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

Supporting Information

Fluoromethylsulfinyl Radicals: Spectroscopic Characterization and Photoisomerization via Intramolecular Hydrogen Shift

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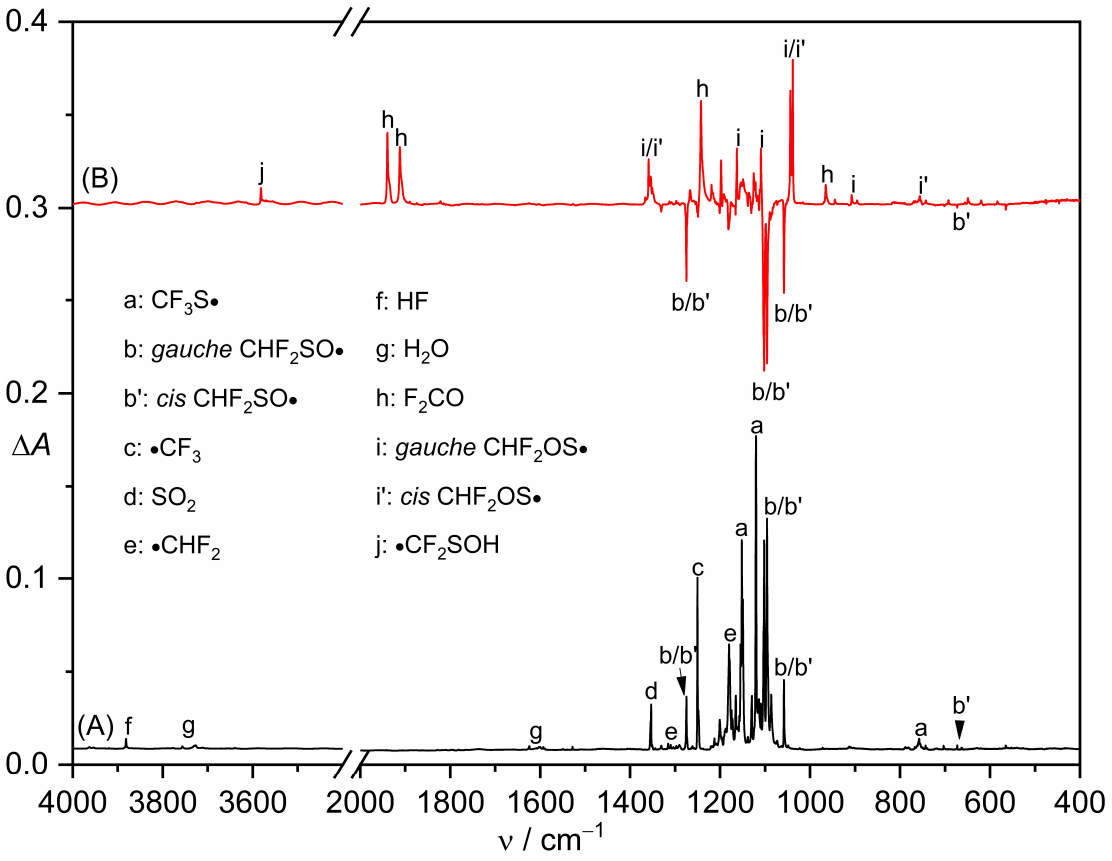

Figure S1. (A) IR spectrum of the high-vacuum flash pyrolysis (HVFP) products of $CHF_2S(O)SCF_3$ in solid Ar-matrix at 10 K. (B) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products upon a 266 nm laser irradiation (40 min).

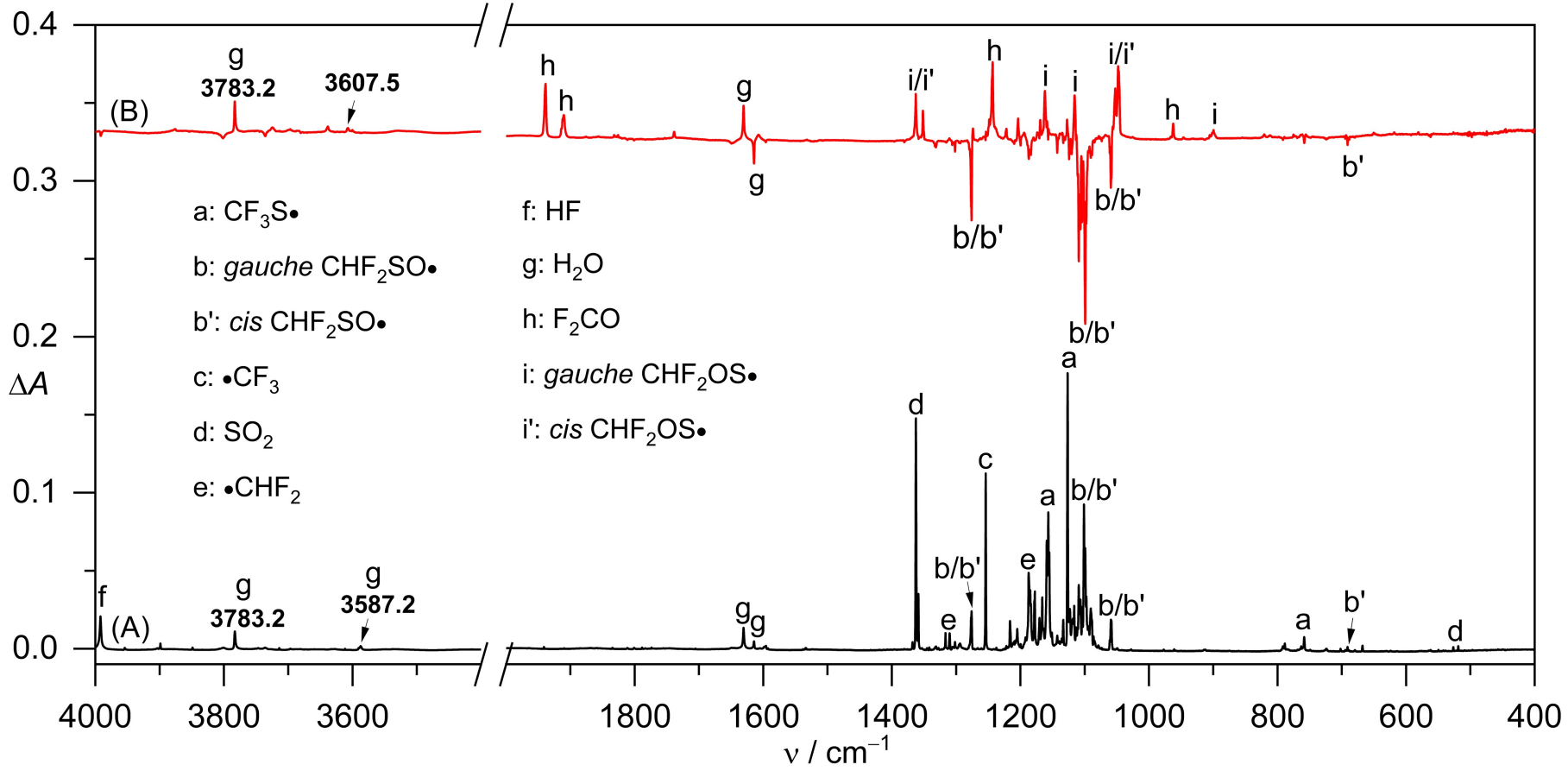

Figure S2. (A) IR spectrum of the high-vacuum flash pyrolysis (HVFP) products of $CHF_2S(O)SCF_3$ in solid Ne-matrix at 3 K. (B) IR difference spectrum reflecting the change of the Ne-matrix isolated HVFP products upon a 266 nm laser irradiation (70 min). For clarity, the band positions for H_2O (g) at 3783.2 and 3587.2 cm^{-1}) and $•CF_2SOH$ (3607.5 cm^{-1}, tentative assignment) are marked.

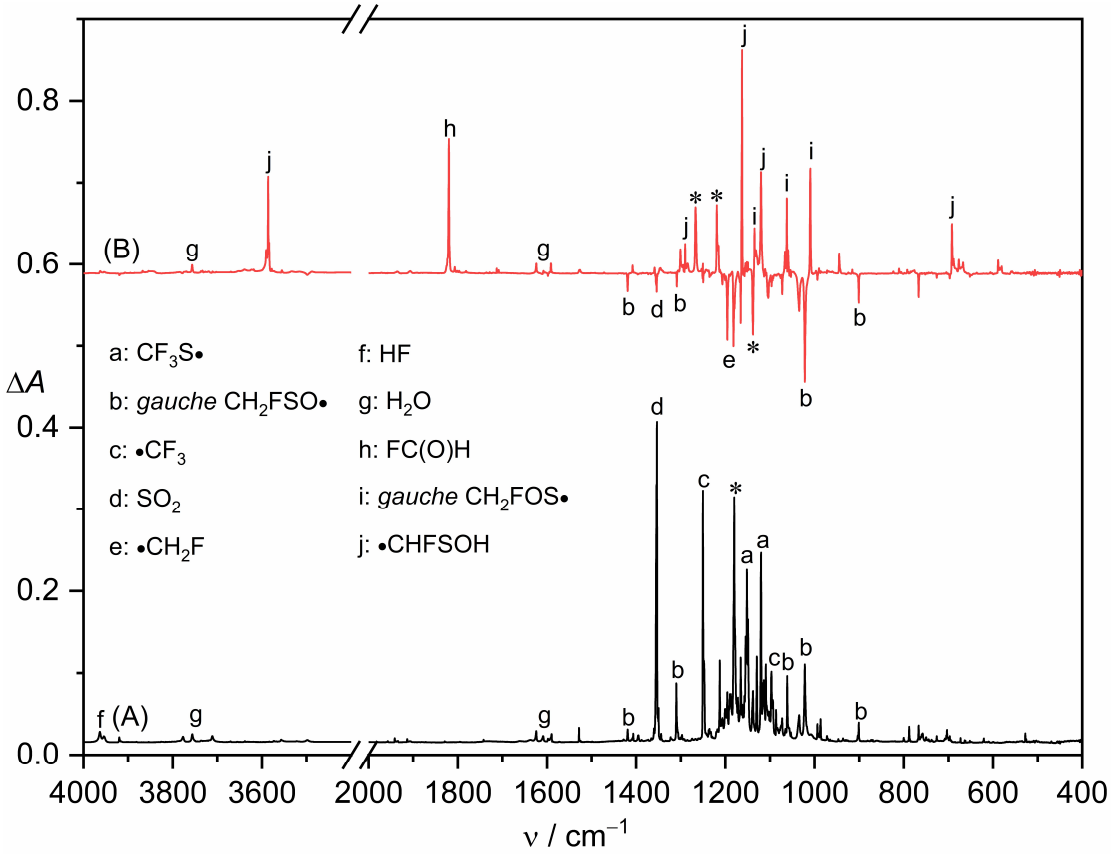

Figure S3. (A) IR spectrum of the high-vacuum flash pyrolysis (HVFP) products of $CH_2FS(O)SCF_3$ in solid Ar-matrix at 10 K. (B) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products upon a 266 nm laser irradiation (35 min). The IR bands for unknown species are marked with asterisks.

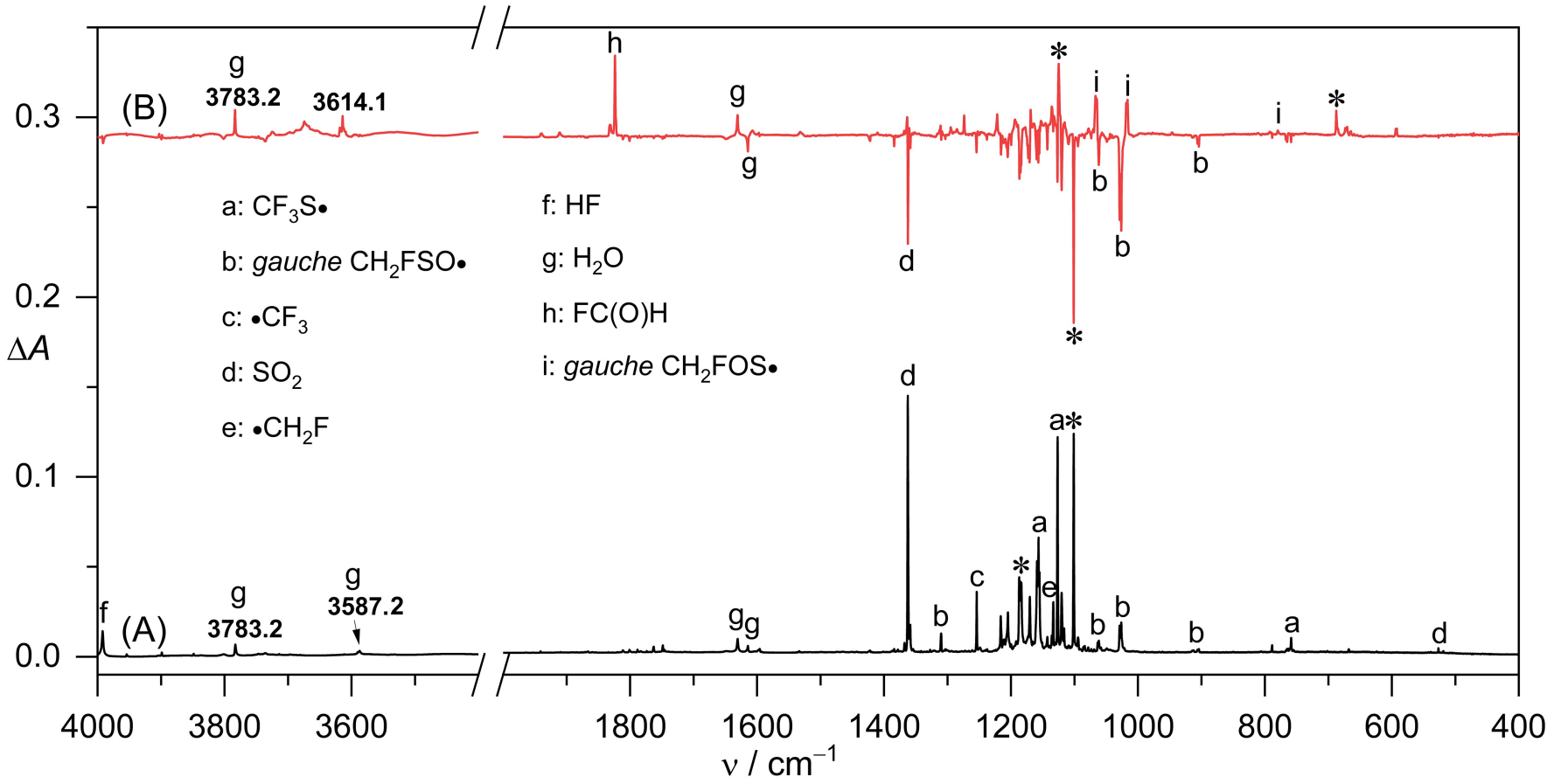

Figure S4. (A) IR spectrum of the high-vacuum flash pyrolysis (HVFP) products of $CH_2FS(O)SCF_3$ in solid Ne-matrix at 3 K. (B) IR difference spectrum reflecting the change of the Ne-matrix isolated HVFP products upon a 266 nm laser irradiation (70 min). The IR bands for unknown species are marked with asterisks. For clarity, the band positions for H_2O (g) at 3783.2 and 3587.2 cm^{-1}) and •CHFSOH (3614.1 cm^{-1}, tentative assignment) are marked.

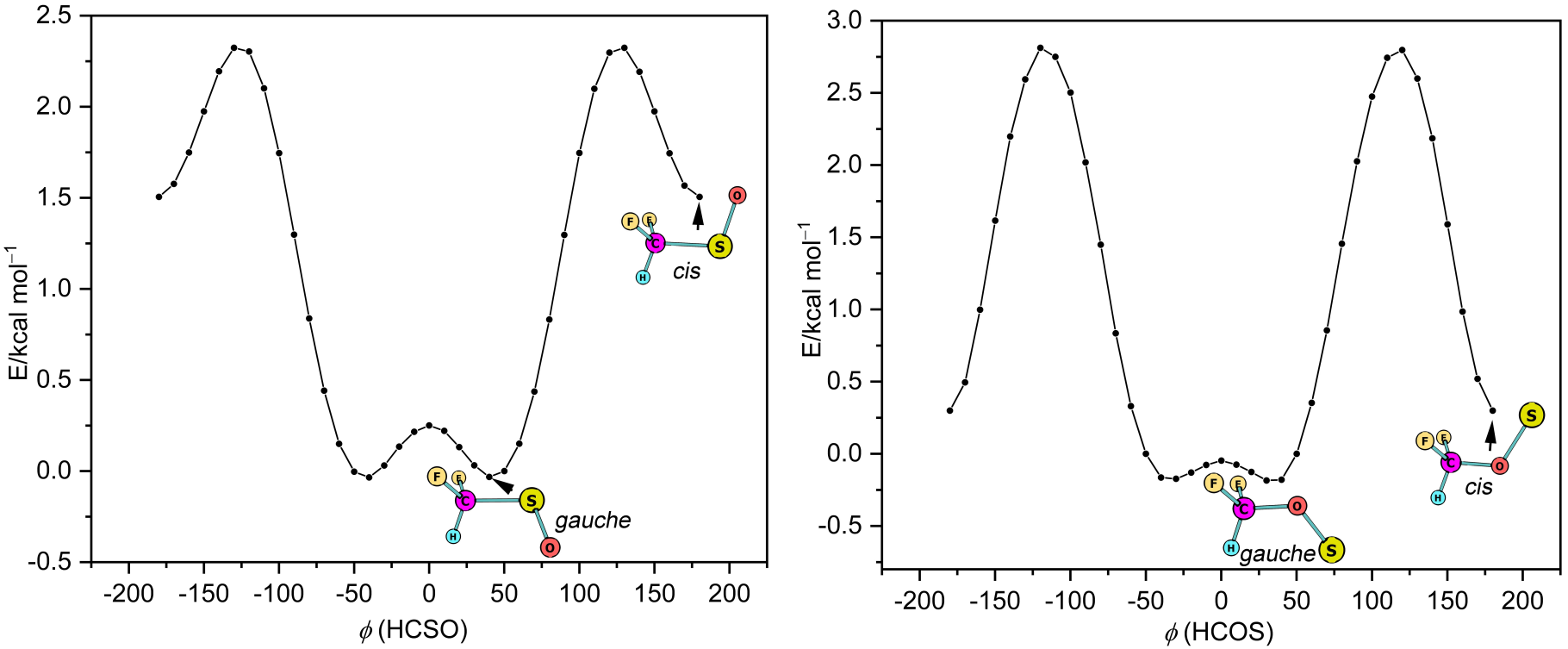

Figure S5. B3LYP/6-311++G(3df,3pd) calculated potential energy curves for the rotation of the C-S and C-O bonds in $CHF_2SO\bullet$ and $CHF_2OS\bullet$, respectively. The calculations were performed by rotating the corresponding dihedral angles in steps of 10° with simultaneous structural optimization of the remaining part of the molecules.

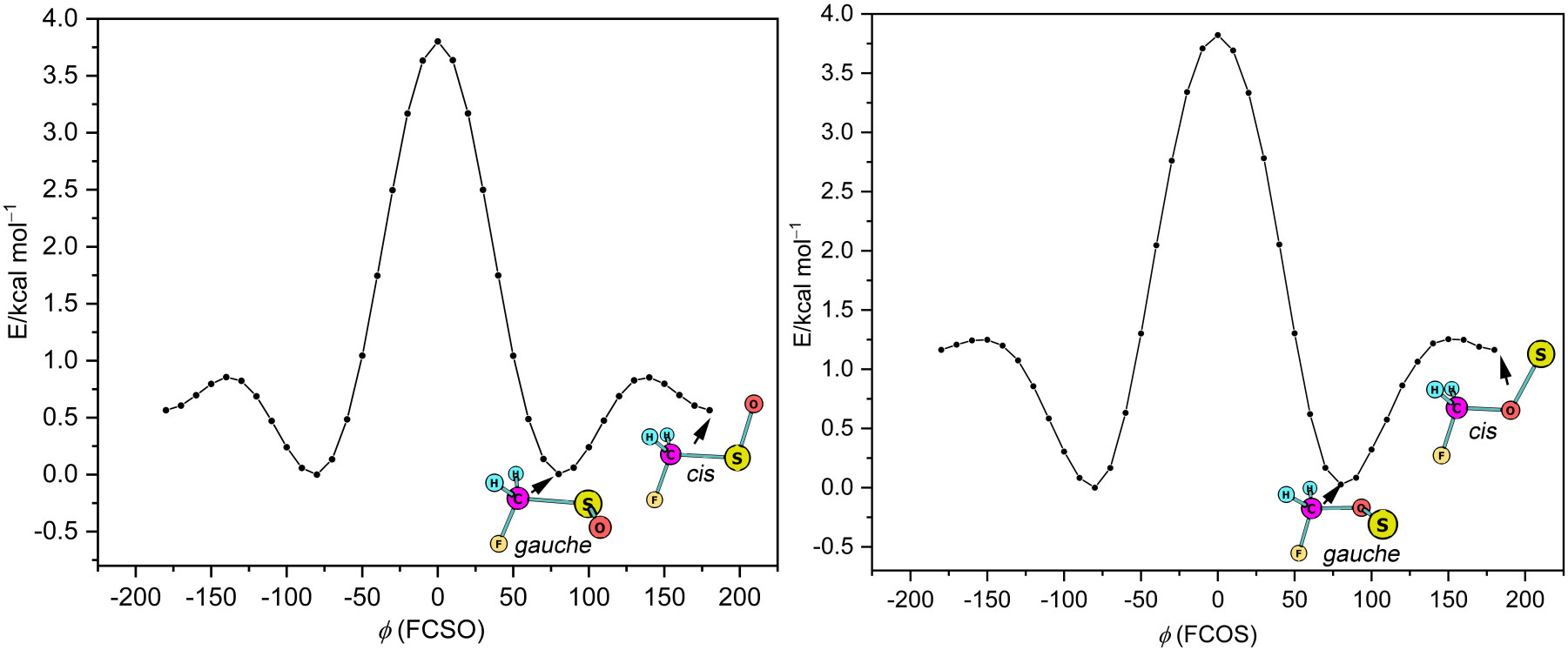

Figure S6. B3LYP/6-311++G(3df,3pd) calculated potential energy curves for the rotation of the C-S and C-O bonds in $CH_2FSO\bullet$ and $CH_2FOS\bullet$, respectively. The calculations were performed by rotating the corresponding dihedral angles in steps of 10° with simultaneous structural optimization of the remaining part of the molecules.

Table S1. Computed vibrational frequencies (cm^{-1}) and intensities (km mol^{-1}, in parentheses) of $CHF_2SO•$, $CHF_2OS•$, and $•CF_2SOH$ at the B3LYP/6-311++G(3df,3pd) level.

$CHF_2SO•$ gauche	$CHF_2SO•$ cis	$CHF_2OS•$ gauche	$CHF_2OS•$ cis	$•CF_2SOH$
3091 (12)	3061 (21)	3114 (12)	3128 (15)	3781 (81)
1345 (8)	1337 (8)	1377 (29)	1382 (30)	1245 (265)
1285 (51)	1314 (42)	1364 (45)	1364 (17)	1201 (227)
1103 (166)	1125 (107)	1151 (169)	1120 (101)	1135 (70)
1094 (194)	1088 (214)	1104 (211)	1095 (257)	690 (10)
1062 (65)	1065 (53)	1030 (434)	1035 (396)	622 (99)
750 (11)	683 (53)	905 (48)	751 (6)	489 (19)
563 (3)	590 (<1)	617 (5)	743 (25)	428 (58)
362 (13)	439 (15)	505 (3)	518 (2)	389 (10)
333 (3)	299 (<1)	427 (7)	478 (3)	335 (41)
202 (9)	197 (3)	278 (<1)	225 (3)	152 (2)
56 (7)	55 (<1)	45 (<1)	104 (3)	85 (3)

Table S2. Computed vibrational frequencies (cm^{-1}) and intensities (km mol^{-1}, in parentheses) of $CH_2FSO•$, $CH_2FOS•$, and •CHFSOH at the B3LYP/6-311++G(3df,3pd) level.

$CH_2FSO•$ gauche	$CH_2FSO•$ cis	$CH_2FOS•$ gauche	$CH_2FOS•$ cis	•CHFSOH
3123 (4)	3126 (5)	3137 (10)	3122 (17)	3788 (82)
3045 (14)	3053 (14)	3061 (34)	3050 (20)	3214 (<1)
1451 (4)	1477 (3)	1503 (2)	1515 (<1)	1305 (37)
1326 (8)	1321 (16)	1432 (16)	1434 (28)	1146 (161)
1245 (<1)	1207 (2)	1281 (<1)	1256 (<1)	1133 (96)
1064 (33)	1073 (130)	1165 (13)	1130 (10)	819 (2)
1029 (143)	1066 (45)	1071 (90)	1120 (134)	655 (108)
917 (7)	875 (<1)	1005 (317)	1001 (276)	478 (5)
646 (2)	732 (<1)	775 (26)	872 (26)	366 (43)
378 (16)	363 (<1)	532 (10)	436 (3)	315 (14)
271 (<1)	214 (18)	349 (4)	276 (3)	290 (79)
84 (6)	51 (14)	88 (4)	36 (2)	173 (3)

Table S3. Computed vertical excitation energies (nm) and oscillator strength of $CHF_2SO•$, $CHF_2OS•$, and $•CF_2SOH$ at the TD-B3LYP/6-311++G(3df,3pd) level.

$CHF_2SO•$ gauche		$CHF_2SO•$ cis		$CHF_2OS•$ gauche		$CHF_2OS•$ cis		$•CF_2SOH$	
λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength
573	0.0004	594	0.0004	1934	0.0000	2356	0.0000	481	0.0018
265	0.0000	259	0.0000	338	0.0000	347	0.0000	312	0.0012
246	0.0344	249	0.0319	268	0.0001	267	0.0000	288	0.0293
233	0.0015	233	0.0000	263	0.0007	266	0.0000	246	0.0064
228	0.0002	230	0.0002	249	0.0217	243	0.0309	228	0.0045
222	0.0005	224	0.0002	237	0.0218	238	0.0040	217	0.0046
205	0.0016	210	0.0018	209	0.0036	213	0.0000	213	0.0132
198	0.0213	199	0.0121	196	0.0204	201	0.0111	205	0.0334
		195	0.0115			192	0.0145	199	0.0009
		194	0.0002					195	0.0007

Table S4. Computed vertical excitation energies (nm) and oscillator strength of $CH_2FSO•$, $CH_2FOS•$, and $•CHFSOH$ at the TD-B3LYP/6-311++G(3df,3pd) level.

$CH_2FSO•$ gauche		$CH_2FSO•$ cis		$CH_2FOS•$ gauche		$CH_2FOS•$ cis		$•CHFSOH$	
λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength	λ	Oscillator strength
543	0.0005	605	0.0005	1879	0.0000	2062	0.0000	436	0.0037
284	0.0000	253	0.0152	333	0.0000	343	0.0000	324	0.0221
253	0.0319	245	0.0166	295	0.0329	282	0.0015	312	0.0009
234	0.0003	244	0.0053	270	0.0003	269	0.0002	249	0.0107
226	0.0002	219	0.0003	262	0.0022	267	0.0006	241	0.0003
218	0.0014	213	0.0002	229	0.0034	242	0.0413	235	0.0096
209	0.0001	211	0.0025	211	0.0153	208	0.0178	221	0.0021
207	0.0173	208	0.0043	203	0.0005	207	0.0010	207	0.0004
199	0.0067	199	0.0071	202	0.0277	202	0.0019	206	0.0022
198	0.0107			200	0.0201	199	0.0393	203	0.0039
				192	0.0118			195	0.0650
				191	0.0328			192	0.0245

Calculated atomic coordinates (in Angstroms) and energies (in Hartrees) for all optimized structures.

***gauche* $CHF_2SO•$**

C	-0.73146200	0.10010700	0.35256800
H	-0.65875600	0.30990100	1.42055100
F	-1.14675200	1.20791400	-0.29696200
F	-1.61965300	-0.89193300	0.11630700
S	0.91796700	-0.45924300	-0.30051600
O	1.90721400	0.44919000	0.36227400

Zero-point correction= 0.025621
Thermal correction to Energy= 0.030940
Thermal correction to Enthalpy= 0.031884
Thermal correction to Gibbs Free Energy= -0.004888
Sum of electronic and zero-point Energies= -711.881452
Sum of electronic and Thermal Energies= -711.876133
Sum of electronic and Thermal Enthalpies= -711.875189
Sum of electronic and Thermal Free Energies= -711.911962

***cis* $CHF_2SO•$**

C	0.82845200	-0.00041300	-0.39569000
H	1.24354100	-0.00333000	-1.40702700
F	1.25048800	1.09374100	0.27020100
F	1.25390100	-1.09103400	0.27522200
S	-1.03001700	-0.00238100	-0.51574100
O	-1.53418300	0.00244400	0.89052800

Zero-point correction= 0.025640
Thermal correction to Energy= 0.030939
Thermal correction to Enthalpy= 0.031883
Thermal correction to Gibbs Free Energy= -0.004842
Sum of electronic and zero-point Energies= -711.878949
Sum of electronic and Thermal Energies= -711.873649
Sum of electronic and Thermal Enthalpies= -711.872705
Sum of electronic and Thermal Free Energies= -711.909430

***gauche* $CHF_2OS•$**

C	0.77534700	-0.00039200	0.29197100
H	0.54412600	0.02615400	1.35623100
F	1.18561800	1.21437600	-0.11668800
F	1.75310300	-0.87721300	0.03394200
O	-0.32716200	-0.39324900	-0.47697200
S	-1.81421300	0.00548200	0.09077700

Zero-point correction= 0.027148
Thermal correction to Energy= 0.032076
Thermal correction to Enthalpy= 0.033020
Thermal correction to Gibbs Free Energy= -0.003194
Sum of electronic and zero-point Energies= -711.875685
Sum of electronic and Thermal Energies= -711.870757
Sum of electronic and Thermal Enthalpies= -711.869813
Sum of electronic and Thermal Free Energies= -711.906027

***cis* $CHF_2OS•$**

C	-0.94253700	0.00023300	0.38849600
H	-1.59608200	0.00024700	1.25901300
F	-1.18249500	-1.08589700	-0.36889400
F	-1.18048900	1.08696400	-0.36785000
O	0.36719700	-0.00116000	0.86159400
S	1.59878600	-0.00012300	-0.24075300

Zero-point correction= 0.027205
Thermal correction to Energy= 0.032027
Thermal correction to Enthalpy= 0.032971
Thermal correction to Gibbs Free Energy= -0.002460
Sum of electronic and zero-point Energies= -711.874817
Sum of electronic and Thermal Energies= -711.869995
Sum of electronic and Thermal Enthalpies= -711.869051
Sum of electronic and Thermal Free Energies= -711.904482

•CF_2SOH

S	0.85419400	-0.44722100	-0.48745500
O	1.75448100	0.34671600	0.72457700
H	2.02293900	1.20512000	0.37359500
C	-0.76625100	-0.05360000	-0.19572900
F	-1.58704700	-0.80759500	0.51925200
F	-1.20499700	1.19629300	-0.20775700

Zero-point correction= 0.024042
Thermal correction to Energy= 0.029808
Thermal correction to Enthalpy= 0.030752
Thermal correction to Gibbs Free Energy= -0.006522
Sum of electronic and zero-point Energies= -711.847151
Sum of electronic and Thermal Energies= -711.841384
Sum of electronic and Thermal Enthalpies= -711.840440
Sum of electronic and Thermal Free Energies= -711.877715

•CF_2OSH

C	-0.83609900	-0.01857200	0.28163600
F	-1.01919900	1.26048200	-0.05134600
O	0.21903700	-0.61623000	-0.32446000
S	1.73937800	0.05302500	-0.00200900
H	2.00257300	-0.69865500	1.08566500
F	-1.93283600	-0.71697800	0.03494000

Zero-point correction= 0.022781
Thermal correction to Energy= 0.028286
Thermal correction to Enthalpy= 0.029230
Thermal correction to Gibbs Free Energy= -0.007636
Sum of electronic and zero-point Energies= -711.838788
Sum of electronic and Thermal Energies= -711.833283
Sum of electronic and Thermal Enthalpies= -711.832339
Sum of electronic and Thermal Free Energies= -711.869205

•$CF_2S(O)H$

C	0.84114600	-0.03389800	-0.33390400
F	1.48799800	-0.97504300	0.33239500

S	-0.98137000	-0.27404400	-0.39349800
H	-1.00409100	0.69527700	-1.37003700
O	-1.65145000	0.27902400	0.80451300
F	1.27541800	1.15955800	0.02686300

Zero-point correction= 0.022835
Thermal correction to Energy= 0.028244
Thermal correction to Enthalpy= 0.029188
Thermal correction to Gibbs Free Energy= -0.007461
Sum of electronic and zero-point Energies= -711.815945
Sum of electronic and Thermal Energies= -711.810537
Sum of electronic and Thermal Enthalpies= -711.809593
Sum of electronic and Thermal Free Energies= -711.846241

TS1 (from $CHF_2SO\bullet$ to $CHF_2OS\bullet$)

C	-0.70739700	-0.01058200	0.34802400
H	-0.63128700	0.07714000	1.42010700
F	-1.49174500	0.85292500	-0.26398600
F	-1.17011100	-1.21010500	-0.04193600
S	1.41964500	-0.35661200	-0.09876100
O	0.76475500	1.11334500	0.10315400

Zero-point correction= 0.024353
Thermal correction to Energy= 0.029133
Thermal correction to Enthalpy= 0.030078
Thermal correction to Gibbs Free Energy= -0.005244
Sum of electronic and zero-point Energies= -711.774115
Sum of electronic and Thermal Energies= -711.769335
Sum of electronic and Thermal Enthalpies= -711.768391
Sum of electronic and Thermal Free Energies= -711.803712

TS2 (from $CHF_2SO\bullet$ to $\bullet CF_2SOH$)

C	-0.85008700	0.00037500	0.31033500
O	1.50215700	0.00146300	0.96374200
S	1.28132800	-0.00083200	-0.60116400
H	0.41925600	0.00171100	1.21995200
F	-1.54667000	1.05188300	-0.06635500
F	-1.54635500	-1.05214500	-0.06400800

Zero-point correction= 0.020019
Thermal correction to Energy= 0.025346
Thermal correction to Enthalpy= 0.026290
Thermal correction to Gibbs Free Energy= -0.010523
Sum of electronic and zero-point Energies= -711.805938
Sum of electronic and Thermal Energies= -711.800612
Sum of electronic and Thermal Enthalpies= -711.799667
Sum of electronic and Thermal Free Energies= -711.836481

TS3 (from $\bullet CF_2SOH$ to $\bullet CF_2S(O)H$)

S	0.83398200	-0.53854200	-0.25190100
O	1.92814100	0.44848000	0.50370200
H	1.45519800	0.58898800	-0.86817100
C	-0.78293400	-0.00416000	-0.18432100
F	-1.72982600	-0.77207800	0.32542400

F	-1.10644400	1.26816600	-0.10599100

Zero-point correction= 0.018505
Thermal correction to Energy= 0.024067
Thermal correction to Enthalpy= 0.025011
Thermal correction to Gibbs Free Energy= -0.011671
Sum of electronic and zero-point Energies= -711.754397
Sum of electronic and Thermal Energies= -711.748835
Sum of electronic and Thermal Enthalpies= -711.747891
Sum of electronic and Thermal Free Energies= -711.784573

TS4 (from $CHF_2SO\bullet$ to $\bullet CF_2S(O)H$)

C	-0.80022000	-0.03710100	0.23557900
H	0.09819200	-0.10087900	1.48535000
F	-1.12744700	1.23651800	0.08932900
F	-1.69218200	-0.81172300	-0.37544600
S	0.95737000	-0.45574200	0.22728700
O	1.84523400	0.47402600	-0.49504500

Zero-point correction= 0.019106
Thermal correction to Energy= 0.024319
Thermal correction to Enthalpy= 0.025263
Thermal correction to Gibbs Free Energy= -0.010808
Sum of electronic and zero-point Energies= -711.783273
Sum of electronic and Thermal Energies= -711.778061
Sum of electronic and Thermal Enthalpies= -711.777117
Sum of electronic and Thermal Free Energies= -711.813188

TS5 (from $CHF_2OS\bullet$ to $\bullet CF_2OSH$)

C	0.65589700	0.00003500	0.09338700
H	-0.46535200	-0.00000800	1.12597600
F	1.42126200	1.08235900	0.12695300
F	1.42141000	-1.08225000	0.12710800
O	-0.27902500	-0.00018700	-0.87250000
S	-1.67636700	0.00001900	0.18794700

Zero-point correction= 0.020164
Thermal correction to Energy= 0.025013
Thermal correction to Enthalpy= 0.025957
Thermal correction to Gibbs Free Energy= -0.010061
Sum of electronic and zero-point Energies= -711.806787
Sum of electronic and Thermal Energies= -711.801938
Sum of electronic and Thermal Enthalpies= -711.800994
Sum of electronic and Thermal Free Energies= -711.837012

***gauche* $CH_2FSO\bullet$**

C	0.94047200	-0.31253600	0.48141200
H	0.85812000	0.15728700	1.46112300
H	1.35914200	-1.31826400	0.54905600
F	1.75136700	0.45818000	-0.32434500
S	-0.74015800	-0.46110600	-0.21498400
O	-1.47248400	0.78628200	0.18252500

Zero-point correction= 0.033213
Thermal correction to Energy= 0.037879

Thermal correction to Enthalpy= 0.038823
Thermal correction to Gibbs Free Energy= 0.004372
Sum of electronic and zero-point Energies= -612.596950
Sum of electronic and Thermal Energies= -612.592285
Sum of electronic and Thermal Enthalpies= -612.591341
Sum of electronic and Thermal Free Energies= -612.625791

***cis* $CH_2FSO•$**

C	-0.85107200	0.60092300	-0.00008200
H	-0.83407100	1.21563800	0.89930100
H	-0.83424200	1.21545400	-0.89959600
F	-1.96889900	-0.19986600	0.00009000
S	0.63399100	-0.49342200	-0.00004300
O	1.79387100	0.45711500	0.00008400

Zero-point correction= 0.033167
Thermal correction to Energy= 0.037967
Thermal correction to Enthalpy= 0.038911
Thermal correction to Gibbs Free Energy= 0.003905
Sum of electronic and zero-point Energies= -612.596091
Sum of electronic and Thermal Energies= -612.591292
Sum of electronic and Thermal Enthalpies= -612.590347
Sum of electronic and Thermal Free Energies= -612.625354

***gauche* $CH_2FOS•$**

C	-1.05795000	0.45999900	0.31991300
H	-0.85168800	0.31808800	1.38001500
H	-1.67456800	1.33247100	0.11124000
F	-1.70773700	-0.65198900	-0.14511600
O	0.13939900	0.64171600	-0.40236800
S	1.44552400	-0.22977400	0.06964100

Zero-point correction= 0.035081
Thermal correction to Energy= 0.039429
Thermal correction to Enthalpy= 0.040373
Thermal correction to Gibbs Free Energy= 0.006501
Sum of electronic and zero-point Energies= -612.582384
Sum of electronic and Thermal Energies= -612.578037
Sum of electronic and Thermal Enthalpies= -612.577093
Sum of electronic and Thermal Free Energies= -612.610965

***cis* $CH_2FOS•$**

C	-0.94329400	0.48139100	-0.00080400
H	-0.87210000	1.08399000	0.90446400
H	-0.87438200	1.08245200	-0.90729200
F	-2.12082700	-0.19408300	0.00113600
O	0.08217500	-0.51004700	-0.00136600
S	1.61476800	0.04827100	0.00052200

Zero-point correction= 0.034736
Thermal correction to Energy= 0.039328
Thermal correction to Enthalpy= 0.040272
Thermal correction to Gibbs Free Energy= 0.005487
Sum of electronic and zero-point Energies= -612.580904

Sum of electronic and Thermal Energies= -612.576313
Sum of electronic and Thermal Enthalpies= -612.575369
Sum of electronic and Thermal Free Energies= -612.610153

•CHFSOH

C	-0.96017600	-0.41151300	0.30095200
H	-1.50868100	-1.13075200	0.89133400
F	-1.70860300	0.59773400	-0.17105000
S	0.62930100	-0.61771900	-0.16907200
O	1.39563000	0.83744900	0.25871200
H	1.41330800	1.40413300	-0.52214000

Zero-point correction= 0.031167
Thermal correction to Energy= 0.036283
Thermal correction to Enthalpy= 0.037227
Thermal correction to Gibbs Free Energy= 0.002458
Sum of electronic and zero-point Energies= -612.567627
Sum of electronic and Thermal Energies= -612.562511
Sum of electronic and Thermal Enthalpies= -612.561567
Sum of electronic and Thermal Free Energies= -612.596336

•CHFOSH

C	1.13107200	0.47836900	0.29271100
H	1.83921800	1.30019800	0.26033400
F	1.67026000	-0.70503700	-0.05043100
O	-0.03529000	0.76821600	-0.31620800
S	-1.34814700	-0.27220200	-0.00694700
H	-1.80531500	0.38442200	1.07809700

Zero-point correction= 0.029783
Thermal correction to Energy= 0.034785
Thermal correction to Enthalpy= 0.035729
Thermal correction to Gibbs Free Energy= 0.000821
Sum of electronic and zero-point Energies= -612.550430
Sum of electronic and Thermal Energies= -612.545428
Sum of electronic and Thermal Enthalpies= -612.544484
Sum of electronic and Thermal Free Energies= -612.579392

•CHFS(O)H

C	-0.94384500	-0.21474800	0.50596200
H	-1.07122100	0.01759200	1.55867600
F	-1.88124300	0.30277600	-0.28284000
S	0.66270100	-0.38838600	-0.23696600
H	0.92803100	-1.40500800	0.65277000
O	1.51677900	0.77063800	0.13622500

Zero-point correction= 0.029762
Thermal correction to Energy= 0.034606
Thermal correction to Enthalpy= 0.035550
Thermal correction to Gibbs Free Energy= 0.000970
Sum of electronic and zero-point Energies= -612.531549
Sum of electronic and Thermal Energies= -612.526705
Sum of electronic and Thermal Enthalpies= -612.525761
Sum of electronic and Thermal Free Energies= -612.560342

TS1 (from $CH_2FSO•$ to $CH_2FOS•$)

C	-0.83373900	-0.59984300	0.18809400
H	-0.75023400	-0.74031600	1.25339100
F	-1.88126600	0.14114800	-0.17087100
S	1.32201100	-0.22094600	-0.07725400
O	0.29095600	1.00791700	0.10745200
H	-0.79577000	-1.45915900	-0.46766800

Zero-point correction= 0.031833
Thermal correction to Energy= 0.036177
Thermal correction to Enthalpy= 0.037121
Thermal correction to Gibbs Free Energy= 0.003511
Sum of electronic and zero-point Energies= -612.486047
Sum of electronic and Thermal Energies= -612.481703
Sum of electronic and Thermal Enthalpies= -612.480759
Sum of electronic and Thermal Free Energies= -612.514369

TS2 (from $CH_2FSO•$ to •CHFSOH)

C	0.75848200	0.37996700	0.32268300
O	-1.48166700	0.72883500	-0.17901200
S	-0.66095800	-0.62901800	0.03525900
H	-0.38199200	1.25879000	-0.10399200
H	0.91499600	0.59347700	1.38225600
F	1.92719600	0.01128200	-0.26071200

Zero-point correction= 0.027113
Thermal correction to Energy= 0.031394
Thermal correction to Enthalpy= 0.032338
Thermal correction to Gibbs Free Energy= -0.000899
Sum of electronic and zero-point Energies= -612.515982
Sum of electronic and Thermal Energies= -612.511701
Sum of electronic and Thermal Enthalpies= -612.510757
Sum of electronic and Thermal Free Energies= -612.543994

TS3 (from •CHFSOH to •CHFS(O)H)

S	-0.66126000	-0.54579900	0.05647500
O	-1.36130100	0.89830700	-0.18985600
H	-1.13944800	0.33758200	1.14187000
C	0.97002700	-0.48169600	-0.14957100
F	1.69661300	0.60810900	0.08684800
H	1.52032700	-1.37406500	-0.41082800

Zero-point correction= 0.025509
Thermal correction to Energy= 0.030219
Thermal correction to Enthalpy= 0.031163
Thermal correction to Gibbs Free Energy= -0.002856
Sum of electronic and zero-point Energies= -612.481114
Sum of electronic and Thermal Energies= -612.476404
Sum of electronic and Thermal Enthalpies= -612.475460
Sum of electronic and Thermal Free Energies= -612.509479

TS4 (from $CH_2FSO•$ to •CHFS(O)H)

C	-0.90543700	0.19067100	0.45749200

H	-0.02999300	-0.79491900	1.27066900
F	-1.97648300	0.08958200	-0.34509500
S	0.66268700	-0.44458600	-0.04863500
O	1.69561900	0.61159700	-0.15406900
H	-0.91698800	1.06525200	1.10094800

Zero-point correction= 0.026788
Thermal correction to Energy= 0.031292
Thermal correction to Enthalpy= 0.032236
Thermal correction to Gibbs Free Energy= -0.001424
Sum of electronic and zero-point Energies= -612.505096
Sum of electronic and Thermal Energies= -612.500592
Sum of electronic and Thermal Enthalpies= -612.499648
Sum of electronic and Thermal Free Energies= -612.533308

TS5 (from $CH_2FOS\bullet$ to $\bullet CHFOSH$)

C	0.83406100	-0.13370100	0.41595800
H	-0.26614100	-1.14607400	0.15829900
F	1.94784400	-0.18801200	-0.31550800
O	-0.02812200	0.83137400	0.00618600
S	-1.44292100	-0.17566700	-0.08425500
H	1.04289900	-0.19993400	1.48411400

Zero-point correction= 0.027736
Thermal correction to Energy= 0.031997
Thermal correction to Enthalpy= 0.032941
Thermal correction to Gibbs Free Energy= -0.000471
Sum of electronic and zero-point Energies= -612.518019
Sum of electronic and Thermal Energies= -612.513759
Sum of electronic and Thermal Enthalpies= -612.512815
Sum of electronic and Thermal Free Energies= -612.546226