

(Supplementary Material for this Article)

THE THERMAL DECOMPOSITION OF CF₃ AND THE REACTION OF CF₂ + OH → CF₂O + H

by

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Table 1S: Supplementary Material*****
CF3

B3LYP/6-311++G**

SCF Done: E(UB+HF-LYP) = -337.670658489 A.U. after 1 cycles

1	6	0	0.000000	0.000000	0.327142
2	9	0	0.000000	1.261852	-0.072698
3	9	0	1.092796	-0.630926	-0.072698
4	9	0	-1.092796	-0.630926	-0.072698

Rotational constants (GHZ): 10.7617454 10.7617454 5.5688045

Frequencies -- 503.0249 503.0289 691.3129

Frequencies -- 1062.7017 1223.2230 1223.2551

CF2

B3LYP/6-311++G**

1	6	0	0.000000	0.000000	0.600032
2	9	0	0.000000	1.034522	-0.200011
3	9	0	0.000000	-1.034522	-0.200011

Rotational constants (GHZ): 86.5775191 12.4276930 10.8676988

SCF Done: E(RB+HF-LYP) = -237.774336386 A.U. after 1 cycles

Frequencies -- 667.1676 1085.7393 1209.0764

CF2O

B3LYP/6-311++G**

SCF Done: E(RB+HF-LYP) = -313.116609693 A.U. after 1 cycles

1	6	0	0.000000	0.000000	0.146257
2	8	0	0.000000	0.000000	1.317148
3	9	0	0.000000	1.066710	-0.634152
4	9	0	0.000000	-1.066710	-0.634152

Rotational constants (GHZ): 11.6890057 11.6818978 5.8427253

Frequencies -- 575.6492 614.8732 772.2069

Frequencies -- 955.6594 1201.6071 1974.3130

CF2OH

B3LYP/6-311++G**

SCF Done: E(UB+HF-LYP) = -313.654951987 A.U. after 1 cycles

1	6	0	-0.003558	-0.015268	0.319372
2	8	0	1.194619	-0.446348	-0.107603
3	9	0	-0.957860	-0.856698	-0.059856
4	9	0	-0.309772	1.243119	-0.075692
5	1	0	1.873082	0.184608	0.164514

Rotational constants (GHZ): 10.7362794 10.4966413 5.4933959

Frequencies -- 299.4687 498.3705 505.4593

Frequencies -- 685.9108 1015.7793 1066.7908

Frequencies -- 1248.1953 1346.2651 3821.1308