

## Supporting Information

A DFT Study on Chemical Degradation of Perfluorobis(sulfonyl)imide Sulfonic Acid

Ionomer Membrane

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Table S1. Calculated ionization energies and electron affinities of small molecules.

Molecule	Total energy + zero point vibrational energy (Hartree)	Ionization potential and Electron affinity (eV)	
		Calculated	Experimental <sup>a</sup>
H <sup>b</sup>	-0.501986		
H <sup>+</sup>	0	13.66	13.6
H <sup>-b</sup>	-0.531708	0.809	0.755
H <sub>2</sub>	-1.161764		
H <sub>2</sub> <sup>+</sup>	-0.594117	15.45	15.43
NH <sub>3</sub>	-56.50166		
NH <sub>3</sub> <sup>+</sup>	-56.132554	10.04	10.07
OH	-75.697844		
OH <sup>+</sup>	-75.21859	13.04	13.017
OH <sup>-</sup>	-75.758202	1.642	1.827
H <sub>2</sub> O	-76.376545		
H <sub>2</sub> O <sup>+</sup>	-75.917136	12.50	12.621
F	-99.702233		
F <sup>+</sup>	-99.055524	17.60	17.423
F <sup>-</sup>	-99.827298	3.40	3.401
HF	-100.406974		
HF <sup>+</sup>	-99.819541	15.98	16.03
N <sub>2</sub> H <sub>4</sub>	-111.777024		
N <sub>2</sub> H <sub>4</sub> <sup>+</sup>	-111.489261	7.83	8.1
NH <sub>2</sub> OH	-131.634353		
NH <sub>2</sub> OH <sup>+</sup>	-131.300307	9.09	9.6
O <sub>2</sub>	-150.273361		
O <sub>2</sub> <sup>+</sup>	-149.809326	12.63	12.07
O <sub>2</sub> <sup>-</sup>	-150.290434	0.46	0.45
HO <sub>2</sub>	-150.844703		
HO <sub>2</sub> <sup>+</sup>	-150.40341	12.01	11.355
HO <sub>2</sub> <sup>-</sup>	-150.876628	0.87	1.078
H <sub>2</sub> O <sub>2</sub>	-151.470639		

H <sub>2</sub> O <sub>2</sub> <sup>+</sup>	-151.085598	10.48	10.58
CO <sub>2</sub>	-188.515148		
CO <sub>2</sub> <sup>+</sup>	-188.008256	13.79	13.777
F <sub>2</sub>	-199.456377		
F <sub>2</sub> <sup>+</sup>	-198.877508	15.75	15.697
F <sub>2</sub> <sup>-</sup>	-199.589278	3.62	3.005
CF <sub>2</sub>	-237.634738		
CF <sub>2</sub> <sup>+</sup>	-237.215035	11.42	11.44
CF <sub>2</sub> <sup>-</sup>	-237.649603	0.40	0.18
CF <sub>2</sub> O	-312.923512		
CF <sub>2</sub> O <sup>+</sup>	-312.447571	12.95	13.04
CF <sub>3</sub> CO <sub>2</sub>	-525.954062		
CF <sub>3</sub> CO <sub>2</sub> <sup>-</sup>	-526.118837	4.48	4.46
SO <sub>2</sub>	-548.521909		
SO <sub>2</sub> <sup>+</sup>	-548.067481	12.37	12.349
SO <sub>2</sub> <sup>-</sup>	-548.578892	1.55	1.107
SO <sub>3</sub>	-623.669469		
SO <sub>3</sub> <sup>+</sup>	-623.19608	12.88	12.8
SO <sub>3</sub> <sup>-</sup>	-623.765012	2.60	1.9
SO <sub>4</sub>	-698.74208		
SO <sub>4</sub> <sup>+</sup>	-698.93217	5.17	5.1
HSO <sub>4</sub>	-699.409448		
HSO <sub>4</sub> <sup>-</sup>	-699.586568	4.82	4.75
H <sub>2</sub> SO <sub>4</sub>	-700.075434		
H <sub>2</sub> SO <sub>4</sub> <sup>+</sup>	-699.647565	11.64	12.4
CF <sub>3</sub> SO <sub>3</sub>	-961.153112		
CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup>	-961.153112	5.28	5.3

<sup>a</sup> NIST webbook.

<sup>b</sup> 6-31++G\*\* basis set.

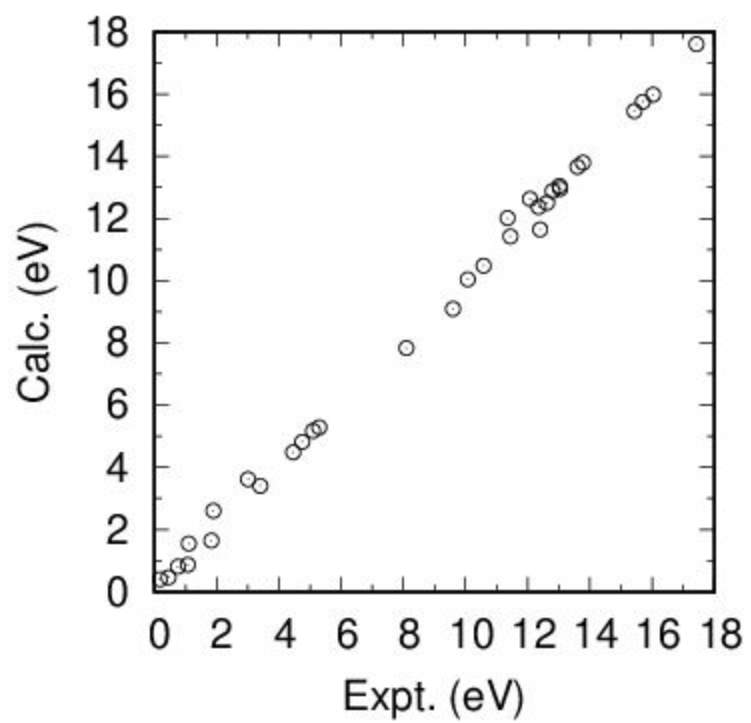


Figure S1 Experimental vs. calculated ionization potentials and electron affinities.

Table S2 Barriers and reaction energies of fluoromethanes and hydrogen.

Molecule	Total energy (Hartree)	Energy difference (kJ mol <sup>-1</sup> )	
		DFT	G2(MP2)
CF <sub>4</sub>	-437.3887625		
CF <sub>4</sub> + H	-437.8893701		
CF <sub>4</sub> H (TS)	-437.8222743	176.0	190.3 <sup>a</sup>
CF <sub>3</sub>	-337.4832935		
CF <sub>3</sub> +HF	-437.8994418	-26.4	
CHF <sub>3</sub>	-338.1617102		
CHF <sub>3</sub> + H	-338.6623178		
CHF <sub>3</sub> H (TS)	-338.598276	168.0	177.1 <sup>a</sup> , 177.2 <sup>b</sup>
CHF <sub>2</sub>	-238.2582189		
CHF <sub>2</sub> + HF	-338.6743672	-31.6	-36.9 <sup>b</sup>
CH <sub>2</sub> F <sub>2</sub>	-238.9297213		
CH <sub>2</sub> F <sub>2</sub> + H	-239.4303289		
CH <sub>2</sub> F <sub>2</sub> H (TS)	-239.3728599	150.7	154.2 <sup>a</sup>
CH <sub>2</sub> F	-139.0343603		
CH <sub>2</sub> F + HF	-239.4505086	-52.9	
CH <sub>3</sub> F	-139.7070167		
CH <sub>3</sub> F + H	-140.2076243		
CH <sub>3</sub> FH (TS)	-140.1582387	129,5	128.5 <sup>a</sup>
CH <sub>3</sub>	-39.8232843		
CH <sub>3</sub> + HF	-140.2394326	-83.4	

a Ref.S1

b Ref.S2

Table S3 Barriers and reaction energies of formamide and hydrogen.

	Total energy	Energy difference (kJ mol <sup>-1</sup> )
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	(Hartree)	DFT	G2(MP2) <sup>a</sup>
NH <sub>2</sub> CHO	- 169.8444218		
NH <sub>2</sub> CHO + H	- 170.3450294		
NH <sub>2</sub> CHOH (TS)	- 170.3243596	54.2	51
<i>syn</i> -NH <sub>2</sub> CHOH	- 170.3682035	-60.8	-47
NH <sub>2</sub> CH <sub>2</sub> O (TS)	- 170.3278421	45.1	49
NH <sub>2</sub> CH <sub>2</sub> O	- 170.3682035	-29.5	2
HNH <sub>2</sub> CHO (TS)	- 170.3175371	72.1	80
NH <sub>3</sub> + HCO	-170.352042	-18.4	-37

a Ref.S3.

Table S4 Cartesian coordinates of optimized geometries (Å) and total energies (Hartree)

PFIS<sup>2-</sup> ((CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NSO<sub>2</sub>C<sub>3</sub>F<sub>6</sub>SO<sub>3</sub><sup>2-</sup>)

Optimized geometry

Total energy -4327.9418656

No.	Atom.No.	x	y	z
1	6	-6.859453	0.290258	0.070411
2	6	-7.552302	0.104722	-1.314885
3	6	-7.284987	1.58504	0.829532
4	9	-7.236494	-0.759029	0.841812
5	9	-7.131557	-1.028567	-1.870446
6	9	-7.265054	1.117594	-2.132076
7	9	-8.882213	0.036418	-1.175135
8	9	-6.661965	1.631233	2.003685
9	9	-6.969449	2.674371	0.130219
10	9	-8.605605	1.591564	1.052299
11	8	-5.49903	0.367001	-0.150665
12	6	-4.600691	-0.549218	0.367507
13	9	-4.889323	-1.784551	-0.066519
14	9	-4.652359	-0.561176	1.708294
15	6	-3.193433	-0.090625	-0.136927
16	9	-3.093344	1.226029	0.11824
17	9	-3.190571	-0.2777	-1.472064
18	6	-1.992098	-0.844124	0.528519
19	9	-2.325377	-2.150801	0.59842
20	9	-1.881763	-0.362833	1.779749
21	6	-0.647542	-0.689961	-0.246298
22	9	-0.558918	0.586042	-0.678279
23	9	-0.720923	-1.493714	-1.327705
24	16	0.891526	-1.120069	0.762076
25	8	1.011551	-0.018232	1.705723
26	8	0.554843	-2.445572	1.274068
27	7	1.994697	-1.265068	-0.362629
28	16	2.953977	-0.081203	-0.919682
29	8	2.533236	1.267859	-0.572144
30	8	3.274393	-0.396065	-2.304389
31	6	4.535827	-0.428441	0.052229
32	9	4.285763	-0.090446	1.331749
33	9	4.762876	-1.752949	-0.000137
34	6	5.808699	0.324123	-0.467015
35	9	6.221494	-0.306663	-1.581817
36	9	5.452049	1.583874	-0.789447
37	6	6.979577	0.385129	0.566495
38	9	6.645423	1.306338	1.501476
39	9	7.053864	-0.819331	1.192076
40	16	8.696934	0.806619	-0.100734
41	8	9.091071	-0.397509	-0.845525
42	8	8.460912	2.007433	-0.916209
43	8	9.44647	1.034734	1.146002

PFIHS<sup>-</sup> ((CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NHSO<sub>2</sub>C<sub>3</sub>F<sub>6</sub>SO<sub>3</sub><sup>-</sup>)

Optimized geometry

Total energy

-4328.4990951

No.	Atom.No.	x	y	z
1	6	6.867511	0.323784	-0.028307
2	6	7.555423	-0.086736	1.309922
3	6	7.274217	1.732163	-0.561571
4	9	7.235999	-0.580783	-0.963334
5	9	7.147338	-1.30728	1.652261
6	9	7.237005	0.762412	2.285294
7	9	8.882339	-0.10521	1.169992
8	9	6.628304	1.96752	-1.70158
9	9	6.956513	2.680316	0.317998
10	9	8.586765	1.784198	-0.796844
11	8	5.496613	0.351877	0.202057
12	6	4.617421	-0.472466	-0.451773
13	9	4.895508	-1.76443	-0.224538
14	9	4.642269	-0.27324	-1.779749
15	6	3.206481	-0.114704	0.117004
16	9	3.0669	1.218994	0.073473
17	9	3.17504	-0.520729	1.401436
18	6	2.016128	-0.768173	-0.658458
19	9	2.318028	-2.05194	-0.919715
20	9	1.860362	-0.109995	-1.820622
21	6	0.670218	-0.725679	0.130797
22	9	0.526394	0.45762	0.732493
23	9	0.67308	-1.697178	1.056847
24	16	-0.824736	-1.006704	-0.979285
25	8	-1.103723	0.233375	-1.64896
26	8	-0.572297	-2.260642	-1.655219
27	7	-1.990866	-1.331105	0.155964
28	16	-3.041706	-0.272615	0.999307
29	8	-2.443829	1.035408	0.982961
30	8	-3.36704	-1.004542	2.200302
31	6	-4.533036	-0.334928	-0.168016
32	9	-4.176452	0.356239	-1.249181
33	9	-4.676232	-1.626205	-0.494566
34	6	-5.826012	0.227107	0.507272
35	9	-6.24817	-0.714207	1.363457
36	9	-5.442268	1.316324	1.206036
37	6	-6.940483	0.601927	-0.513297
38	9	-6.555846	1.755564	-1.106193
39	9	-6.939234	-0.366404	-1.470515
40	16	-8.676288	0.788581	0.203638
41	8	-9.048975	-0.59661	0.509025
42	8	-8.4292	1.654953	1.36322
43	8	-9.387955	1.406136	-0.919347
44	1	-2.118983	-2.318148	0.363886



PFISH<sup>-</sup> ((CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NSO<sub>2</sub>C<sub>3</sub>F<sub>6</sub>SO<sub>3</sub>H<sup>-</sup>)

Optimized geometry

Total energy -4328.4975964

No.	Atom.No.	x	y	z
1	6	6.865974	0.337197	-0.016707
2	6	7.586541	-0.306533	1.207877
3	6	7.264088	1.82056	-0.290434
4	9	7.225946	-0.376826	-1.109617
5	9	7.198604	-1.573953	1.328422
6	9	7.286954	0.343671	2.331662
7	9	8.912911	-0.284018	1.041799
8	9	6.594444	2.264812	-1.351061
9	9	6.973905	2.591962	0.756639
10	9	8.572879	1.91931	-0.544274
11	8	5.506059	0.315114	0.242284
12	6	4.60757	-0.380432	-0.538587
13	9	4.906857	-1.687108	-0.561139
14	9	4.617882	0.066625	-1.804424
15	6	3.208703	-0.144973	0.118043
16	9	3.082063	1.175899	0.33297
17	9	3.226366	-0.78135	1.306045
18	6	2.000734	-0.643431	-0.744589
19	9	2.33292	-1.83883	-1.271711
20	9	1.838523	0.239727	-1.745902
21	6	0.675761	-0.792728	0.064467
22	9	0.565133	0.252575	0.907189
23	9	0.768024	-1.919409	0.794473
24	16	-0.871883	-0.874283	-1.007244
25	8	-1.064566	0.48118	-1.497302
26	8	-0.569159	-1.939893	-1.951211
27	7	-1.953313	-1.419022	0.039953
28	16	-2.917494	-0.506457	0.932427
29	8	-2.505195	0.871791	1.141336
30	8	-3.382468	-1.295132	2.06332
31	6	-4.444207	-0.394534	-0.165269
32	9	-4.180868	0.430225	-1.199823
33	9	-4.730267	-1.613424	-0.658383
34	6	-5.720106	0.130282	0.561631
35	9	-6.255846	-0.855908	1.304959
36	9	-5.418161	1.164503	1.361333
37	6	-6.824935	0.625653	-0.424602
38	9	-6.532336	1.842111	-0.887261
39	9	-6.96748	-0.217854	-1.463
40	16	-8.532977	0.734127	0.356024
41	8	-9.06398	-0.601186	0.510892
42	8	-8.503511	1.707987	1.413335
43	8	-9.297017	1.429821	-0.890817
44	1	-9.617266	0.73045	-1.484732

PFIHSH ((CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NHSO<sub>2</sub>C<sub>3</sub>F<sub>6</sub>SO<sub>3</sub>H)

Optimized geometry

Total energy

-4328.9726676

No.	Atom.No.	x	y	z
1	6	-6.891254	0.353	0.014548
2	6	-7.587996	-0.185759	-1.272635
3	6	-7.279991	1.812458	0.404266
4	9	-7.25509	-0.449428	1.038245
5	9	-7.181789	-1.43495	-1.494247
6	9	-7.270793	0.562787	-2.327599
7	9	-8.911769	-0.186663	-1.122844
8	9	-6.632688	2.14797	1.51902
9	9	-6.942287	2.66384	-0.562365
10	9	-8.590555	1.904579	0.625841
11	8	-5.51732	0.345821	-0.224679
12	6	-4.644193	-0.413941	0.501801
13	9	-4.925863	-1.721711	0.411053
14	9	-4.647162	-0.081321	1.803786
15	6	-3.234452	-0.129105	-0.109091
16	9	-3.072454	1.199298	-0.199118
17	9	-3.206037	-0.663053	-1.345743
18	6	-2.044748	-0.715366	0.719098
19	9	-2.344544	-1.963259	1.112267
20	9	-1.854491	0.054791	1.805036
21	6	-0.70724	-0.767137	-0.084803
22	9	-0.536256	0.348255	-0.794226
23	9	-0.711469	-1.824673	-0.906477
24	16	0.78886	-0.957298	1.047109
25	8	1.129885	0.334572	1.574194
26	8	0.55605	-2.137892	1.843711
27	7	1.953704	-1.4165	-0.078629
28	16	2.994965	-0.465792	-0.997226
29	8	2.425103	0.842877	-1.153592
30	8	3.417626	-1.31911	-2.081054
31	6	4.459314	-0.337187	0.182499
32	9	4.12546	0.511478	1.15637
33	9	4.658806	-1.555935	0.700384
34	6	5.754036	0.147704	-0.541121
35	9	6.264908	-0.879268	-1.236633
36	9	5.425221	1.138115	-1.384757
37	6	6.840768	0.677184	0.444266
38	9	6.51284	1.900195	0.862563
39	9	6.935667	-0.145335	1.504239
40	16	8.548008	0.763895	-0.329296
41	8	9.079405	-0.576478	-0.389792
42	8	8.459756	1.650234	-1.455177
43	8	9.286711	1.557539	0.857197
44	1	2.043669	-2.419842	-0.223565
45	1	9.731015	0.919431	1.441978

PFIHS<sup>-</sup> + H

Transition state of reaction (6)

Total energy

-4328.9496885

No.	Atom.No.	x	y	z
1	6	6.818339	0.395965	0.043543
2	6	7.544747	-0.020011	1.331568
3	6	7.271554	1.695035	-0.640425
4	9	7.263581	-0.760433	-1.025758
5	9	7.110791	-1.214775	1.730472
6	9	7.295306	0.86215	2.309069
7	9	8.863775	-0.080411	1.147882
8	9	6.601697	1.863065	-1.779107
9	9	7.02116	2.746461	0.151822
10	9	8.577462	1.673432	-0.907766
11	8	5.468416	0.403474	0.236891
12	6	4.593562	-0.457339	-0.388902
13	9	4.873079	-1.732304	-0.095353
14	9	4.63183	-0.318273	-1.721143
15	6	3.178998	-0.072712	0.15195
16	9	3.038979	1.256904	0.041371
17	9	3.138862	-0.414926	1.454389
18	6	1.99553	-0.765857	-0.599266
19	9	2.30267	-2.060035	-0.795764
20	9	1.847071	-0.165325	-1.793138
21	6	0.644137	-0.688639	0.1776
22	9	0.493542	0.522334	0.719482
23	9	0.6432	-1.613695	1.150037
24	16	-0.841987	-1.028134	-0.928297
25	8	-1.123194	0.179028	-1.654672
26	8	-0.577187	-2.309345	-1.54612
27	7	-2.014081	-1.30934	0.211971
28	16	-3.071807	-0.219764	1.006052
29	8	-2.480927	1.089342	0.930689
30	8	-3.394533	-0.898065	2.238784
31	6	-4.560993	-0.343536	-0.159084
32	9	-4.206889	0.300725	-1.269637
33	9	-4.696216	-1.648877	-0.427831
34	6	-5.858066	0.240245	0.48946
35	9	-6.276417	-0.665627	1.384846
36	9	-5.481244	1.360636	1.141086
37	6	-6.972913	0.56476	-0.547733
38	9	-6.59456	1.695118	-1.187597
39	9	-6.963536	-0.442669	-1.463709
40	16	-8.711071	0.769786	0.15848
41	8	-9.077025	-0.604628	0.516329
42	8	-8.470586	1.681405	1.284267
43	8	-9.423952	1.339845	-0.988586
44	1	-2.136235	-2.286739	0.464302
45	1	7.577879	-1.705292	-1.89369

PFIHS<sup>-</sup> + H

Transition state of reaction (10)

Total energy

-4328.9644134

No.	Atom.No.	x	y	z
1	6	6.641635	0.546948	0.035903
2	6	7.154401	0.900469	1.46591
3	6	7.08655	1.545206	-1.077077
4	9	7.151122	-0.664004	-0.285142
5	9	6.725705	-0.023958	2.323269
6	9	6.697205	2.090208	1.851718
7	9	8.488599	0.920937	1.494799
8	9	6.599669	1.136327	-2.246815
9	9	6.629804	2.77011	-0.824234
10	9	8.417853	1.5902	-1.162255
11	8	5.252453	0.568603	0.076301
12	6	4.484267	-0.539299	-0.175525
13	9	4.756803	-1.530031	0.686281
14	9	4.68227	-1.009044	-1.418349
15	6	3.002941	-0.069404	-0.009831
16	9	2.845277	1.060686	-0.715573
17	9	2.809206	0.195548	1.296935
18	6	1.93964	-1.114095	-0.487099
19	9	2.310342	-2.332446	-0.057654
20	9	1.919499	-1.101114	-1.832171
21	6	0.502176	-0.809045	0.033511
22	9	0.245913	0.486709	-0.094479
23	9	0.40359	-1.179714	1.322376
24	16	-0.838654	-1.810449	-0.917159
25	8	-1.353478	-0.966192	-1.96632
26	8	-0.230752	-3.108065	-1.158423
27	7	-2.253932	-2.310975	0.148834
28	16	-3.091004	-1.035645	1.072324
29	8	-2.319984	0.173586	0.908912
30	8	-3.360547	-1.637561	2.358367
31	6	-4.698005	-0.901962	0.049754
32	9	-4.34614	-1.046499	-1.223879
33	9	-5.460738	-1.925287	0.430763
34	6	-5.391049	0.475518	0.318945
35	9	-5.254938	0.7027	1.644444
36	9	-4.698669	1.396291	-0.360761
37	6	-6.896163	0.489799	-0.07972
38	9	-6.995578	-0.186004	-1.257107
39	9	-7.55665	-0.230815	0.856444
40	16	-7.680297	2.199005	-0.247216
41	8	-7.247741	2.845833	0.998069
42	8	-7.07463	2.713185	-1.479003
43	8	-9.102694	1.854747	-0.331361
44	1	-1.820678	-2.916679	0.855912
45	1	-3.433198	-3.3382	0.016616

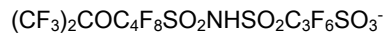
PFHS<sup>-</sup> + H

Transition state of reaction (11)

Total energy

-4328.9600598

No.	Atom.No.	x	y	z
1	6	-6.640106	-0.651967	0.033218
2	6	-6.940645	-1.934148	0.869033
3	6	-7.251242	-0.654192	-1.401967
4	9	-7.179321	0.395839	0.696388
5	9	-6.381272	-1.810429	2.071011
6	9	-6.443198	-3.015157	0.271493
7	9	-8.256109	-2.094362	1.026003
8	9	-6.937659	0.488868	-2.008798
9	9	-6.771537	-1.66835	-2.119078
10	9	-8.580706	-0.755614	-1.34592
11	8	-5.259256	-0.564401	-0.106611
12	6	-4.529537	0.488052	0.381545
13	9	-4.664178	0.604678	1.710364
14	9	-4.902658	1.653156	-0.174066
15	6	-3.043211	0.173554	0.015294
16	9	-2.995851	-0.161456	-1.282994
17	9	-2.657697	-0.880458	0.759364
18	6	-2.057733	1.363471	0.261637
19	9	-2.352152	1.936168	1.440123
20	9	-2.229582	2.263464	-0.722732
21	6	-0.560731	0.920634	0.281118
22	9	-0.336946	0.024192	-0.681465
23	9	-0.272392	0.382323	1.476399
24	16	0.611073	2.386664	0.030279
25	8	0.725805	2.638847	-1.381065
26	8	0.151454	3.371941	0.986713
27	7	2.141878	1.798114	0.568439
28	16	2.759062	0.085795	-0.291796
29	8	2.535085	0.161591	-1.717414
30	8	2.364229	-1.043748	0.533632
31	6	4.568971	0.536617	0.107708
32	9	4.861454	1.571594	-0.673389
33	9	4.562165	0.925629	1.388426
34	6	5.526341	-0.679023	-0.11318
35	9	5.316584	-1.516335	0.912328
36	9	5.124874	-1.273827	-1.255408
37	6	7.025089	-0.267442	-0.212099
38	9	7.196398	0.290424	-1.432552
39	9	7.226377	0.711312	0.712733
40	16	8.271334	-1.661056	0.048112
41	8	8.161053	-1.924579	1.486335
42	8	7.73906	-2.704958	-0.836535
43	8	9.51534	-1.020682	-0.388621
44	1	2.036211	1.505068	1.548547
45	1	2.72246	3.195353	1.027462



Optimized geometry of product of reaction (6)

Total energy

-4228.6238322

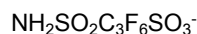
No.	Atom.No.	x	y	z
1	6	6.971844	0.190868	-0.469521
2	6	7.679655	1.488059	-0.179189
3	6	7.708169	-1.062006	-0.879411
4	9	6.877736	2.31189	0.498218
5	9	8.056129	2.119234	-1.306875
6	9	8.782653	1.268618	0.551094
7	9	7.047629	-1.702947	-1.847493
8	9	8.934573	-0.762639	-1.32955
9	9	7.852032	-1.911155	0.153237
10	8	5.639911	0.278169	-0.668065
11	6	4.770003	-0.34617	0.205398
12	9	5.103212	-0.064698	1.472038
13	9	4.81619	-1.679049	0.059115
14	6	3.346444	0.193058	-0.132261
15	9	3.176631	0.101438	-1.459923
16	9	3.31244	1.489417	0.230571
17	6	2.185669	-0.573173	0.581716
18	9	2.53319	-0.782708	1.863899
19	9	2.028438	-1.760263	-0.029175
20	6	0.828451	0.196294	0.552567
21	9	0.641373	0.751075	-0.647712
22	9	0.849354	1.158375	1.488095
23	16	-0.641686	-0.920943	0.921574
24	8	-0.946753	-1.642811	-0.282412
25	8	-0.340756	-1.543426	2.192415
26	7	-1.812445	0.21113	1.236375
27	16	-2.904029	1.001205	0.176605
28	8	-2.351434	0.924519	-1.148997
29	8	-3.209484	2.234452	0.861688
30	6	-4.385517	-0.167795	0.348069
31	9	-4.04764	-1.279282	-0.303256
32	9	-4.480537	-0.432841	1.657688
33	6	-5.701202	0.47536	-0.19849
34	9	-6.093743	1.3735	0.716103
35	9	-5.360206	1.123176	-1.33247
36	6	-6.822599	-0.566108	-0.48451
37	9	-6.477639	-1.208955	-1.623822
38	9	-6.778933	-1.478474	0.525316
39	16	-8.56782	0.135506	-0.637601
40	8	-8.891899	0.495928	0.746576
41	8	-8.357451	1.259462	-1.558878
42	8	-9.295523	-1.014292	-1.182743
43	1	-1.910646	0.460039	2.217373



Optimized geometry of product of reaction (10)

Total energy -2387.6258635

No.	Atom.No.	x	y	z
1	6	2.871335	0.06133	-0.282891
2	6	3.625637	-1.223426	0.178556
3	6	3.488264	1.399343	0.228949
4	9	2.907397	0.089675	-1.632626
5	9	3.014701	-2.29109	-0.332557
6	9	3.620251	-1.320458	1.507003
7	9	4.886814	-1.20553	-0.250342
8	9	2.759121	2.414576	-0.231169
9	9	3.488738	1.438492	1.560264
10	9	4.73859	1.536484	-0.209984
11	8	1.575738	-0.012702	0.228211
12	6	0.468962	-0.073181	-0.571401
13	9	0.489579	-1.148819	-1.37127
14	9	0.347121	1.016165	-1.348263
15	6	-0.747846	-0.159552	0.405037
16	9	-0.624007	0.80938	1.324763
17	9	-0.700515	-1.358106	1.018764
18	6	-2.142227	-0.004201	-0.287224
19	9	-2.168092	-0.732938	-1.412853
20	9	-2.327189	1.290764	-0.593635
21	6	-3.326435	-0.469883	0.614766
22	9	-3.1892	-0.025979	1.862415
23	9	-3.425532	-1.798139	0.610616
24	16	-5.038028	0.199591	-0.009231
25	8	-5.115596	1.593661	0.436585
26	8	-5.107353	-0.181751	-1.424445

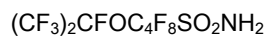


Optimized geometry of product of reaction (10)

Total energy -1941.4532715

No.	Atom.No.	x	y	z
1	7	3.964146	0.658825	-0.450353
2	16	2.833447	-0.41855	0.121695
3	8	3.040616	-0.509561	1.550121
4	8	2.851301	-1.559923	-0.766623
5	6	1.22752	0.520529	-0.182071
6	9	1.27725	1.585662	0.640049
7	9	1.30494	0.966747	-1.45188
8	6	-0.074586	-0.313387	0.027667
9	9	-0.182786	-1.124359	-1.036358
10	9	0.116956	-1.062733	1.131872
11	6	-1.352952	0.562843	0.194521
12	9	-1.314477	1.078761	1.445957
13	9	-1.24084	1.605608	-0.674694
14	16	-3.001223	-0.310855	-0.085702
15	8	-3.016167	-0.520557	-1.537674
16	8	-2.850788	-1.519967	0.733928
17	8	-3.947964	0.690198	0.418683
18	1	3.86889	0.838021	-1.44498

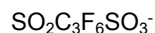
19 1 4.001234 1.512087 0.098861



Optimized geometry of product of reaction (11)

Total energy -2443.5980269

No.	Atom.No.	x	y	z
1	6	3.113449	0.045825	-0.250299
2	6	3.837948	-1.268121	0.175322
3	6	3.738381	1.351454	0.330938
4	9	3.18582	0.128853	-1.596854
5	9	3.223803	-2.305017	-0.392042
6	9	3.801637	-1.418924	1.498415
7	9	5.109337	-1.253504	-0.22423
8	9	3.036856	2.397001	-0.103146
9	9	3.708105	1.335972	1.662583
10	9	5.001505	1.486965	-0.072105
11	8	1.806401	-0.029831	0.225603
12	6	0.716588	-0.029941	-0.602338
13	9	0.739375	-1.068737	-1.449761
14	9	0.640301	1.095604	-1.331713
15	6	-0.525024	-0.134761	0.340673
16	9	-0.395789	0.786829	1.308246
17	9	-0.511325	-1.361958	0.897238
18	6	-1.897674	0.087177	-0.375017
19	9	-1.898489	-0.576175	-1.54351
20	9	-2.039813	1.402071	-0.617755
21	6	-3.118348	-0.402896	0.464439
22	9	-2.96241	-0.06162	1.75225
23	9	-3.212269	-1.736624	0.369958
24	16	-4.750293	0.321524	-0.114873
25	8	-4.811719	1.679988	0.376636
26	8	-4.867371	-0.041181	-1.511202
27	7	-5.77555	-0.601265	0.784702
28	1	-6.290844	-1.291558	0.250432
29	1	-6.325819	-0.064849	1.445855



Optimized geometry of product of reaction (11)

Total energy -1885.486

No.	Atom.No.	x	y	z
1	16	-3.124142	-0.235492	-0.015282
2	8	-3.364742	-0.128216	-1.461009
3	8	-3.085166	-1.538959	0.663074
4	6	-1.419207	0.64761	0.355001
5	9	-1.470547	1.775341	-0.350984
6	9	-1.463513	0.930805	1.656562
7	6	-0.181909	-0.234954	-0.007035
8	9	-0.094228	-1.176796	0.941615
9	9	-0.452445	-0.821072	-1.188626
10	6	1.139438	0.58842	-0.107676
11	9	1.081469	1.279609	-1.269422
12	9	1.12151	1.497937	0.904571
13	16	2.740659	-0.412168	-0.032042
14	8	2.795461	-0.828346	1.372984



15	8	2.479354	-1.47858	-1.006479
16	8	3.72579	0.59706	-0.434568
PFBI <sup>-</sup> ((CF <sub>3</sub> ) <sub>2</sub> CFOC <sub>4</sub> F <sub>8</sub> SO <sub>2</sub> NSO <sub>2</sub> C <sub>4</sub> F <sub>9</sub> ) <sup>-</sup>				
Optimized geometry				
Total energy				-4041.75477
No.	Atom.No.	x	y	z
1	6	6.651216	0.319884	-0.021837
2	6	7.371819	-0.272328	1.228444
3	6	7.047974	1.791083	-0.356411
4	9	7.012482	-0.438605	-1.083965
5	9	6.979309	-1.531784	1.404784
6	9	7.076966	0.427442	2.323474
7	9	8.697936	-0.262363	1.059322
8	9	6.384349	2.188015	-1.439289
9	9	6.749244	2.60576	0.654864
10	9	8.358286	1.882417	-0.605775
11	8	5.291542	0.306292	0.238259
12	6	4.392301	-0.413579	-0.519697
13	9	4.686873	-1.721289	-0.493676
14	9	4.408138	-0.012932	-1.800821
15	6	2.992583	-0.149073	0.124056
16	9	2.871742	1.179203	0.291988
17	9	3.004363	-0.743126	1.333901
18	6	1.784881	-0.672124	-0.724285
19	9	2.113402	-1.887248	-1.207014
20	9	1.631304	0.175426	-1.757177
21	6	0.456315	-0.785923	0.08471
22	9	0.350134	0.288292	0.89121
23	9	0.540235	-1.887403	0.853571
24	16	-1.088767	-0.894549	-0.988726
25	8	-1.268146	0.444523	-1.526536
26	8	-0.788626	-1.994466	-1.893659
27	7	-2.177507	-1.394842	0.071868
28	16	-3.136002	-0.444468	0.932041
29	8	-2.710941	0.936806	1.093317
30	8	-3.600994	-1.189805	2.092608
31	6	-4.664495	-0.361194	-0.166883
32	9	-4.39301	0.419719	-1.230952
33	9	-4.958012	-1.597172	-0.6113
34	6	-5.932223	0.197926	0.548368
35	9	-6.458801	-0.763782	1.33389
36	9	-5.607267	1.25249	1.317658
37	6	-7.053155	0.672826	-0.433225
38	9	-6.706362	1.857062	-0.969197
39	9	-7.212486	-0.224844	-1.427295
40	6	-8.455082	0.865122	0.223446
41	9	-9.004245	-0.303125	0.555278
42	9	-8.380103	1.631544	1.313203
43	9	-9.266325	1.466933	-0.656473

PFBIH ((CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NHSO<sub>2</sub>C<sub>4</sub>F<sub>9</sub>)

Optimized geometry

Total energy

-4042.231226

No.	Atom.No.	x	y	z
1	6	6.6795	0.331495	-0.01591
2	6	7.373379	-0.201887	1.275033
3	6	7.075549	1.786303	-0.415502
4	9	7.039573	-0.479674	-1.034024
5	9	6.961951	-1.447985	1.504319
6	9	7.058657	0.554585	2.325104
7	9	8.697232	-0.209092	1.126069
8	9	6.429329	2.117915	-1.532007
9	9	6.742887	2.645763	0.54578
10	9	8.386448	1.870176	-0.638405
11	8	5.305599	0.332446	0.223415
12	6	4.428609	-0.426292	-0.499617
13	9	4.703034	-1.735088	-0.401529
14	9	4.434373	-0.10075	-1.803307
15	6	3.020131	-0.130377	0.10893
16	9	2.865534	1.199395	0.191813
17	9	2.988221	-0.657476	1.348491
18	6	1.827632	-0.714442	-0.716699
19	9	2.120541	-1.966408	-1.102078
20	9	1.64306	0.050348	-1.80733
21	6	0.489267	-0.753425	0.086508
22	9	0.325323	0.366867	0.790147
23	9	0.486707	-1.806469	0.914158
24	16	-1.007522	-0.940031	-1.044896
25	8	-1.338403	0.350937	-1.580139
26	8	-0.782005	-2.127321	-1.833551
27	7	-2.175595	-1.38441	0.083472
28	16	-3.209659	-0.420972	0.997301
29	8	-2.635677	0.888371	1.13376
30	8	-3.624929	-1.258747	2.096481
31	6	-4.681183	-0.30813	-0.175783
32	9	-4.340855	0.507053	-1.174308
33	9	-4.894906	-1.539909	-0.656304
34	6	-5.96525	0.207667	0.546283
35	9	-6.472177	-0.800293	1.27473
36	9	-5.614218	1.211928	1.369024
37	6	-7.060662	0.72831	-0.437738
38	9	-6.67782	1.922584	-0.91529
39	9	-7.174356	-0.14078	-1.461646
40	6	-8.47521	0.898637	0.198584
41	9	-9.015905	-0.285314	0.475513
42	9	-8.398398	1.617335	1.31899
43	9	-9.260202	1.534219	-0.669464
44	1	-2.269509	-2.386075	0.236926

PFBIH + H

Transition state of reaction (12)

Total energy

-4042.681698

No.	Atom.No.	x	y	z
1	6	6.628361	0.399796	0.072495
2	6	7.36058	-0.207683	1.278626
3	6	7.06963	1.791851	-0.404858
4	9	7.061925	-0.576187	-1.164225
5	9	6.922025	-1.447714	1.494068
6	9	7.11668	0.517654	2.37865
7	9	8.676216	-0.243066	1.079242
8	9	6.39918	2.120862	-1.508609
9	9	6.801803	2.708092	0.535289
10	9	8.374624	1.82367	-0.665782
11	8	5.27535	0.375703	0.271871
12	6	4.404083	-0.392297	-0.459506
13	9	4.686267	-1.69604	-0.356557
14	9	4.416417	-0.064326	-1.75959
15	6	2.992755	-0.100888	0.144247
16	9	2.832524	1.22828	0.224097
17	9	2.958951	-0.6261	1.384387
18	6	1.806245	-0.691831	-0.685053
19	9	2.106775	-1.943504	-1.066102
20	9	1.623674	0.069318	-1.778486
21	6	0.464511	-0.734877	0.11223
22	9	0.292468	0.386565	0.81202
23	9	0.46338	-1.785668	0.942725
24	16	-1.026207	-0.931764	-1.025393
25	8	-1.359536	0.355865	-1.567078
26	8	-0.791703	-2.120962	-1.808574
27	7	-2.197645	-1.376662	0.098944
28	16	-3.240557	-0.413829	1.003712
29	8	-2.672561	0.898333	1.137898
30	8	-3.657866	-1.249147	2.103954
31	6	-4.706344	-0.311803	-0.177551
32	9	-4.363933	0.50054	-1.177666
33	9	-4.912571	-1.546418	-0.654033
34	6	-5.996229	0.201817	0.535671
35	9	-6.503133	-0.805338	1.265232
36	9	-5.653451	1.210521	1.356431
37	6	-7.088241	0.714492	-0.456276
38	9	-6.707357	1.908436	-0.93619
39	9	-7.192881	-0.158883	-1.477512
40	6	-8.50693	0.881686	0.171582
41	9	-9.044481	-0.303333	0.450062
42	9	-8.439098	1.604943	1.289618
43	9	-9.289568	1.510847	-0.703226
44	1	-2.288317	-2.378116	0.255714
45	1	7.382114	-1.374036	-2.170193

PFBIH + H

Transition state of reaction (13)

Total energy

-4042.695654

No.	Atom.No.	x	y	z
1	6	6.476824	0.472186	0.046183
2	6	7.004411	0.729	1.491294
3	6	6.930078	1.525901	-1.010844
4	9	6.951629	-0.728265	-0.351145
5	9	6.558599	-0.237523	2.292405
6	9	6.569631	1.901584	1.949523
7	9	8.336486	0.721611	1.512396
8	9	6.424036	1.192723	-2.197069
9	9	6.493225	2.740402	-0.682652
10	9	8.258916	1.553054	-1.104647
11	8	5.0844	0.519002	0.102625
12	6	4.294617	-0.54954	-0.217952
13	9	4.543553	-1.606458	0.568863
14	9	4.462436	-0.936753	-1.493659
15	6	2.825056	-0.062301	-0.005277
16	9	2.676571	1.118091	-0.624836
17	9	2.636323	0.107661	1.318013
18	6	1.736672	-1.046983	-0.549054
19	9	2.073324	-2.303815	-0.221378
20	9	1.686866	-0.928143	-1.887648
21	6	0.312746	-0.752224	0.014529
22	9	0.064865	0.549258	-0.017505
23	9	0.205361	-1.21811	1.269159
24	16	-1.052742	-1.655006	-0.997956
25	8	-1.623927	-0.713951	-1.929196
26	8	-0.494423	-2.936174	-1.377849
27	7	-2.453774	-2.245994	0.122005
28	16	-3.25052	-1.031111	1.098399
29	8	-2.51475	0.204005	0.970877
30	8	-3.565192	-1.643252	2.366293
31	6	-4.851117	-0.833041	0.096712
32	9	-4.560519	-1.004071	-1.190032
33	9	-5.704939	-1.773371	0.504521
34	6	-5.462415	0.584794	0.330985
35	9	-5.376093	0.862562	1.645718
36	9	-4.744157	1.478008	-0.363186
37	6	-6.960735	0.687203	-0.100602
38	9	-7.114084	0.078747	-1.292684
39	9	-7.716744	0.058671	0.813514
40	6	-7.493288	2.147465	-0.239211
41	9	-7.214176	2.849479	0.859736
42	9	-6.952112	2.751441	-1.293272
43	9	-8.81455	2.105745	-0.401203
44	1	-1.984704	-2.882342	0.778796
45	1	-3.652662	-3.262348	0.041127

PFBIH + H

Transition state of reaction (14)

Total energy

-4042.690516

No.	Atom.No.	x	y	z
1	6	6.561589	-0.481547	0.047489
2	6	7.019763	-1.419296	-1.111481
3	6	7.046674	-0.911752	1.466121
4	9	7.069791	0.745213	-0.198823
5	9	6.547564	-0.945643	-2.263626
6	9	6.552623	-2.653383	-0.930614
7	9	8.349375	-1.463711	-1.179764
8	9	6.601129	-0.02994	2.359502
9	9	6.575902	-2.117317	1.779502
10	9	8.37769	-0.938275	1.517303
11	8	5.166932	-0.501219	0.069222
12	6	4.409708	0.612936	-0.158354
13	9	4.641483	1.135047	-1.371333
14	9	4.63626	1.573196	0.753942
15	6	2.924797	0.136478	-0.059064
16	9	2.780232	-0.570025	1.071461
17	9	2.67561	-0.662105	-1.115433
18	6	1.877358	1.297894	-0.052505
19	9	2.208818	2.20329	-0.984333
20	9	1.885878	1.880873	1.158865
21	6	0.424312	0.805107	-0.342757
22	9	0.175848	-0.338396	0.293988
23	9	0.254591	0.625105	-1.662731
24	16	-0.866413	2.083184	0.199039
25	8	-1.151584	1.915162	1.596666
26	8	-0.438273	3.323391	-0.40232
27	7	-2.300787	1.569007	-0.65983
28	16	-2.937357	-0.229256	-0.219253
29	8	-2.592545	-0.676013	1.111234
30	8	-2.813129	-1.040126	-1.419303
31	6	-4.721851	0.401398	-0.16304
32	9	-4.819352	1.20211	0.898962
33	9	-4.930532	1.103184	-1.281598
34	6	-5.754915	-0.765468	-0.077437
35	9	-5.847879	-1.326175	-1.295044
36	9	-5.29867	-1.682396	0.792381
37	6	-7.173341	-0.302589	0.385869
38	9	-7.134211	-0.057794	1.704932
39	9	-7.496553	0.832951	-0.263715
40	6	-8.310837	-1.338205	0.124533
41	9	-8.561176	-1.44778	-1.17781
42	9	-7.972204	-2.533936	0.607282
43	9	-9.416547	-0.921566	0.738752
44	1	-2.062427	1.445	-1.65318
45	1	-2.863562	3.017053	-0.973225

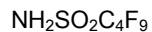


Optimized geometry of product of reaction (12)

Total energy

-3942.355272

No.	Atom.No.	x	y	z
1	6	-6.776375	0.347796	-0.340877
2	6	-7.48242	-0.9485	-0.680122
3	6	-7.511544	1.661887	-0.290913
4	9	-6.633597	-1.811368	-1.241518
5	9	-8.490445	-0.730356	-1.53816
6	9	-8.002362	-1.521624	0.415983
7	9	-6.868821	2.52621	0.500161
8	9	-7.607344	2.22141	-1.509552
9	9	-8.749306	1.483756	0.183637
10	8	-5.439788	0.438386	-0.539059
11	6	-4.57225	0.03006	0.448672
12	9	-4.904823	-1.180957	0.915764
13	9	-4.593329	0.882067	1.484853
14	6	-3.153455	-0.001768	-0.197086
15	9	-2.962596	1.153796	-0.850203
16	9	-3.128405	-1.019237	-1.079107
17	6	-1.988293	-0.193246	0.827231
18	9	-2.328211	-1.144223	1.711918
19	9	-1.794214	0.966515	1.479152
20	6	-0.642818	-0.610502	0.153992
21	9	-0.440387	0.081247	-0.967371
22	9	-0.662462	-1.920232	-0.124712
23	16	0.833492	-0.308458	1.287492
24	8	1.198467	1.077612	1.197031
25	8	0.556785	-1.010837	2.517326
26	7	2.001352	-1.238541	0.510795
27	16	3.073845	-0.813358	-0.715395
28	8	2.533355	0.297597	-1.447769
29	8	3.484489	-2.066924	-1.300492
30	6	4.529559	-0.198023	0.313162
31	9	4.19648	0.991624	0.813858
32	9	4.701217	-1.072623	1.312706
33	6	5.838103	-0.096911	-0.531869
34	9	6.329266	-1.335882	-0.696644
35	9	5.526244	0.416516	-1.735181
36	6	6.93152	0.80302	0.126714
37	9	6.573052	2.088538	-0.013858
38	9	7.006197	0.506337	1.439354
39	6	8.3596	0.635528	-0.479303
40	9	8.872791	-0.550681	-0.162581
41	9	8.318665	0.754302	-1.806702
42	9	9.147726	1.58806	0.015676
43	1	2.068885	-2.202639	0.829724

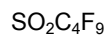


Optimized geometry of product of reaction (13)

Total energy

-1655.191707

No.	Atom.No.	x	y	z
1	7	3.80964	0.670399	-0.363864
2	16	2.664526	-0.398733	0.122481
3	8	2.800675	-0.559347	1.550121
4	8	2.643908	-1.488336	-0.82533
5	6	1.064783	0.548938	-0.161066
6	9	1.039885	1.562265	0.722935
7	9	1.124434	1.066888	-1.402014
8	6	-0.219914	-0.322043	-0.025164
9	9	-0.343142	-1.063569	-1.139472
10	9	-0.076367	-1.139003	1.032294
11	6	-1.525682	0.512123	0.172705
12	9	-1.549179	0.986815	1.429001
13	9	-1.520575	1.55015	-0.688189
14	6	-2.847657	-0.283555	-0.058808
15	9	-3.007885	-0.574473	-1.347615
16	9	-2.844082	-1.414043	0.647549
17	9	-3.874055	0.468833	0.338075
18	1	3.828026	0.872577	-1.357019
19	1	3.944928	1.46828	0.246964



Optimized geometry of product of reaction (14)

Total energy

-1599.2192685

No.	Atom.No.	x	y	z
1	16	-2.954443	-0.190014	-0.024794
2	8	-3.147598	-0.112235	-1.475498
3	8	-2.899034	-1.466123	0.697364
4	6	-1.252893	0.669772	0.337274
5	9	-1.226793	1.769946	-0.412131
6	9	-1.270306	0.996487	1.628424
7	6	-0.039595	-0.257502	0.022323
8	9	0.060723	-1.161962	1.008406
9	9	-0.279234	-0.892173	-1.137425
10	6	1.312193	0.516457	-0.103373
11	9	1.321757	1.176142	-1.272446
12	9	1.398354	1.406884	0.904721
13	6	2.584429	-0.385209	-0.050824
14	9	2.760004	-0.884714	1.169705
15	9	2.480958	-1.38743	-0.923712
16	9	3.645574	0.355262	-0.366724

PFIHS<sup>-</sup> + OH

Transition state of reaction (15)

Total energy

-4404.1943312

No.	Atom.No.	x	y	z
1	6	6.927056	0.36446	-0.096237
2	6	7.72243	-0.638985	0.794188
3	6	7.327166	1.86017	0.093315
4	9	7.177192	0.042906	-1.385436
5	9	7.316264	-1.877675	0.521728
6	9	7.514203	-0.392661	2.086357
7	9	9.030456	-0.555054	0.544139
8	9	6.579604	2.614078	-0.709685
9	9	7.131016	2.245577	1.353092
10	9	8.610678	2.046343	-0.22007
11	8	5.584961	0.250971	0.250194
12	6	4.622718	-0.158483	-0.636175
13	9	4.875644	-1.391366	-1.098981
14	9	4.533167	0.667626	-1.691259
15	6	3.281935	-0.147557	0.16643
16	9	3.181987	1.033913	0.794341
17	9	3.353247	-1.13098	1.084589
18	6	2.005673	-0.355474	-0.713503
19	9	2.241954	-1.337745	-1.600935
20	9	1.763736	0.786355	-1.379736
21	6	0.740912	-0.737312	0.118566
22	9	0.678043	0.002374	1.228629
23	9	0.808226	-2.034242	0.446017
24	16	-0.859464	-0.471803	-0.839868
25	8	-1.132381	0.94133	-0.859733
26	8	-0.719778	-1.269	-2.047165
27	7	-1.887872	-1.303681	0.166297
28	16	-3.090314	-0.639916	1.20292
29	8	-2.439783	0.393657	1.973237
30	8	-3.685507	-1.813794	1.790509
31	6	-4.31438	0.180529	-0.020667
32	9	-3.923263	1.445045	-0.134775
33	9	-4.150933	-0.44706	-1.189785
34	6	-5.783006	0.071242	0.497385
35	9	-6.152737	-1.207251	0.348989
36	9	-5.732634	0.37565	1.812579
37	6	-6.766989	1.030863	-0.237093
38	9	-6.521677	2.27711	0.229355
39	9	-6.425079	1.01751	-1.554641
40	16	-8.600158	0.622393	-0.050107
41	8	-8.746547	-0.58798	-0.865074
42	8	-8.718956	0.43504	1.401438
43	8	-9.221983	1.833805	-0.593762
44	1	-2.084335	-2.496628	-0.195067
45	8	-2.584576	-3.190312	-0.964626
46	1	-2.168116	-2.938916	-1.814147



PFIS-

reaction product of (15)

Total energy

-4327.8200894

No.	Atom.No.	x	y	z
1	6	-6.831369	0.343856	0.042656
2	6	-7.550717	-0.14708	-1.251355
3	6	-7.220672	1.788302	0.484997
4	9	-7.201187	-0.489983	1.043418
5	9	-7.163346	-1.390929	-1.523719
6	9	-7.249196	0.634138	-2.287927
7	9	-8.877074	-0.143605	-1.08511
8	9	-6.563299	2.096632	1.600157
9	9	-6.907858	2.67515	-0.458938
10	9	-8.532295	1.869871	0.730254
11	8	-5.470291	0.342357	-0.211753
12	6	-4.579946	-0.445735	0.485642
13	9	-4.887182	-1.744182	0.354506
14	9	-4.592412	-0.149541	1.794946
15	6	-3.176982	-0.144675	-0.134577
16	9	-3.041788	1.191329	-0.19511
17	9	-3.193002	-0.639651	-1.388138
18	6	-1.974915	-0.745938	0.668483
19	9	-2.312404	-1.994078	1.049312
20	9	-1.814449	0.012351	1.767587
21	6	-0.646433	-0.802584	-0.147006
22	9	-0.529914	0.333652	-0.860942
23	9	-0.735751	-1.836117	-1.003964
24	16	0.895301	-1.011919	0.915706
25	8	1.087562	0.275681	1.563303
26	8	0.589016	-2.182377	1.724032
27	7	1.985236	-1.428621	-0.182584
28	16	2.947366	-0.41354	-0.956237
29	8	2.519635	0.974282	-1.022887
30	8	3.441372	-1.069858	-2.157455
31	6	4.462106	-0.396237	0.16394
32	9	4.187135	0.322326	1.27185
33	9	4.759859	-1.65387	0.53674
34	6	5.734289	0.213824	-0.498378
35	9	6.29751	-0.691049	-1.326431
36	9	5.422767	1.31389	-1.197866
37	6	6.832632	0.617516	0.534647
38	9	6.547352	1.788251	1.111787
39	9	6.98624	-0.318743	1.475346
40	16	8.524308	0.847759	-0.25097
41	8	9.110652	-0.511822	-0.471006
42	8	8.396945	1.713351	-1.397044
43	8	9.393414	1.318816	0.870058



Optimized geometry of product of reaction (16)

Total energy

-3704.1274659

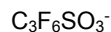
No.	Atom.No.	x	y	z
1	6	-5.792706	0.189462	-0.048979
2	6	-6.484903	-1.058653	-0.678597
3	6	-6.270136	1.553671	-0.635937
4	9	-6.106448	0.195149	1.268467
5	9	-6.017988	-2.160558	-0.096486
6	9	-6.241277	-1.127173	-1.987028
7	9	-7.80798	-1.010145	-0.492545
8	9	-5.629137	2.543152	-0.018742
9	9	-6.017404	1.625152	-1.942214
10	9	-7.583502	1.716279	-0.445574
11	8	-4.435402	0.086809	-0.300293
12	6	-3.496405	-0.036872	0.702242
13	9	-3.738571	-1.121431	1.452179
14	9	-3.509695	1.034704	1.510795
15	6	-2.118681	-0.16397	-0.025289
16	9	-2.05361	0.820612	-0.938236
17	9	-2.127295	-1.351381	-0.66324
18	6	-0.877231	-0.067794	0.924137
19	9	-1.1505	-0.779185	2.036294
20	9	-0.739453	1.226403	1.263091
21	6	0.440277	-0.604152	0.284509
22	9	0.486777	-0.204557	-1.001724
23	9	0.386777	-1.948902	0.309275
24	16	2.008116	-0.028516	1.15767
25	8	2.143131	1.374227	0.798471
26	8	1.764925	-0.38959	2.54695
27	7	3.094743	-1.035261	0.555566
28	16	4.002223	-0.758692	-0.735476
29	8	3.529571	0.262601	-1.656626
30	8	4.455877	-2.038086	-1.259871
31	6	5.550397	-0.03162	0.049973
32	9	5.257201	1.194524	0.532491
33	9	5.930558	-0.806767	1.085019
34	6	6.781425	0.114486	-0.896209
35	9	7.300789	-1.108246	-1.139538
36	9	6.402256	0.673116	-2.063199
37	6	7.912718	0.974612	-0.341562
38	9	7.697423	2.280217	-0.323345
39	9	8.443081	0.560087	0.801053



Optimized geometry of product of reactions (17)

Total energy -2990.835457

No.	Atom.No.	x	y	z
1	6	-3.905985	-0.052578	0.003167
2	6	-4.549438	0.913338	-1.038749
3	6	-4.465584	0.085003	1.452624
4	9	-4.153527	-1.314955	-0.407833
5	9	-3.987586	0.703991	-2.228192
6	9	-4.351624	2.183052	-0.687582
7	9	-5.858744	0.689357	-1.138571
8	9	-3.852964	-0.800041	2.237176
9	9	-4.243368	1.308571	1.929277
10	9	-5.77538	-0.157925	1.47369
11	8	-2.544984	0.247124	0.060016
12	6	-1.575958	-0.653663	-0.282782
13	9	-1.696372	-1.05643	-1.555704
14	9	-1.602441	-1.745609	0.499524
15	6	-0.219812	0.097972	-0.089609
16	9	-0.220264	0.669743	1.124506
17	9	-0.144151	1.060544	-1.02901
18	6	1.043382	-0.817494	-0.198677
19	9	0.910317	-1.64699	-1.245688
20	9	1.144932	-1.543511	0.927063
21	6	2.366674	-0.014593	-0.394398
22	9	2.405995	1.047485	0.427377
23	9	2.462185	0.405023	-1.657062
24	16	3.904416	-1.037217	-0.014111
25	8	3.997994	-1.223195	1.412711
26	8	3.948118	-2.121386	-0.958866
27	7	5.050101	0.089978	-0.580256
28	16	5.696173	1.160457	0.304675
29	8	5.360293	1.36399	1.688166
30	8	6.681971	1.962177	-0.366706

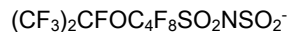


Optimized geometry of product of reactions (17)

Total energy -1336.9419103

No.	Atom.No.	x	y	z
1	6	2.373265	-0.178595	-0.007889
2	9	2.810067	0.887199	0.654976
3	9	2.728572	-0.115611	-1.284597
4	6	0.930886	-0.594844	0.274199
5	9	0.702241	-1.69824	-0.467684
6	9	0.879604	-0.927343	1.584589
7	6	-0.140382	0.495301	-0.027686
8	9	0.021239	1.462579	0.910088
9	9	0.191494	1.046974	-1.227839
10	16	-1.944763	-0.054143	-0.070322
11	8	-2.015218	-0.857707	-1.296326
12	8	-2.077511	-0.800514	1.187974
13	8	-2.640441	1.237609	-0.120699



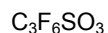


Optimized geometry of product of reactions (18)

Total energy

-2990.9792703

No.	Atom.No.	x	y	z
1	6	-3.909285	-0.030978	-0.08199
2	6	-4.526236	1.314649	-0.5742
3	6	-4.538288	-0.581502	1.235204
4	9	-4.145397	-0.95148	-1.047187
5	9	-3.933303	1.681696	-1.707567
6	9	-4.354426	2.276432	0.332236
7	9	-5.83578	1.177327	-0.807527
8	9	-3.951866	-1.733031	1.552737
9	9	-4.370088	0.27865	2.239026
10	9	-5.847683	-0.802925	1.078061
11	8	-2.56592	0.190865	0.163569
12	6	-1.561593	-0.457781	-0.525795
13	9	-1.652332	-0.211476	-1.840437
14	9	-1.635989	-1.786516	-0.349426
15	6	-0.222833	0.104039	0.053992
16	9	-0.313621	0.04658	1.394684
17	9	-0.151873	1.395876	-0.323688
18	6	1.056968	-0.669271	-0.411424
19	9	0.918197	-0.935874	-1.725346
20	9	1.080432	-1.831164	0.268134
21	6	2.382438	0.11751	-0.176917
22	9	2.305594	0.718823	1.026345
23	9	2.465721	1.068758	-1.127012
24	16	3.933994	-0.961117	-0.239811
25	8	3.984961	-1.570167	1.087891
26	8	3.683403	-1.799398	-1.405567
27	7	5.122626	0.042354	-0.576351
28	16	5.895839	0.835309	0.654972
29	8	5.093692	1.955403	1.199394
30	8	7.251237	1.149716	0.156131



Optimized geometry of product of reactions (18)

Total energy

-1336.8829678

No.	Atom.No.	x	y	z
1	6	2.373265	-0.178595	-0.007889
1	6	2.373265	-0.178595	-0.007889
2	9	2.810067	0.887199	0.654976
3	9	2.728572	-0.115611	-1.284597
4	6	0.930886	-0.594844	0.274199
5	9	0.702241	-1.69824	-0.467684
6	9	0.879604	-0.927343	1.584589
7	6	-0.140382	0.495301	-0.027686
8	9	0.021239	1.462579	0.910088
9	9	0.191494	1.046974	-1.227839
10	16	-1.944763	-0.054143	-0.070322
11	8	-2.015218	-0.857707	-1.296326
12	8	-2.077511	-0.800514	1.187974
13	8	-2.640441	1.237609	-0.120699

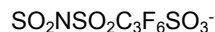




Optimized geometry of product of reaction (19)

Total energy -1839.0891556

No.	Atom.No.	x	y	z
1	6	-2.028228	0.007582	-0.23356
2	6	-2.673067	1.340537	0.256361
3	6	-2.70522	-1.284724	0.318319
4	9	-2.138072	-0.023422	-1.579827
5	9	-2.016892	2.364633	-0.286559
6	9	-2.60095	1.438815	1.582896
7	9	-3.951418	1.407212	-0.114303
8	9	-2.075024	-2.348181	-0.177904
9	9	-2.63338	-1.324038	1.647755
10	9	-3.985473	-1.33689	-0.048234
11	8	-0.707271	-0.000537	0.209409
12	6	0.360754	-0.022552	-0.646397
13	9	0.368193	1.043962	-1.45983
14	9	0.364134	-1.124229	-1.414804
15	6	1.628753	-0.00612	0.262993
16	9	1.512026	-0.991651	1.171028
17	9	1.656155	1.177273	0.908877
18	6	2.994164	-0.191643	-0.474326
19	9	3.046399	0.660076	-1.518612
20	9	3.060149	-1.459139	-0.929792
21	6	4.225532	0.058011	0.385275
22	9	4.357215	-0.737234	1.431219
23	9	4.46383	1.319231	0.689506



Optimized geometry of product of reaction (19)

Total energy -2488.6967701

No.	Atom.No.	x	y	z
1	16	-3.959644	-0.71037	-0.01964
2	8	-3.775288	-1.207374	1.320243
3	8	-5.007582	-1.23441	-0.861637
4	7	-3.121872	0.389323	-0.659583
5	16	-1.825625	1.20568	0.148475
6	8	-2.03417	1.179248	1.576692
7	8	-1.671124	2.428561	-0.596735
8	6	-0.463197	-0.012392	-0.349618
9	9	-0.798084	-1.161423	0.260005
10	9	-0.575412	-0.173121	-1.668553
11	6	0.96819	0.473701	0.046554
12	9	1.291499	1.435011	-0.830974
13	9	0.86588	1.019037	1.274725
14	6	2.024065	-0.671494	0.05164
15	9	1.792572	-1.407408	1.164085
16	9	1.754366	-1.465759	-1.020706
17	16	3.829787	-0.124616	0.001849
18	8	3.979022	0.368148	-1.371073
19	8	3.863652	0.896918	1.055955
20	8	4.519124	-1.382627	0.304987



Optimized geometry of reaction intermediate (20)

Total energy

-2565.1181088

No.	Atom.No.	x	y	z
1	16	-3.959644	-0.71037	-0.01964
1	16	3.751683	-0.677063	0.397492
2	8	3.139022	-1.852082	-0.174893
3	8	5.054664	-0.745756	1.00021
4	7	2.924196	0.534699	0.843053
5	16	1.603319	1.176661	0.039943
6	8	1.954093	1.299042	-1.378793
7	8	1.214166	2.329473	0.808375
8	6	0.25577	-0.157123	0.169645
9	9	0.493586	-1.01531	-0.824765
10	9	0.450111	-0.767685	1.342417
11	6	-1.179307	0.453461	0.067371
12	9	-1.429515	1.05732	1.236384
13	9	-1.12404	1.381094	-0.912413
14	6	-2.273842	-0.605059	-0.263794
15	9	-2.131393	-0.920563	-1.573055
16	9	-1.978294	-1.721823	0.455789
17	16	-4.054775	-0.081055	0.076342
18	8	-4.120291	-0.083925	1.541305
19	8	-4.108233	1.239102	-0.564582
20	8	-4.802026	-1.149464	-0.595264
21	8	4.354897	0.119321	-1.574009
22	1	3.570477	0.678487	-1.79042
23	1	4.326372	-0.628732	-2.188701



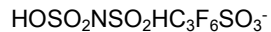
HOSO<sub>2</sub>NSO<sub>2</sub>HC<sub>3</sub>F<sub>6</sub>SO<sub>3</sub><sup>-</sup>

Optimized geometry of reaction intermediate (20)

Total energy

-2565.1374461

No.	Atom.No.	x	y	z
1	16	-3.835084	-0.586689	0.05878
2	8	-5.19314	-0.509701	-0.39474
3	8	-3.544643	-0.599364	1.502662
4	7	-2.964576	0.586721	-0.667022
5	16	-1.676486	1.238003	-0.081063
6	8	-1.719365	1.279208	1.495824
7	8	-1.348034	2.522824	-0.627738
8	6	-0.272182	0.022966	-0.405776
9	9	-0.622395	-1.06497	0.329218
10	9	-0.369643	-0.292895	-1.694677
11	6	1.162646	0.52474	-0.04351
12	9	1.521449	1.357255	-1.030247
13	9	1.059344	1.219351	1.105211
14	6	2.184874	-0.639011	0.124302
15	9	1.91297	-1.221617	1.317167
16	9	1.903795	-1.555937	-0.842957
17	16	4.005909	-0.152398	0.040149
18	8	4.185076	0.166982	-1.379172
19	8	4.050654	0.986849	0.964743
20	8	4.652537	-1.38314	0.504164
21	8	-3.274113	-1.961815	-0.551691
22	1	-2.369087	0.587202	1.814903
23	1	-2.361796	-2.114505	-0.247537



Transition state of the first H migration in reaction (20)

Total energy

-2565.1374461

No.	Atom.No.	x	y	z
1	16	-4.122157	-0.506658	0.11188
2	8	-5.393146	0.164664	0.00921
3	8	-3.625104	-0.785347	1.469023
4	7	-2.852878	0.337828	-0.762807
5	16	-1.601909	1.068145	-0.113275
6	8	-1.807821	1.085624	1.442244
7	8	-1.268645	2.37198	-0.610787
8	6	-0.181309	-0.157203	-0.387446
9	9	-0.501397	-1.200042	0.383559
10	9	-0.279248	-0.509908	-1.670465
11	6	1.221766	0.438681	-0.048007
12	9	1.526857	1.272799	-1.050735
13	9	1.062856	1.148315	1.087979
14	6	2.316488	-0.65177	0.142974
15	9	2.080424	-1.230124	1.344122
16	9	2.09848	-1.597918	-0.81108
17	16	4.099254	-0.038697	0.053596
18	8	4.261583	0.260998	-1.372071
19	8	4.055199	1.122043	0.951452
20	8	4.830928	-1.207727	0.548284
21	8	-3.889092	-1.631512	-0.900005
22	1	-2.403332	0.323091	1.725153
23	1	-2.97417	-0.824659	-1.315074



Optimized geometry after the first H migration in reaction (20)

Total energy -2565.1635901

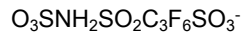
No.	Atom.No.	x	y	z
1	16	4.088596	-0.577811	0.02493
2	8	5.133095	-0.651035	1.011579
3	8	4.60075	0.446726	-1.092909
4	7	2.836365	0.268481	0.787003
5	16	1.563345	1.005478	-0.048584
6	8	1.883661	0.894642	-1.462779
7	8	1.327419	2.268341	0.610939
8	6	0.154584	-0.186744	0.375028
9	9	0.425016	-1.311149	-0.284119
10	9	0.255169	-0.400785	1.689471
11	6	-1.2403	0.411653	-0.001095
12	9	-1.523969	1.331979	0.931447
13	9	-1.076364	1.028618	-1.190963
14	6	-2.365208	-0.659774	-0.09708
15	9	-2.158805	-1.341059	-1.247899
16	9	-2.168373	-1.529841	0.93109
17	16	-4.13124	0.003953	-0.046605
18	8	-4.27974	0.420138	1.351756
19	8	-4.06992	1.08948	-1.033751
20	8	-4.89732	-1.181425	-0.442761
21	8	3.52006	-1.731276	-0.615796
22	1	3.865415	0.592322	-1.726637
23	1	3.136237	0.787001	1.609187



Transition state of the second H migration in reaction (20)

Total energy -2565.1043854

No.	Atom.No.	x	y	z
1	16	4.552073	-0.206391	0.064707
2	8	4.806219	0.986217	-0.695402
3	8	4.311124	-1.480643	-0.749627
4	7	2.710436	-0.387165	0.428495
5	16	1.521976	0.768459	-0.129424
6	8	1.781084	0.949134	-1.533309
7	8	1.470176	1.844268	0.830451
8	6	0.037562	-0.385185	0.120419
9	9	0.176191	-1.343414	-0.799137
10	9	0.202992	-0.922694	1.340831
11	6	-1.326572	0.366672	0.009166
12	9	-1.470154	1.055391	1.14971
13	9	-1.191715	1.23385	-1.015429
14	6	-2.53158	-0.588187	-0.236487
15	9	-2.462543	-0.976727	-1.5306
16	9	-2.316009	-1.694021	0.529782
17	16	-4.23409	0.132867	0.139923
18	8	-4.237665	0.192292	1.604923
19	8	-4.166552	1.424834	-0.553769
20	8	-5.113437	-0.874647	-0.459451
21	8	5.194654	-0.416341	1.340556
22	1	3.120046	-1.360987	-0.337686
23	1	2.577446	-0.580011	1.424933



Optimized geometry after the second H migration in reaction (20)

Total energy -2565.1539223

No.	Atom.No.	x	y	z
1	16	4.901316	-0.104964	0.067374
2	8	4.834167	1.330492	-0.016405
3	8	5.029382	-0.890681	-1.137587
4	7	2.671302	-0.560063	0.327747
5	16	1.48578	0.585129	-0.198847
6	8	1.690961	0.731758	-1.616632
7	8	1.528561	1.663486	0.7557
8	6	-0.058972	-0.461888	0.112442
9	9	0.027857	-1.475993	-0.762396
10	9	0.090179	-0.955831	1.353641
11	6	-1.393444	0.335634	-0.024932
12	9	-1.49459	1.088234	1.079817
13	9	-1.243152	1.142307	-1.094653
14	6	-2.638618	-0.582316	-0.205449
15	9	-2.603083	-1.039444	-1.478836
16	9	-2.4571	-1.655956	0.613733
17	16	-4.307929	0.220475	0.152689
18	8	-4.288346	0.359978	1.612168
19	8	-4.206308	1.469475	-0.611938
20	8	-5.231469	-0.786017	-0.378777
21	8	5.212255	-0.728089	1.335831
22	1	2.576628	-1.433242	-0.194355
23	1	2.56918	-0.738204	1.327658

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>

Transition state of SO<sub>2</sub> dissociation reaction (22)

Total energy

-2387.6169798

No.	Atom.No.	x	y	z
1	6	2.920464	0.098649	-0.304964
2	6	3.704259	-1.201516	0.052559
3	6	3.531639	1.410084	0.277667
4	9	2.920602	0.215221	-1.650328
5	9	3.094522	-2.243011	-0.511339
6	9	3.735053	-1.38445	1.371629
7	9	4.953321	-1.136892	-0.406027
8	9	2.778049	2.441794	-0.098703
9	9	3.563852	1.36358	1.608419
10	9	4.769043	1.593715	-0.180389
11	8	1.639873	-0.030212	0.232756
12	6	0.512687	-0.050684	-0.540322
13	9	0.524292	-1.067753	-1.413917
14	9	0.356324	1.087659	-1.235237
15	6	-0.675667	-0.224465	0.45725
16	9	-0.554537	0.690243	1.432642
17	9	-0.586712	-1.455493	1.000497
18	6	-2.097996	-0.071416	-0.176393
19	9	-2.163431	-0.792035	-1.307023
20	9	-2.305957	1.22641	-0.454244
21	6	-3.229343	-0.549039	0.747978
22	9	-3.233317	0.002124	1.942259
23	9	-3.37217	-1.854894	0.809523
24	16	-5.367917	0.20648	-0.17022
25	8	-5.453618	1.581694	0.300575
26	8	-5.238753	-0.045146	-1.599456

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub> + H<sub>2</sub>O<sub>2</sub>

Transition state of reaction (23)

Total energy

-1990.5747092

No.	Atom.No.	x	y	z
1	6	-2.587878	-0.041202	-0.303425
2	6	-3.309163	1.296955	0.045602
3	6	-3.255596	-1.315729	0.298825
4	9	-2.607525	-0.172441	-1.647887
5	9	-2.659069	2.30405	-0.534859
6	9	-3.321437	1.495673	1.362742
7	9	-4.564323	1.28346	-0.402254
8	9	-2.553689	-2.386823	-0.068239
9	9	-3.277952	-1.251956	1.629174
10	9	-4.503405	-1.448388	-0.149721
11	8	-1.299586	0.035118	0.221628
12	6	-0.176892	-0.0192	-0.559353
13	9	-0.142877	0.982304	-1.450184
14	9	-0.093448	-1.175796	-1.238252
15	6	1.027761	0.102866	0.425533
16	9	0.860672	-0.7954	1.412271
17	9	1.00088	1.341727	0.957015
18	6	2.436808	-0.128132	-0.209257
19	9	2.52642	0.572405	-1.351274
20	9	2.558859	-1.448509	-0.485651
21	6	3.612359	0.263979	0.6845
22	9	3.60651	-0.32722	1.870352
23	9	3.816502	1.557355	0.79155
24	8	5.273784	-0.293974	-0.253215
25	1	5.130201	-1.254324	-0.280356
26	8	6.698839	-0.32113	-0.966656
27	1	7.186066	0.163031	-0.281326

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>OH

Intermediate of reaction (23)

Total energy

-1914.9714159

No.	Atom.No.	x	y	z
1	6	-2.25426	-0.007573	-0.246938
2	6	-2.914199	1.343249	0.168373
3	6	-2.934339	-1.275739	0.355071
4	9	-2.343646	-0.103491	-1.59197
5	9	-2.258006	2.344285	-0.415849
6	9	-2.860625	1.507479	1.489266
7	9	-4.188373	1.382737	-0.221361
8	9	-2.285824	-2.3582	-0.071404
9	9	-2.893163	-1.246471	1.686154
10	9	-4.205733	-1.357629	-0.037034
11	8	-0.941671	0.012709	0.216951
12	6	0.140631	-0.043005	-0.620015
13	9	0.151806	0.984452	-1.481934
14	9	0.160541	-1.180057	-1.335733
15	6	1.394578	0.025055	0.310319
16	9	1.235254	-0.877456	1.293126
17	9	1.42838	1.257672	0.850833
18	6	2.746871	-0.270314	-0.414274
19	9	2.769435	0.377914	-1.595817
20	9	2.814656	-1.593034	-0.645922
21	6	4.017271	0.153802	0.383048
22	9	3.912316	-0.273173	1.668621
23	9	4.088422	1.506684	0.442799
24	8	5.090976	-0.368924	-0.231603
25	1	5.897294	-0.048527	0.199744



(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>7</sub>O HF

Transition state of reaction (23)

Total energy

-1914.8946704

No.	Atom.No.	x	y	z
1	6	-2.255129	0.015421	-0.248299
2	6	-2.872079	1.385318	0.170648
3	6	-2.974631	-1.233467	0.347986
4	9	-2.34208	-0.073387	-1.593463
5	9	-2.182958	2.366189	-0.409667
6	9	-2.81443	1.542774	1.492005
7	9	-4.143362	1.465885	-0.220705
8	9	-2.358386	-2.333174	-0.08278
9	9	-2.933281	-1.210935	1.679022
10	9	-4.246877	-1.274125	-0.045975
11	8	-0.94198	-0.00786	0.218616
12	6	0.137992	-0.089269	-0.616014
13	9	0.184321	0.940097	-1.473804
14	9	0.132248	-1.224375	-1.336115
15	6	1.39146	-0.060597	0.315883
16	9	1.218702	-0.978067	1.284221
17	9	1.45879	1.158372	0.875429
18	6	2.736449	-0.374946	-0.41079
19	9	2.800347	0.287439	-1.572238
20	9	2.787717	-1.701463	-0.66416
21	6	4.028891	-0.0751	0.396397
22	9	3.910154	-0.40237	1.662019
23	9	4.093067	1.692536	0.391065
24	8	5.15795	-0.096216	-0.156874
25	1	5.038772	1.129878	-0.092491

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>3</sub>F<sub>6</sub>CFO

Intermediate of reaction (23)

Total energy

-1814.5375604

No.	Atom.No.	x	y	z
1	6	2.018835	-0.02341	-0.242239
2	6	2.690891	-1.318589	0.30876
3	6	2.685726	1.307043	0.224826
4	9	2.102088	-0.065284	-1.589678
5	9	2.045205	-2.37925	-0.173045
6	9	2.634183	-1.348734	1.639138
7	9	3.965745	-1.383531	-0.072948
8	9	2.02235	2.332494	-0.307076
9	9	2.647719	1.412344	1.552006
10	9	3.954105	1.362332	-0.178994
11	8	0.704886	-0.010281	0.224648
12	6	-0.376578	-0.040194	-0.611223
13	9	-0.390155	-1.145442	-1.369363
14	9	-0.409611	1.023521	-1.432469
15	6	-1.629262	-0.015849	0.318014
16	9	-1.4844	0.981283	1.204618
17	9	-1.681307	-1.188681	0.985637
18	6	-2.99383	0.169198	-0.414273
19	9	-3.031204	-0.61458	-1.501059
20	9	-3.129234	1.455196	-0.794749
21	6	-4.191666	-0.210884	0.490588
22	9	-4.295121	0.647965	1.505851
23	8	-4.927132	-1.116044	0.318162

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>3</sub>F<sub>6</sub>CFO+H<sub>2</sub>O

Transition state of reaction (23)

Total energy

-1890.8825953

No.	Atom.No.	x	y	z
1	6	2.270235	0.020912	-0.258851
2	6	3.010005	-1.233615	0.299372
3	6	2.891641	1.387013	0.165883
4	9	2.324808	-0.046631	-1.607394
5	9	2.38708	-2.329306	-0.13262
6	9	3.003726	-1.231915	1.630835
7	9	4.271717	-1.262779	-0.128766
8	9	2.185012	2.373575	-0.382695
9	9	2.866351	1.524171	1.490124
10	9	4.152817	1.478492	-0.255809
11	8	0.969428	-0.01718	0.239446
12	6	-0.130434	-0.084605	-0.568838
13	9	-0.140038	-1.206566	-1.311691
14	9	-0.199125	0.95967	-1.407758
15	6	-1.361415	-0.076654	0.393244
16	9	-1.416675	1.126423	0.979862
17	9	-1.17087	-1.020057	1.330121
18	6	-2.721918	-0.374032	-0.308801
19	9	-2.782683	-1.691335	-0.618625
20	9	-2.815244	0.309873	-1.46657
21	6	-3.933648	-0.105124	0.605108
22	9	-4.11279	1.695974	0.38728
23	8	-4.089682	-0.472267	1.708039
24	8	-5.253685	-0.022376	-0.329318
25	1	-5.060162	1.06319	-0.214853
26	1	-5.08188	-0.288274	-1.24985

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>3</sub>F<sub>6</sub>COOH  
product of reaction (23)

Total energy

-1790.5299652

No.	Atom.No.	x	y	z
1	6	-2.020594	-0.024015	-0.241098
2	6	-2.717789	1.283849	0.245099
3	6	-2.668225	-1.342078	0.283995
4	9	-2.097512	-0.044924	-1.589758
5	9	-2.076331	2.331728	-0.269005
6	9	-2.686016	1.368754	1.573613
7	9	-3.98629	1.316676	-0.161889
8	9	-1.995743	-2.380938	-0.210233
9	9	-2.62051	-1.393368	1.613821
10	9	-3.938385	-1.429385	-0.108721
11	8	-0.70972	0.008016	0.232118
12	6	0.376291	0.011052	-0.598117
13	9	0.391869	1.085106	-1.404793
14	9	0.411056	-1.08374	-1.375281
15	6	1.62474	0.037997	0.337336
16	9	1.674536	-1.146172	0.991162
17	9	1.468108	1.023588	1.229921
18	6	2.995291	0.230383	-0.372893
19	9	3.09385	1.477122	-0.848728
20	9	3.061976	-0.63798	-1.426955
21	6	4.183224	-0.045523	0.597876
22	8	4.481199	0.750844	1.436825
23	8	4.806068	-1.207798	0.41873
24	1	4.436535	-1.696689	-0.332956

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub> + H<sub>2</sub>O<sub>2</sub>

Transition state of reaction (24)

Total energy

-2539.1020081

No.	Atom.No.	x	y	z
1	6	-3.401983	-0.043265	-0.159564
2	6	-4.052681	1.37367	-0.195764
3	6	-4.041546	-1.029528	0.865696
4	9	-3.546869	-0.586966	-1.387452
5	9	-3.426729	2.113475	-1.109722
6	9	-3.943879	1.971716	0.989383
7	9	-5.341463	1.289657	-0.522902
8	9	-3.407221	-2.198537	0.793138
9	9	-3.931366	-0.55647	2.105781
10	9	-5.33016	-1.223748	0.588099
11	8	-2.068227	0.125697	0.210521
12	6	-1.026296	-0.227716	-0.600581
13	9	-1.052317	0.438575	-1.763823
14	9	-1.02699	-1.542332	-0.878502
15	6	0.267205	0.141268	0.194556
16	9	0.162089	-0.364193	1.433061
17	9	0.334395	1.484482	0.270739
18	6	1.590452	-0.394445	-0.443843
19	9	1.564043	-0.189543	-1.770376
20	9	1.678313	-1.714734	-0.204931
21	6	2.86994	0.293772	0.1244
22	9	2.803745	0.406229	1.4495
23	9	3.029476	1.495759	-0.431298
24	16	4.45995	-0.693602	-0.2612
25	8	4.54407	-1.796777	0.67727
26	8	4.517239	-0.862506	-1.710664
27	8	5.775807	0.77936	0.430621
28	1	6.008124	1.222865	-0.405166
29	8	6.633579	1.833568	1.3842
30	1	7.096775	1.147153	1.893135

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>3</sub>F<sub>6</sub>CO<sub>2</sub><sup>-</sup>

Optimized geometry

Total energy

-1790.0208856

No.	Atom.No.	x	y	z
1	6	-1.969585	0.02086	-0.245105
2	6	-2.644986	1.333244	0.260796
3	6	-2.678866	-1.282962	0.236205
4	9	-2.05978	0.033346	-1.599798
5	9	-1.99129	2.385185	-0.224704
6	9	-2.630845	1.396121	1.592735
7	9	-3.918378	1.404272	-0.151082
8	9	-2.042184	-2.341092	-0.259028
9	9	-2.679983	-1.365963	1.566957
10	9	-3.948954	-1.320968	-0.189654
11	8	-0.681968	-0.005342	0.239078
12	6	0.438126	0.013882	-0.584897
13	9	0.418268	1.111211	-1.356407
14	9	0.434486	-1.057162	-1.397301
15	6	1.679265	-0.0033	0.365411
16	9	1.450232	-0.977903	1.265129
17	9	1.665713	1.191488	1.004045
18	6	3.054898	-0.208071	-0.330158
19	9	3.004077	0.487895	-1.503337
20	9	3.129159	-1.531612	-0.677875
21	6	4.299132	0.195855	0.576641
22	8	4.269396	-0.364006	1.685595
23	8	5.094747	0.975546	0.037767

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>3</sub><sup>-</sup>

Optimized geometry

Total energy

-2462.9770677

No.	Atom.No.	x	y	z
1	6	3.060356	0.053524	-0.253363
2	6	3.800485	-1.25957	0.148487
3	6	3.692586	1.350916	0.339165
4	9	3.143554	0.155675	-1.602112
5	9	3.199727	-2.297855	-0.427528
6	9	3.782501	-1.431923	1.470297
7	9	5.07462	-1.230181	-0.258852
8	9	2.994418	2.406746	-0.069964
9	9	3.684363	1.319156	1.671905
10	9	4.956914	1.494551	-0.07454
11	8	1.76761	-0.033433	0.225693
12	6	0.658486	-0.023129	-0.601063
13	9	0.707272	-1.048752	-1.463317
14	9	0.604494	1.11237	-1.313674
15	6	-0.576811	-0.148147	0.349223
16	9	-0.411223	0.757137	1.331813
17	9	-0.518195	-1.384666	0.885595
18	6	-1.959001	0.087601	-0.350084
19	9	-1.917424	-0.546285	-1.542057
20	9	-2.053031	1.41117	-0.57101
21	6	-3.181056	-0.425051	0.46846
22	9	-2.952331	-0.128732	1.775287
23	9	-3.188846	-1.775374	0.356161
24	16	-4.860822	0.26313	-0.047683
25	8	-4.803061	1.652966	0.418912
26	8	-4.83522	0.078152	-1.505021
27	8	-5.774134	-0.615721	0.691158

(CF<sub>3</sub>)<sub>2</sub>CFOC<sub>4</sub>F<sub>8</sub>SO<sub>2</sub>NH<sub>2</sub> + H

Transition state of reaction (25)

Total energy

-2444.073856

No.	Atom.No.	x	y	z
1	6	3.143624	0.051452	-0.237699
2	6	3.858267	-1.290091	0.111523
3	6	3.771559	1.315281	0.426827
4	9	3.225233	0.216943	-1.575957
5	9	3.243373	-2.286591	-0.523465
6	9	3.810562	-1.521734	1.422424
7	9	5.132594	-1.25731	-0.276812
8	9	3.080633	2.390165	0.051162
9	9	3.729658	1.219377	1.754684
10	9	5.038778	1.46568	0.042821
11	8	1.832389	-0.047542	0.223633
12	6	0.748719	0.015617	-0.608813
13	9	0.770611	-0.961191	-1.526971
14	9	0.681012	1.190021	-1.257904
15	6	-0.500026	-0.14946	0.315906
16	9	-0.372428	0.694446	1.351635
17	9	-0.503337	-1.415633	0.776859
18	6	-1.865216	0.137223	-0.390272
19	9	-1.864028	-0.433091	-1.606283
20	9	-2.001547	1.468044	-0.529584
21	6	-3.094915	-0.405994	0.400852
22	9	-2.952131	-0.169603	1.709968
23	9	-3.214847	-1.723418	0.194539
24	16	-4.714549	0.392371	-0.141515
25	8	-4.79338	1.699778	0.485864
26	8	-4.810936	0.175696	-1.57786
27	7	-5.765078	-0.783629	0.826781
28	1	-6.247108	-1.324442	0.103784
29	1	-6.451238	-0.153512	1.251769
30	1	-5.947195	-1.867183	1.894118



$\text{NH}_2\text{SO}_2\text{C}_3\text{F}_6\text{SO}_3^- + \text{H}$

Transition state of reaction (26)

Total energy

-1941.9323153

No.	Atom.No.	x	y	z
1	7	4.107466	0.685383	-0.460023
2	16	2.797284	-0.462445	0.126371
3	8	3.038475	-0.609294	1.547669
4	8	2.822803	-1.5756	-0.801173
5	6	1.176199	0.509414	-0.13047
6	9	1.246942	1.526195	0.744589
7	9	1.282538	1.014275	-1.375073
8	6	-0.133942	-0.318391	0.031852
9	9	-0.228695	-1.093359	-1.059297
10	9	0.039031	-1.102488	1.114796
11	6	-1.407655	0.56272	0.208435
12	9	-1.378256	1.042846	1.474121
13	9	-1.275414	1.628736	-0.629204
14	16	-3.058315	-0.29141	-0.116885
15	8	-3.054073	-0.459956	-1.574025
16	8	-2.924502	-1.52359	0.670345
17	8	-4.004223	0.701686	0.403615
18	1	3.850989	0.915776	-1.423005
19	1	3.988393	1.53278	0.100675
20	1	5.574089	0.88118	-0.669018

NH<sub>2</sub>SO<sub>2</sub>C<sub>4</sub>F<sub>9</sub> + H

Transition state of reaction (27)

Total energy

-1655.6686036

No.	Atom.No.	x	y	z
1	7	3.990162	0.639763	-0.381017
2	16	2.633118	-0.422995	0.129179
3	8	2.804745	-0.606772	1.553375
4	8	2.612333	-1.509053	-0.827354
5	6	1.007506	0.541572	-0.122727
6	9	0.999906	1.5244	0.791895
7	9	1.091893	1.094516	-1.347479
8	6	-0.28242	-0.320192	-0.016949
9	9	-0.389498	-1.048925	-1.140975
10	9	-0.15427	-1.147445	1.03493
11	6	-1.588433	0.516008	0.171354
12	9	-1.623041	0.983291	1.430153
13	9	-1.567629	1.559724	-0.682651
14	6	-2.910931	-0.272098	-0.080797
15	9	-3.054437	-0.55707	-1.372865
16	9	-2.921222	-1.405396	0.620866
17	9	-3.939116	0.483143	0.305417
18	1	3.812064	0.907171	-1.351818
19	1	3.94584	1.477618	0.203801
20	1	5.506848	0.663499	-0.518796

Table S5 Frequencies and absorption intensities of normal modes

Species	No.	Frequency (cm <sup>-1</sup> )	Intensity(KM/mol)	Assignment
PFIS <sup>2-</sup>	70	574	153	$\delta(\text{CF}_2)$
	73	593	215	$\delta(\text{SNS})$
	78	645	77	$\delta(\text{SO}_3)$
	81	696	44	$\delta(\text{SNS})$
	88	872	237	(Backbone)
	89	1013	31	$\nu_s(\text{SO}_3^-)+\delta(\text{CCC})$
	91	1050	357	$\nu_s(\text{SO}_3^-)+\delta(\text{CCC})$
	92	1076	357	$\nu_{as}(\text{SNS})$
	96	1154	182	(Backbone)
	102	1187	409	$\nu_{as}(\text{CF}_2)$
	103	1189	237	$\nu_s(\text{SO}_2)$
	105	1208	155	$\nu_{as}(\text{CF}_2)$
	108	1225	254	$\nu_{as}(\text{CF}_2)$
	109	1230	106	$\nu_{as}(\text{CF}_2)$
	110	1237	527	$\nu_{as}(\text{CF}_2)$
	111	1245	700	$\nu_{as}(\text{CF}_2)$
	112	1262	122	$\nu_{as}(\text{CF}_2)$
	113	1269	426	(Backbone)
	114	1271	332	$\nu(\text{CC})+\nu_{as}(\text{SO}_3)$
	115	1277	261	$\nu_{as}(\text{CF}_2)$
	116	1284	430	$\nu_{as}(\text{SO}_3)$
	119	1326	128	(Backbone)
	120	1339	113	$\nu_{as}(\text{SO}_2)$
122	1367	483	$\nu_{as}(\text{SO}_2)$	
PFIHS <sup>-</sup>	70	554	166	$\delta(\text{SO}_2)+\delta(\text{CF}_2)$
	73	574	98	$\delta(\text{SO}_2)+\delta(\text{CF}_2)$

	74	590	157	$\rho(\text{CF}_2)$
	85	748	60	$\delta(\text{SNS})+\omega(\text{CF}_2)$
	87	806	114	$\delta(\text{COC})$
	89	874	236	(Backbone)
	90	886	389	$\nu_{\text{as}}(\text{SNS})$
	93	1049	101	$\nu_{\text{s}}(\text{SO}_3)$
	97	1151	160	$\nu_{\text{as}}(\text{CF}_2)$
	101	1181	164	$\nu_{\text{as}}(\text{CF}_2)$
	102	1191	178	$\nu_{\text{s}}(\text{SO}_2)$
	105	1218	261	(Backbone)
	110	1243	362	$\nu_{\text{as}}(\text{CF}_2)$
	111	1247	166	$\nu_{\text{as}}(\text{CF}_2)$
	112	1259	751	$\nu(\text{CO})+\nu_{\text{s}}(\text{CF}_2)$
	114	1280	344	(Backbone)
	115	1287	382	$\nu_{\text{as}}(\text{CC})$
	116	1294	352	$\nu_{\text{as}}(\text{SO}_3^-)$
	117	1298	430	$\nu_{\text{as}}(\text{SO}_3^-)$
	120	1325	141	(Backbone)
	124	1446	378	$\nu_{\text{as}}(\text{SO}_3^-)$
	125	1455	149	$\nu_{\text{as}}(\text{SO}_2)$
	126	3618	100	$\delta(\text{NH})$
PFIHSH	71	549	202	$\delta(\text{SO}_2)+\delta(\text{CF}_2)$
	75	588	130	$\rho(\text{CF}_2)$
	86	754	100	$\delta(\text{SNS})+\omega(\text{CF}_2)$
	87	789	114	$\delta(\text{COC})$
	90	857	94	$\nu(\text{S-OH})$
	91	869	479	$\nu_{\text{as}}(\text{SNS})$
	92	874	237	(Backbone)
	93	1038	42	$\nu(\text{CC})$
	102	1185	318	$\nu_{\text{s}}(\text{CF}_2)$

	103	1196	293	$\nu_s(\text{SO}_2)$
	106	1215	217	(Backbone)
	111	1245	146	$\nu_{\text{as}}(\text{CF}_2)$
	112	1246	340	$\nu_{\text{as}}(\text{CF}_2)$
	113	1252	144	$\nu_{\text{as}}(\text{CF}_2)$
	115	1264	762	$\nu_{\text{as}}(\text{CF}_2)$
	116	1284	222	$\nu(\text{CC})$
	118	1291	466	$\nu(\text{CC})$
	120	1324	142	(Backbone)
	125	1451	172	$\nu_{\text{as}}(\text{SO}_2)$ in $\text{SO}_3\text{H}$
	126	1458	451	$\nu_{\text{as}}(\text{SO}_2)$
	127	1463	139	$\delta(\text{NH})$
	128	3607	112	$\nu(\text{NH})$
	129	3768	176	$\nu(\text{OH})$
PFBI-	63	504	204	$\delta(\text{SO}_2)$
	70	575	141	$\omega(\text{CF}_2)$
	72	589	150	$\omega(\text{SO}_2)$
	75	613	140	$\omega(\text{SO}_2)$
	88	874	237	(Backbone)
	91	1071	687	$\nu(\text{SNS})$
	98	1172	169	$\nu_s(\text{CF}_2)$
	99	1187	497	$\nu_s(\text{CF}_2)$
	102	1196	102	$\nu_{\text{as}}(\text{CF}_2)$
	104	1212	119	$\nu_{\text{as}}(\text{CF}_2)$
	105	1222	290	(Backbone)
	107	1229	165	$\nu_{\text{as}}(\text{CF}_2)$
	109	1237	184	$\nu_{\text{as}}(\text{CF}_2)$
	110	1240	636	$\nu_{\text{as}}(\text{CF}_2)$
	111	1251	721	$\nu(\text{CO})$
	112	1265	447	$\nu_{\text{as}}(\text{CF}_2)$

	113	1273	385	(Backbone)
	114	1279	123	$\nu(\text{CC})$
	115	1281	257	$\nu(\text{CC})$
	118	1326	133	(Backbone)
	121	1374	503	$\nu_{\text{as}}(\text{SO}_2)$
	122	1379	113	$\nu(\text{CC})$
PFBIH	63	486	219	$\delta(\text{SO}_2)$
	72	578	109	$\omega(\text{SO}_2)$
	73	584	96	$\omega(\text{CF}_2)$
	86	802	148	$\delta(\text{COC})$
	89	871	384	$\nu_{\text{as}}(\text{SNS})$
	90	874	239	(Backbone)
	99	1182	225	$\nu_{\text{s}}(\text{CF}_2)$
	100	1196	291	$\nu_{\text{s}}(\text{SO}_2)$
	103	1215	257	(Backbone)
	108	1246	293	$\nu_{\text{as}}(\text{CF}_2)$
	109	1251	193	$\nu_{\text{as}}(\text{CF}_2)$
	110	1252	227	$\nu_{\text{as}}(\text{CF}_2)$
	111	1255	156	$\nu_{\text{as}}(\text{CF}_2)$
	112	1264	663	$\nu(\text{CC}) + \nu_{\text{s}}(\text{CF}_2)$
	113	1275	489	$\nu_{\text{as}}(\text{CF}_2)$
	114	1284	209	$\nu(\text{CC})$
	115	1288	105	$\nu(\text{CC})$
	116	1291	488	$\nu(\text{CC})$
	117	1318	101	$\nu(\text{CC})$
	119	1324	142	(Backbone)
	122	1381	105	$\nu(\text{CC})$
	124	1458	378	$\nu_{\text{as}}(\text{SO}_2)$
	125	1463	133	$\delta(\text{NH})$
	126	3608	112	$\nu(\text{NH})$

$(\text{CF}_3)_2\text{CFOC}_4\text{F}_8\text{SO}_2\text{NH}_2$	40	495	176	$\omega(\text{NH}_2)$
	45	578	151	$\omega(\text{SO}_2) + \omega(\text{NH}_2)$
	55	873	239	(Backbone)
	56	911	93	$\nu(\text{SN})$
	63	1181	188	$\nu_s(\text{CF}_2)$
	64	1195	118	$\nu_s(\text{SO}_2)$
	66	1213	117	$\nu_{as}(\text{CF}_2)$
	67	1218	201	$\nu_{as}(\text{CF}_2)$
	70	1245	457	$\nu_{as}(\text{CF}_2)$
	71	1260	712	$\nu_{as}(\text{CF}_2)$
	72	1282	226	$\nu(\text{CC})$
	73	1289	507	$\nu(\text{CC})$
	75	1324	142	(Backbone)
	78	1425	286	$\nu_{as}(\text{SO}_2)$
	79	1617	51	$\delta(\text{NH}_2)$
$(\text{CF}_3)_2\text{CFOC}_3\text{F}_6\text{CO}_2^-$	40	708	87	$\omega(\text{CF}_2) + \delta(\text{CO}_2)$
	42	794	80	$\delta(\text{CO}_2)$
	44	873	242	(Backbone)
	51	1168	133	$\nu_s(\text{CF}_2)$
	53	1217	141	$\nu_{as}(\text{CF}_2)$
	54	1218	201	$\nu_{as}(\text{CF}_2)$
	55	1228	217	$\nu(\text{CO})$
	56	1234	961	$\nu_{as}(\text{COC})$
	57	1265	565	(Backbone)
	59	1327	130	(Backbone)
	60	1340	282	$\nu(\text{CC})$
	62	1401	80	$\nu_s(\text{CO}_2)$
	63	1831	629	$\nu_{as}(\text{CO}_2)$
$(\text{CF}_3)_2\text{CFOC}_4\text{F}_8\text{SO}_3^-$	43	581	137	$\omega(\text{CF}_2)$
	45	616	103	$\omega(\text{CF}_2)$

	53	873	239	(Backbone)
	55	1053	143	$\nu_s(\text{SO}_3)$
	59	1157	119	$\nu_{as}(\text{CF}_2)$
	64	1223	143	$\nu_{as}(\text{CF}_2)$
	65	1226	218	$\nu_{as}(\text{CF}_2)$
	66	1236	350	$\nu_s(\text{CF}_2)$
	67	1244	662	(Backbone)
	68	1269	306	(Backbone)
	69	1276	363	$\nu(\text{CC})$
	70	1286	366	$\nu_{as}(\text{SO}_3)$
	71	1293	503	$\nu_{as}(\text{SO}_3)$
	73	1327	147	(Backbone)



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