753	0.722673	-1.584883
F	-2.609106	-0.357869	1.636445
F	-3.299208	-1.147256	-0.251594
F	-3.766121	0.885796	0.304229

Rotational constants (GHz): 1.0204300 0.2618200 0.2522100

Vibrational harmonic frequencies (cm-1):

i637.7006	15.3815	25.9253
30.2346	56.8616	61.0620
94.5499	113.3189	160.5478
198.5264	207.9359	216.9138
229.3846	251.7007	268.2121
294.0742	347.0120	376.8656
387.5068	400.3001	448.4497
468.5426	515.0990	536.7430
545.4631	590.1878	617.0924

635.6812	685.2136	687.7473
703.0208	793.5411	823.1225
1042.3569	1102.6734	1114.6394
1203.5455	1226.8610	1263.7533
1280.4653	1281.7647	1328.9630
1372.2514	1376.8522	1391.2825
1421.4414	1567.6720	3850.9890

Zero-point correction (Hartree): 0.076573

TS.C3F7OCFOCF2OH.C3F7O+HOFCF2CFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1415.26721882

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-2.915408	-0.641585	-0.074455
C	-2.290592	0.775847	0.044256
O	-0.617992	0.323854	0.583806
F	-2.707921	1.374490	1.142193
C	0.455118	0.476983	-0.213978
F	0.738144	1.758338	-0.463901
F	0.338738	-0.152760	-1.386969
C	1.646847	-0.156094	0.588295
F	-2.861443	-1.252677	1.099857
O	-4.217908	-0.544357	-0.441673
F	-2.206932	-1.341807	-0.968917
H	-4.274857	-0.319013	-1.378270
O	-1.956305	1.424442	-0.936017
C	2.976021	-0.223250	-0.208310
F	1.857867	0.577570	1.682561
F	1.325102	-1.402934	0.940153
F	3.314704	0.971931	-0.666025
F	2.874288	-1.067113	-1.222313
F	3.925294	-0.654362	0.611639

Rotational constants (GHz): 0.9093400 0.2425000 0.2362900

Vibrational harmonic frequencies (cm-1):

i587.4444	11.5437	27.4714
42.0515	50.3890	80.2417
89.2237	141.7015	186.3239
218.6902	223.1083	231.4429
236.2670	254.1206	260.6598
292.4921	308.3162	337.9692
356.4365	380.0014	382.7604
449.8106	471.1282	501.1426
546.1771	551.6532	572.8114
591.9935	611.8523	625.1807
681.1023	695.1792	750.4729
813.6767	826.6112	990.3196
1126.0945	1138.6978	1145.2827
1191.4071	1227.8326	1255.2469
1267.6833	1273.3097	1305.0086
1306.5892	1323.9079	1384.6481
1405.4677	1553.5975	3842.1881

Zero-point correction (Hartree): 0.080960

TS.C3F7OCFOHCF2.C3F7OCFCF2+OH

E(UM062X/Aug-CC-pVTZ) (Hartree): -1339.98913032

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.836375	0.650732	-0.031783
C	2.043245	-0.404333	-0.268579
O	0.830469	-0.548908	0.315851
F	2.352749	-1.291222	-1.178728
C	-0.239912	0.006809	-0.347563
F	-0.325998	-0.456730	-1.594612
F	-0.116324	1.335801	-0.418956
C	-1.504559	-0.368957	0.456079
F	2.535157	1.588307	0.817631
F	3.990722	0.806893	-0.595644
O	3.281101	-1.213635	1.312063
H	2.723667	-0.963153	2.065815
C	-2.819636	0.245538	-0.079058
F	-1.343535	0.045993	1.717126
F	-1.631941	-1.698469	0.437169
F	-3.012895	-0.096230	-1.344700
F	-2.789937	1.566495	0.014709
F	-3.825699	-0.213644	0.650038

Rotational constants (GHz): 0.9933900 0.2641500 0.2595200

Vibrational harmonic frequencies (cm-1):

i216.0272	10.0545	22.0677
56.3275	69.2458	92.6508
112.7143	135.6534	153.5310
177.8639	213.9673	223.8361
230.7282	239.9893	265.5619
297.9158	327.2046	340.3255
383.5592	387.8304	411.9593
480.4400	511.6316	541.0392
544.4416	574.8986	591.4815
606.1208	643.6673	681.2347

706.3489	762.8213	825.7523
840.2967	1030.7787	1191.9764
1202.5456	1222.8415	1236.5420
1270.4689	1293.5125	1301.4408
1367.3172	1389.6382	1424.6880
1437.9977	1801.3990	3782.7618

Zero-point correction (Hartree): 0.076130

TS.C3F7OCFCF2OH.C3F7OCF2CFOH

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.01682076

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-3.089686	0.457456	-0.236504
C	-2.034281	-0.386859	-0.499672
O	-0.810076	0.050610	-0.768032
F	-2.249251	-1.665616	-0.636337
C	0.204509	-0.084473	0.182515
F	0.157645	-1.272144	0.766257
F	0.113650	0.866007	1.098574
C	1.526644	0.068793	-0.605946
F	-2.896336	1.735585	-0.282000
O	-4.322403	0.082664	-0.051509
F	-2.350147	-0.283066	1.526642
H	-4.317803	-0.666345	0.568216
C	2.802582	0.071745	0.268420
F	1.492080	1.221495	-1.282686
F	1.619631	-0.948830	-1.468877
F	2.863640	-1.026371	1.007607
F	2.824656	1.131990	1.060698
F	3.859877	0.112081	-0.530407

Rotational constants (GHz): 1.0604700 0.2683400 0.2645900

Vibrational harmonic frequencies (cm-1):

i287.9297	18.4743	34.0051
55.5682	77.1814	89.2440
133.8410	145.4915	170.7673
212.5438	228.9552	241.1472
259.2525	293.8053	301.9975
310.6096	333.0210	343.3949
385.6506	393.4906	452.9948
479.5484	537.6951	540.7768
548.4169	574.3697	588.1060
617.2729	653.6692	684.9979
761.8479	822.4239	841.9195
1020.9888	1166.0681	1174.4846
1202.2605	1266.9935	1268.5386
1276.3309	1285.9032	1315.5461
1380.9703	1389.1755	1439.8472
1516.5754	1741.7152	3735.0584

Zero-point correction (Hartree): 0.078171

TS.C3F7OCFCF2OH.CF2OH+C3F7OCFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1415.29360842

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.796818	-0.586977	-0.158286
C	1.933817	0.840899	0.213899
O	0.638540	0.793065	-0.310896
F	2.541863	1.769888	-0.545852
C	-0.315263	-0.084848	0.114221
F	-0.257035	-0.330877	1.422547
F	-0.207571	-1.255750	-0.527933
C	-1.681327	0.558297	-0.231907
F	2.580018	-0.798536	-1.438851
O	4.098223	-0.416783	0.057648
F	2.255234	-1.574150	0.551501
H	4.249023	-0.145672	0.972950
O	2.124658	0.903893	1.466962
C	-2.915300	-0.330232	0.053189
F	-1.808177	1.677186	0.490546
F	-1.696198	0.865862	-1.532495
F	-2.941759	-0.704843	1.324540
F	-2.907822	-1.408075	-0.716446
F	-4.008870	0.372788	-0.208598

Rotational constants (GHz): 0.9392400 0.2575400 0.2467700

Vibrational harmonic frequencies (cm-1):

i320.0899	17.4220	32.6160
58.9685	78.6457	90.3269
127.4938	153.8605	195.6197
222.9457	226.2857	228.5729
243.9852	287.9423	299.6369
323.1769	343.6900	347.1939
365.4578	384.6599	392.3541
435.9346	469.6481	533.0047
548.9888	557.9298	569.7914
595.9548	618.1953	652.4500
693.2060	739.3986	765.9553
836.6957	881.8443	1006.5146

1068.6626	1152.2060	1176.3305
1191.2279	1224.9162	1245.4837
1267.7761	1298.4191	1300.9516
1313.3750	1373.7854	1389.0300
1412.1898	1442.2563	3822.5747

Zero-point correction (Hartree): 0.082027

TS.C3F7OCFOHCF2.C3F7OCFOCF2H

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.00257586

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.058337	-0.379023	0.175332
C	3.270459	0.512859	0.062286
F	4.300136	0.041786	-0.607862
O	0.884584	0.263000	-0.185997
F	3.074509	1.790782	-0.177525
F	2.163027	-1.547502	-0.478836
O	2.259250	-0.524605	1.533077
H	3.317531	0.235874	1.355098
C	-0.285127	-0.442637	-0.122934
C	-1.427107	0.587426	0.040234
F	-0.291583	-1.294000	0.906920
F	-0.480639	-1.151105	-1.239650
C	-2.854209	-0.004954	-0.028956
F	-1.320222	1.504072	-0.927808
F	-1.284053	1.180941	1.229880
F	-3.724675	0.955373	0.250560
F	-2.997008	-0.984112	0.853448
F	-3.110861	-0.472352	-1.241073

Rotational constants (GHz): 1.0604700 0.2656400 0.2519800

Vibrational harmonic frequencies (cm-1):

i2010.7944	18.6312	36.0507
50.2292	68.2639	84.0812
111.2346	146.8498	198.8027
221.6769	228.9841	239.1301
274.3464	298.3435	328.2019
341.3432	377.1462	384.7558
420.0767	458.3822	513.8601
539.2271	560.6607	571.2493
598.7020	631.6228	680.0097
686.2124	735.5210	774.7722
848.2894	852.4315	1035.0283
1082.5865	1141.1913	1173.8352
1184.5428	1206.6064	1232.2356
1257.5080	1267.7503	1300.5675
1301.8372	1331.9104	1385.4668
1415.2390	1479.1775	2022.9199

Zero-point correction (Hartree): 0.075402

TS.C3F7OCFCF2OH.C3F7OCFCF2+OH

E(UM062X/Aug-CC-pVTZ) (Hartree): -1339.98959329

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-2.861503	-0.482991	-0.302776
C	-1.994903	0.519037	-0.127658
O	-0.805624	0.373006	0.490416
F	-2.319355	1.756106	-0.452709
C	0.276665	0.141534	-0.326124
F	0.392835	1.099688	-1.249159
F	0.146910	-1.021817	-0.968862
C	1.525396	0.115604	0.582519
F	-2.581039	-1.719223	-0.034792
O	-3.471376	0.034645	1.774731
F	-4.007114	-0.323006	-0.899811
H	-3.945828	0.871232	1.639452
C	2.854876	-0.183983	-0.149527
F	1.351178	-0.824929	1.514792
F	1.640691	1.311222	1.168934
F	3.081026	0.716529	-1.095397
F	2.826758	-1.390150	-0.696535
F	3.841294	-0.136380	0.733624

Rotational constants (GHz): 1.0026300 0.2566800 0.2541100

Vibrational harmonic frequencies (cm-1):

i277.8676	11.1167	25.6672
56.6045	61.3663	88.6998
94.8296	116.7176	164.8271
180.7593	195.0638	222.6095
228.2866	231.5068	248.2044
297.4339	327.8858	340.1747
383.7350	388.3339	413.6890
480.5385	511.8753	540.2520
542.8391	579.9381	599.6992
608.3302	634.3765	643.4735
684.9851	763.3343	827.0215
842.5046	1030.7485	1192.7396
1206.6130	1217.0963	1234.8670
1271.7000	1293.1361	1300.4713

1355.8108 1390.6488 1422.5233
1431.2545 1801.4602 3772.5903
Zero-point correction (Hartree): 0.075768

TS.C3F7OCFOCF2OH.F+HOCF2COOC3F7

E(UM062X/Aug-CC-pVTZ) (Hartree): -1415.25049917

Electronic state : 2-A

Cartesian coordinates (Angs):

C	3.065475	-0.556519	0.041190
C	1.857995	0.391680	0.225011
O	0.706622	-0.230347	-0.026378
F	2.161568	1.483100	-1.264988
C	-0.492284	0.416989	0.255110
F	-0.572364	1.573832	-0.386890
F	-0.604237	0.635264	1.561661
C	-1.609768	-0.539967	-0.222553
F	2.964953	-1.218102	-1.111240
O	4.233976	0.091034	0.112569
F	2.951811	-1.475447	1.029182
H	4.101772	0.986107	0.452220
O	1.967930	1.460948	0.822562
C	-3.048360	-0.019238	0.007434
F	-1.451120	-0.748009	-1.532345
F	-1.480467	-1.696642	0.433765
F	-3.242753	1.117244	-0.644573
F	-3.272725	0.175931	1.298463
F	-3.900036	-0.926822	-0.445191

Rotational constants (GHz): 0.9231200 0.2395600 0.2296600

Vibrational harmonic frequencies (cm-1):

i587.3251	11.1458	38.3318
52.7529	64.9157	74.6890
96.3398	139.5269	149.5063
201.9668	211.1327	226.9523
232.2404	237.9895	246.9814
298.6187	321.1272	338.5278
356.8095	361.4421	386.7549
442.7261	465.0774	516.3872
542.7545	554.0440	576.3051
610.1504	624.1778	651.3442
681.8742	692.5153	771.2125
823.3585	888.9120	1020.6899
1103.9433	1174.7295	1187.0825
1200.9922	1261.1622	1267.5234
1273.0628	1292.1334	1309.6599
1359.4709	1385.3070	1411.7186
1448.7103	1607.3223	3809.4870

Zero-point correction (Hartree): 0.082018

TS.C3F7OCFOHCF2.C3F7OCOCF2+HF

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.00972409

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.809359	-0.688208	-0.117809
C	2.126711	0.524717	-0.402664
O	0.836919	0.513911	-0.767383
F	2.101461	1.324768	1.343900
C	-0.139935	-0.283256	-0.196003
F	0.139355	-0.588191	1.062359
F	-0.269120	-1.414054	-0.893537
C	-1.454675	0.529794	-0.273560
F	4.056260	-0.674837	0.193751
F	2.233538	-1.832369	0.047524
O	2.808519	1.567588	-0.723608
H	2.697572	1.935756	0.301150
C	-2.710129	-0.219670	0.232473
F	-1.666107	0.865063	-1.550785
F	-1.306149	1.632524	0.460810
F	-3.745802	0.603382	0.168141
F	-2.546610	-0.610543	1.487821
F	-2.957831	-1.279967	-0.523078

Rotational constants (GHz): 0.9859500 0.2916700 0.2712800

Vibrational harmonic frequencies (cm-1):

i1238.4115	15.7112	31.4677
69.0783	76.7018	95.5891
112.7913	140.9724	173.8124
200.0861	225.7581	236.7746
241.5676	265.8444	300.0864
339.9625	356.8568	370.6835
386.2781	410.4618	468.8950
505.1916	511.5435	539.8753
554.6021	597.9026	609.2538
637.8791	686.2907	762.7556
768.0253	828.4608	857.4878
928.3866	1038.1860	1182.1437
1190.3773	1234.6277	1263.9989
1276.6089	1291.9056	1306.3714
1380.8527	1415.9428	1463.0417

1473.9708 1666.5093 2306.0158
Zero-point correction (Hartree): 0.074718

TS.C3F7OCFCF2OH.C3F7OCFCFO+HF

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.01553943

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.959723	-0.195754	-0.412945
C	1.990515	0.836967	-0.215240
O	0.733469	0.776792	-0.646277
F	2.284861	1.818291	0.580496
C	-0.188171	0.052953	0.112244
F	-0.074918	0.370640	1.396160
F	0.021848	-1.249021	-0.024402
C	-1.584474	0.437693	-0.425452
F	2.616335	-1.070935	-1.314813
O	4.181091	-0.079542	-0.072978
F	2.757010	-1.151923	1.188905
H	3.929438	-0.676190	0.839105
C	-2.754399	-0.357047	0.201451
F	-1.782233	1.735702	-0.176773
F	-1.604132	0.228820	-1.745119
F	-2.735798	-0.243280	1.521567
F	-2.676630	-1.636705	-0.127300
F	-3.893574	0.137225	-0.259323

Rotational constants (GHz): 1.0196200 0.2736100 0.2656100

Vibrational harmonic frequencies (cm-1):

i1375.4290	19.0883	32.4315
50.2409	65.9395	88.3205
109.1690	112.0125	168.2731
195.1259	225.5397	233.6822
241.0178	291.5270	299.2066
332.0799	341.8488	384.5216
390.3586	449.9761	477.0138
526.1249	540.5195	553.9528
569.0852	584.4742	613.6735
648.5554	680.9224	759.4648
790.0543	821.8169	840.2846
921.5552	1013.5858	1161.8667
1199.5555	1234.2375	1262.7125
1271.7483	1289.8233	1310.4316
1384.6133	1398.2973	1437.9893
1491.9100	1646.9005	2220.1605

Zero-point correction (Hartree): 0.074454

TS.C3F7OCFOCFO.C3F7OCFO+CFO

E(UM062X/Aug-CC-pVTZ) (Hartree): -1314.82113750

Electronic state : 2-A

Cartesian coordinates (Angs):

C	3.098674	0.823256	0.170030
C	2.137832	-0.759631	-0.113661
O	0.917141	-0.466830	0.482437
F	2.774503	-1.565947	0.731661
C	-0.170532	-0.282009	-0.334583
F	-0.392307	-1.357309	-1.090401
F	-0.018803	0.771183	-1.139050
C	-1.375136	-0.044254	0.607650
F	2.446683	1.806533	-0.371185
O	4.128784	0.825001	0.700836
O	2.313149	-0.822642	-1.322386
C	-2.721502	0.219153	-0.107351
F	-1.105930	1.019184	1.374079
F	-1.527179	-1.122730	1.381772
F	-3.046087	-0.802825	-0.885178
F	-2.656815	1.320605	-0.840348
F	-3.661688	0.373158	0.814249

Rotational constants (GHz): 0.9959500 0.2858400 0.2750400

Vibrational harmonic frequencies (cm-1):

i372.4881	14.8615	38.4612
43.7194	59.8698	90.0011
96.5323	151.5365	197.7253
206.6273	225.9445	228.6765
241.0017	297.5274	299.8227
341.4360	349.1968	385.0725
412.4747	417.9495	489.2743
542.1014	573.4949	578.4149
609.9337	629.7231	645.9607
694.0616	697.6834	769.2518
856.7606	889.9092	1055.9160
1135.3232	1192.9684	1194.6234
1231.0489	1243.7003	1268.0010
1295.9196	1304.3999	1382.2067
1409.5129	1576.7605	2023.7183

Zero-point correction (Hartree): 0.066953

TS.C3F7OCFOHCF2.C3F7OCHOHF3

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.01245377
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	2.706335	-0.583059	-0.276254
C	2.078660	0.644065	-0.217762
O	0.779755	0.861048	0.012250
C	-0.184396	-0.118552	-0.012433
F	-0.123016	-0.890599	1.066889
F	-0.054869	-0.887555	-1.097641
C	-1.543124	0.621851	-0.055344
F	3.928227	-0.675477	-0.683089
F	2.181764	-1.709063	0.061337
O	2.726812	1.742995	-0.534422
H	3.477021	1.806986	0.082631
F	3.039106	0.382683	1.541250
C	-2.781857	-0.301765	0.030965
F	-1.610430	1.297759	-1.206934
F	-1.597285	1.476683	0.968003
F	-3.869224	0.437956	-0.126087
F	-2.744213	-1.221122	-0.924122
F	-2.837090	-0.901771	1.209252

Rotational constants (GHz): 1.0296500 0.2755000 0.2610000
 Vibrational harmonic frequencies (cm-1):

i325.0359	15.6889	25.8759
65.5239	76.3166	88.0583
150.1953	173.0345	183.4848
198.5391	229.4652	245.4089
257.7090	271.3674	299.6031
327.1062	340.3856	360.3420
371.6996	387.3961	444.0301
475.5126	511.2056	536.1123
550.3110	580.4574	596.6829
603.3757	630.0431	689.6350
766.8893	795.9531	869.8592
1035.3135	1174.5375	1206.8575
1215.7351	1244.8566	1273.3357
1275.1991	1295.1237	1305.1799
1382.7099	1413.8970	1454.0658
1473.8768	1738.0610	3705.0066

Zero-point correction (Hartree): 0.078166

TS.C3F7OCFCF2OH.C3F7OCFHCF2O

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.00916577
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-3.176753	-0.396867	0.082420
C	-1.984025	0.516840	-0.070141
O	-0.812701	-0.094648	-0.400242
F	-4.275590	0.012801	-0.553354
F	-2.193021	1.663908	-0.701260
F	-2.977975	-1.676128	-0.233773
O	-3.221638	-0.178512	1.435466
H	-2.190193	0.616038	1.231147
C	0.332392	0.374345	0.196686
F	0.276110	0.190959	1.518985
F	0.495073	1.680033	-0.022206
C	1.509792	-0.424837	-0.405787
C	2.905503	-0.029758	0.132271
F	1.511394	-0.234813	-1.728653
F	1.316659	-1.719436	-0.139968
F	2.965335	-0.201991	1.444621
F	3.174708	1.235600	-0.152820
F	3.812135	-0.803055	-0.445532

Rotational constants (GHz): 1.0744300 0.2521000 0.2437500
 Vibrational harmonic frequencies (cm-1):

i1993.7624	10.6755	20.3456
48.8214	59.9571	86.3784
102.1118	160.3548	217.9406
220.3296	228.6636	233.7382
281.2469	297.1319	339.8526
341.0310	376.9179	392.0677
407.3365	489.1059	525.6977
544.1300	548.6933	582.8707
587.4075	630.6307	673.0616
690.9996	732.8352	766.7387
826.0681	899.1862	1025.6790
1088.2560	1163.3352	1187.5083
1198.3787	1205.2644	1231.5855
1263.4173	1272.7281	1283.5069
1301.8005	1306.9296	1389.9999
1419.8398	1460.3115	2016.7102

Zero-point correction (Hartree): 0.075493

TS.C3F7OCFOCF2O.C3F7OCOCFO+F

E(UM062X/Aug-CC-pVTZ) (Hartree): -1314.78277426
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	3.387744	0.463106	-0.252043
C	2.029872	-0.602956	0.001244
O	0.916277	0.155060	0.000150
F	2.859266	0.040480	1.369918
C	-0.294754	-0.523098	-0.065025
F	-0.393565	-1.405026	0.921842
F	-0.417735	-1.160616	-1.224383
C	-1.390340	0.561558	0.068480
F	2.950195	1.688723	-0.308266
O	4.415864	0.039124	-0.601084
O	2.164046	-1.754034	-0.185760
C	-2.839069	0.029437	-0.044884
F	-1.207579	1.465848	-0.898409
F	-1.255973	1.147544	1.260537
F	-3.068755	-0.893222	0.877505
F	-3.051958	-0.490861	-1.243909
F	-3.672809	1.041631	0.139267
Rotational constants (GHz): 1.0837400 0.2682300 0.2537000			
Vibrational harmonic frequencies (cm-1):			
i443.3035	13.6951	31.3617	
48.0745	70.2712	87.5241	
144.8231	157.7952	202.9404	
215.4778	227.9604	237.3243	
275.5637	295.9086	329.9331	
343.1692	365.8582	386.7149	
395.3756	424.2560	465.9938	
538.9460	551.1464	561.5147	
591.7474	626.8740	675.8749	
680.0031	692.0336	708.3967	
783.2693	879.1773	1002.4309	
1093.6596	1146.8665	1186.6463	
1207.3072	1258.5966	1274.0034	
1293.2112	1308.9652	1382.2637	
1411.1595	1851.2518	1946.8708	
Zero-point correction (Hartree): 0.066915			

TS.C3F7OCOHCF3.C3F7OCOCF2+HF

E(UM062X/Aug-CC-pVTZ) (Hartree): -1340.02417702

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-2.701457	-0.510405	0.122295
C	-1.955538	0.700037	0.109012
O	-0.714183	0.814152	-0.415226
C	0.256582	-0.130943	-0.173915
F	0.326287	-0.991581	-1.188633
F	-0.000720	-0.820806	0.941273
C	1.600770	0.621336	-0.031678
F	-3.376050	-0.868766	1.165274
F	-2.337371	-1.515973	-0.597119
O	-2.636133	1.765014	0.275293
H	-3.608528	1.352558	-0.112641
F	-4.201830	0.348957	-0.637233
C	2.845226	-0.288663	0.097103
F	1.528324	1.383524	1.064218
F	1.768103	1.397106	-1.105457
F	3.903623	0.472750	0.328023
F	2.695947	-1.137966	1.104752
F	3.042305	-0.971029	-1.020077
Rotational constants (GHz): 1.0810600 0.2607800 0.2467100			
Vibrational harmonic frequencies (cm-1):			
i1015.9835	19.4256	31.7943	
44.2086	65.4260	87.2923	
148.1026	151.0487	203.1822	
220.8761	229.1427	241.1544	
265.5756	299.0525	329.7325	
344.5752	360.4435	381.5658	
393.6150	460.0547	504.1156	
529.8944	549.4091	580.3667	
590.6983	597.5838	630.6786	
684.4394	694.9698	763.7945	
794.8649	860.0420	896.6751	
1037.1365	1171.1127	1191.2736	
1203.3319	1239.6886	1251.9082	
1273.0972	1294.8023	1303.7357	
1379.9582	1412.5354	1425.7480	
1522.4945	1693.7510	2021.2397	
Zero-point correction (Hartree): 0.076035			

TS.C3F7OCFCFO.CFOCFO+C3F7

E(UM062X/Aug-CC-pVTZ) (Hartree): -1239.57913566

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-3.076285	-0.749283	-0.107823
C	-2.412243	0.496895	0.377566
O	-1.374628	0.551557	1.009900
F	-3.036996	1.592598	-0.009083
C	0.206334	0.760019	-0.131218

F	0.528867	2.017841	-0.048991	
F	-0.292865	0.444052	-1.298375	
C	1.203514	-0.220527	0.448935	
F	-2.338665	-1.810852	0.197725	
O	-4.107045	-0.816099	-0.672805	
C	2.574315	-0.231088	-0.269160	
F	0.687534	-1.449886	0.363103	
F	1.414200	0.101201	1.729289	
F	3.144154	0.962866	-0.173558	
F	2.402742	-0.524441	-1.552884	
F	3.366538	-1.135574	0.280933	
Rotational constants (GHz):	1.0499300	0.3167600	0.2906100	
Vibrational harmonic frequencies (cm-1):				
i527.8243		20.6060		27.1724
40.9214		53.4789		66.6951
85.3671		124.9172		152.4080
195.5050		208.6155		230.5272
272.9029		285.2634		346.4716
376.4822		382.5158		425.3542
438.5181		515.4084		522.2974
545.8050		572.9320		617.8116
656.4255		677.1947		689.8995
775.8235		796.4217		846.9252
1038.3959		1170.9425		1206.2555
1266.8564		1273.0399		1282.4883
1292.7924		1370.2354		1380.1064
1424.0744		1593.4342		1931.5974
Zero-point correction (Hartree):	0.061923			

TS.C3F7OCFOCFO.FCOCFO+C3F7O

E(UM062X/Aug-CC-pVTZ) (Hartree): -1314.79528957

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.779660	0.856354	-0.260803
C	2.566195	-0.635453	0.052244
O	0.851053	-0.665574	0.653371
F	3.152169	-0.960029	1.189879
C	-0.139293	-0.449154	-0.239342
F	-0.485506	-1.547037	-0.910234
F	0.192430	0.493433	-1.134244
C	-1.360658	0.055673	0.601748
F	2.544337	1.599557	0.806151
O	3.132016	1.274150	-1.295113
O	2.352467	-1.466844	-0.814223
C	-2.671957	0.190438	-0.214617
F	-1.051926	1.255328	1.099014
F	-1.588333	-0.798346	1.601244
F	-3.119971	-0.999696	-0.577822
F	-2.477274	0.933633	-1.293366
F	-3.580145	0.774156	0.554085

Rotational constants (GHz): 0.9448000 0.2949600 0.2876600

Vibrational harmonic frequencies (cm-1):				
i613.7454		18.1683		31.7017
36.6959		67.1362		80.7522
94.4162		157.6634		180.0132
212.5249		228.2004		230.5616
241.9576		267.5471		293.3036
337.0115		353.5382		380.4792
397.1770		449.3258		468.9193
533.7249		547.8424		571.8080
586.8153		628.4650		675.1577
682.3022		748.2127		765.1600
814.9544		830.4069		993.8103
1153.0909		1158.5502		1191.5747
1232.0246		1258.7766		1273.6550
1303.1480		1306.1717		1320.1010
1385.3744		1571.2045		1988.1260
Zero-point correction (Hartree):	0.066175			

CF3CF=CF2 + OH : M06-2X/aug-cc-pVTZ 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

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