

Table S1: Fragment charge analysis for C-TEMPYLNO with ILs using geodesic charge scheme

Anion	Cation	Configuration	Charge on Cation	Charge on Anion	Charge on Radical
N(CN) ₂	C ₁ mim	configuration 1	0.85	-0.87	0.02
N(CN) ₂	C ₁ mim	configuration 2	0.83	-0.85	0.02
N(CN) ₂	P _{1,1,1,1}	configuration 1	0.84	-0.86	0.02
N(CN) ₂	C ₁ mpyr	configuration 1	0.82	-0.87	0.04
N(CN) ₂	C ₁ mpyr	configuration 2	0.9	-0.88	-0.02
SO ₃ CH ₃	C ₁ mim	configuration 1	0.82	-0.84	0.01
SO ₃ CH ₃	C ₁ mim	configuration 2	0.9	-0.89	-0.02
SO ₃ CH ₃	P _{1,1,1,1}	configuration 1	0.85	-0.89	0.03
SO ₃ CH ₃	C ₁ mpyr	configuration 1	0.91	-0.86	-0.05
SO ₃ CH ₃	C ₁ mpyr	configuration 2	0.96	-0.89	-0.07
N(SO ₂ CF ₃) ₂	C ₁ mim	configuration 1	0.81	-0.7	-0.11
N(SO ₂ CF ₃) ₂	C ₁ mim	configuration 2	0.84	-0.79	-0.05
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 1	0.98	-0.99	0
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 2	0.85	-0.92	0.07
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 1	0.75	-0.92	0.17
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 2	0.87	-0.88	0
BF ₄	C ₁ mim	configuration 1	0.82	-0.89	0.07
BF ₄	C ₁ mim	configuration 2	0.92	-0.92	0
BF ₄	P _{1,1,1,1}	configuration 1	0.85	-0.93	0.07
BF ₄	P _{1,1,1,1}	configuration 2	0.88	-0.92	0.04
BF ₄	C ₁ mpyr	configuration 1	0.92	-0.89	-0.04
SO ₃ CF ₃	C ₁ mim	configuration 1	0.8	-0.94	0.14
SO ₃ CF ₃	C ₁ mim	configuration 2	0.97	-0.96	-0.01
SO ₃ CF ₃	P _{1,1,1,1}	configuration 1	0.93	-0.98	0.05
SO ₃ CF ₃	C ₁ mpyr	configuration 1	1.04	-0.13	-0.91
SO ₃ CF ₃	C ₁ mpyr	configuration 2	1.09	-0.1	-0.99

Table S2: Interaction energies between radicals and ILs in kJ mol⁻¹

Anion	Cation	Configuration	HF/cc-pVTZ Reference Energy	SRS/MP2 Correlation Energy	Total SRS/MP2 Electronic Energy
N(CN) ₂	C ₁ mim	configuration 1	20.0	-50.4	-30.4
N(CN) ₂	C ₁ mim	configuration 2	9.0	-53.8	-44.8
N(CN) ₂	P _{1,1,1,1}	configuration 1	20.4	-52.2	-31.8
N(CN) ₂	P _{1,1,1,1}	configuration 2	-5.4	-58.2	-63.6
N(CN) ₂	C ₁ mpyr	configuration 1	0.5	-49.3	-48.8
N(CN) ₂	C ₁ mpyr	configuration 2	1.2	-57.3	-56.1
SO ₃ CH ₃	C ₁ mim	configuration 1	-3.6	-74.2	-77.8
SO ₃ CH ₃	C ₁ mim	configuration 2	-10.8	-57.5	-68.2
SO ₃ CH ₃	P _{1,1,1,1}	configuration 1	22.4	-50.7	-28.2
SO ₃ CH ₃	C ₁ mpyr	configuration 1	2.6	-53.0	-50.4
SO ₃ CH ₃	C ₁ mpyr	configuration 2	7.4	-58.9	-51.5
N(SO ₂ CF ₃) ₂	C ₁ mim	configuration 1	-2.2	-79.0	-81.2
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 1	6.8	-65.8	-59.0
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 2	5.9	-59.4	-53.5
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 1	-15.4	-55.5	-70.9
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 2	7.4	-59.1	-51.6
BF ₄	C ₁ mim	configuration 1	0.7	-54.4	-53.6
BF ₄	C ₁ mim	configuration 2	-10.3	-54.7	-64.9
BF ₄	P _{1,1,1,1}	configuration 1	27.0	-44.1	-17.1
BF ₄	P _{1,1,1,1}	configuration 2	18.0	-48.1	-30.1
BF ₄	C ₁ mpyr	configuration 1	0.4	-49.0	-48.6
SO ₃ CF ₃	C ₁ mim	configuration 1	-9.0	-76.6	-85.6
SO ₃ CF ₃	C ₁ mim	configuration 2	-8.3	-57.0	-65.3
SO ₃ CF ₃	P _{1,1,1,1}	configuration 1	22.2	-51.1	-28.9
SO ₃ CF ₃	C ₁ mpyr	configuration 1	-10.5	-70.3	-80.9
SO ₃ CF ₃	C ₁ mpyr	configuration 2	8.9	-58.2	-49.3

Table S3: Bond distances between O radical centre and cation/anion in Å

Anion	Cation	Configuration	Distance to anion	Distance to Cation
N(CN) ₂	C ₁ mim	configuration 1	4.15	2.097
N(CN) ₂	C ₁ mim	configuration 2	4.734	2.118
N(CN) ₂	P _{1,1,1,1}	configuration 1	4.749	2.241
N(CN) ₂	C ₁ mpyr	configuration 1	3.164	2.356
N(CN) ₂	C ₁ mpyr	configuration 2	3.241	2.35
SO ₃ CH ₃	C ₁ mim	configuration 1	5.029	3.365
SO ₃ CH ₃	C ₁ mim	configuration 2	3.619	2.53
SO ₃ CH ₃	P _{1,1,1,1}	configuration 1	4.131	2.286
SO ₃ CH ₃	C ₁ mpyr	configuration 1	4.617	2.319
SO ₃ CH ₃	C ₁ mpyr	configuration 2	4.608	2.292
N(SO ₂ CF ₃) ₂	C ₁ mim	configuration 1	4.783	2.153
N(SO ₂ CF ₃) ₂	C ₁ mim	configuration 2	4.66	2.058
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 1	4.564	2.21
N(SO ₂ CF ₃) ₂	P _{1,1,1,1}	configuration 2	4.564	2.226
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 1	2.842	2.424
N(SO ₂ CF ₃) ₂	C ₁ mpyr	configuration 2	3.877	2.368
BF ₄	C ₁ mim	configuration 1	4.46	2.4
BF ₄	C ₁ mim	configuration 2	3.297	2.512
BF ₄	P _{1,1,1,1}	configuration 1	4.262	2.244
BF ₄	P _{1,1,1,1}	configuration 2	3.878	2.292
BF ₄	C ₁ mpyr	configuration 1	4.493	2.318
SO ₃ CF ₃	C ₁ mim	configuration 1	4.951	3.122
SO ₃ CF ₃	C ₁ mim	configuration 2	3.559	2.425
SO ₃ CF ₃	P _{1,1,1,1}	configuration 1	4.131	2.286
SO ₃ CF ₃	C ₁ mpyr	configuration 1	4.477	2.447
SO ₃ CF ₃	C ₁ mpyr	configuration 2	4.593	2.322

Table S4: Comparison of TEMPO and **Rad-1** maximum interaction energy to investigate effect of carboxylic acid group. All energies in kJ mol⁻¹.

Radical	Ionic Liquid	Dispersion Energy	Electrostatic Energy	Total Energy
Rad-1	[C ₁ mim][CF ₃ SO ₃]	-9.0	-76.6	-85.6
TEMPO	[C ₁ mim][CF ₃ SO ₃]	-12.7	-70.2	-82.9
Rad-1	[C ₁ mpyr][N(CF ₃ SO ₂) ₂]	-15.4	-55.5	-70.9
TEMPO	[C ₁ mpyr][N(CF ₃ SO ₂) ₂]	-8.6	-65.7	-74.3
Rad-1	[C ₁ mpyr][CF ₃ SO ₃]	-10.5	-70.3	-80.9
TEMPO	[C ₁ mpyr][CF ₃ SO ₃]	-6.3	-70.6	-76.9

Figure S1: Structures of TEMPO and **Rad-1** structures used for Table S4

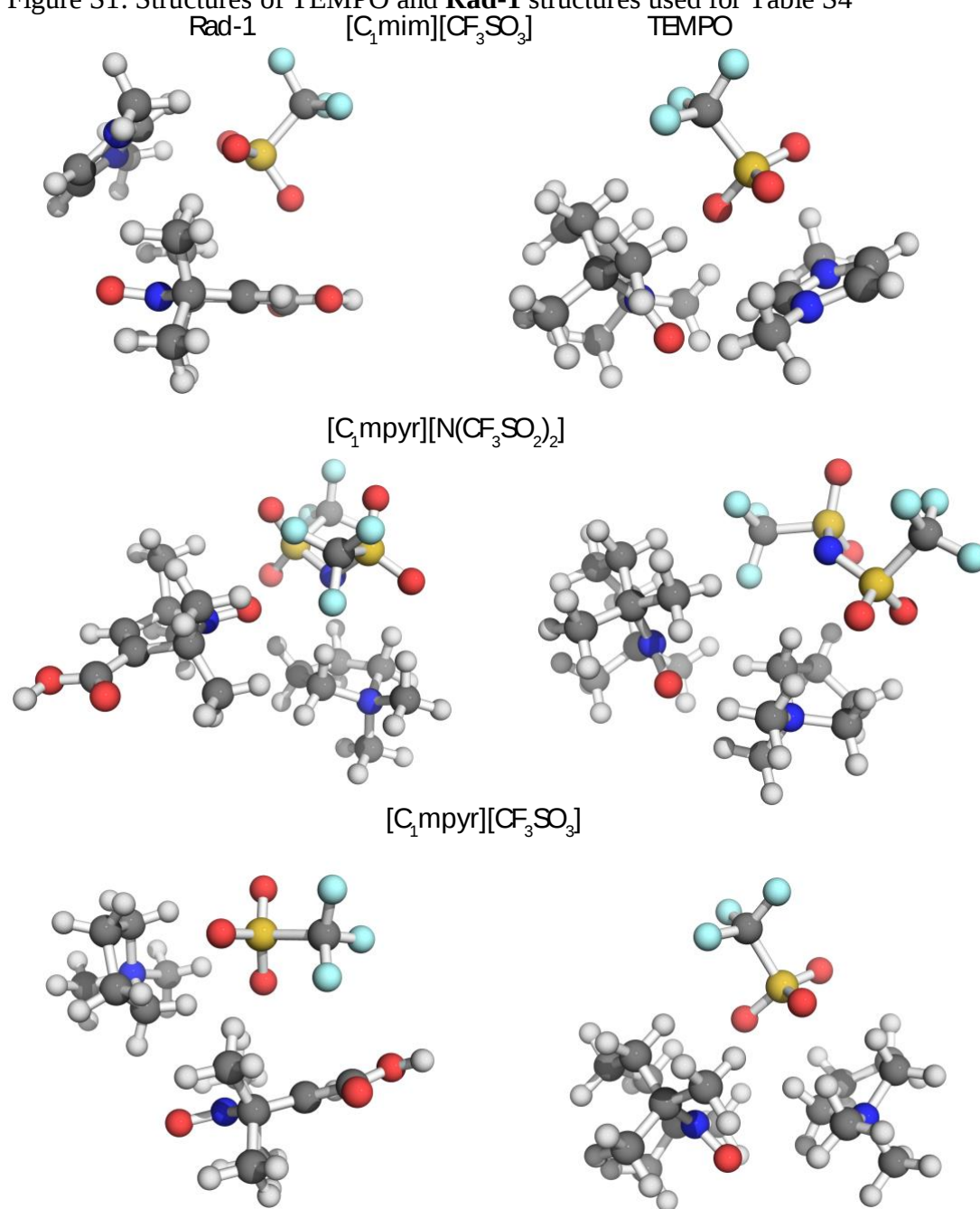


Table S5: Partial atomic charges of the NO group on **Rad-1** calculated with the Geodesic scheme.

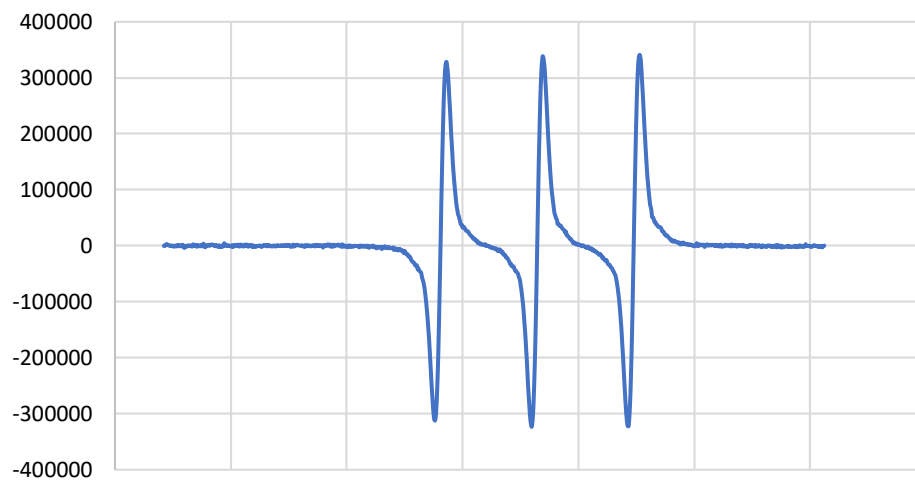
Ionic Liquid	Configuration	With the IL present		With no IL Present	
		N Charge	O Charge	N Charge	O Charge
[C ₁ mim][CF ₃ SO ₃]	1	-0.0198	-0.4293	0.0611	-0.4072
[C ₁ mim][CF ₃ SO ₃]	2	0.0107	-0.415	0.0676	-0.4155
[C ₁ mpyr][N(CF ₃ SO ₂) ₂]	1	0.0695	-0.4831	0.1088	-0.4236

Each room temperature experimental EPR spectrum had present the three peaks characteristic of the nitroxide. The first derivative spectra produced as an instrumental response was doubly integrated to give the area of the first, second, and third peak of the nitroxides spectrum. These peaks are designated as I-1, I₀ and I+1 respectively. The ratio of areas of I₀/I-1 as well as I₀/I+1 are reported along with their average and the 95% confidence intervals. For all experimental samples, serial dilutions from a stock of the radical were performed to ensure a consistent number of spins per unit volume. The EPR tubes used have small variations in their pathlength resulting in differences in the number of radicals present in the path of detection, however, the concentration of radical present remains consistent throughout the sample. We attribute increased signal to noise ratio in some samples to this diminished pathlength effect. In other words, some samples have less radicals in the path of detection and therefore a smaller signal which manifests the appearance of a higher signal to noise ratio. For a given solvent inclusion of a replicate with this feature does not correlate to increased error margins. Because each rotational diffusion coefficient was determined not from absolute intensities in comparison to other spectra but through an internal reference to the central peak and the concentration of radical was consistent among the samples the variation in pathlength had no observable effect on the calculated relative peak areas or the corresponding rotational diffusion coefficients. All replicates for a particular solvent show agreement within a 95% confidence interval.

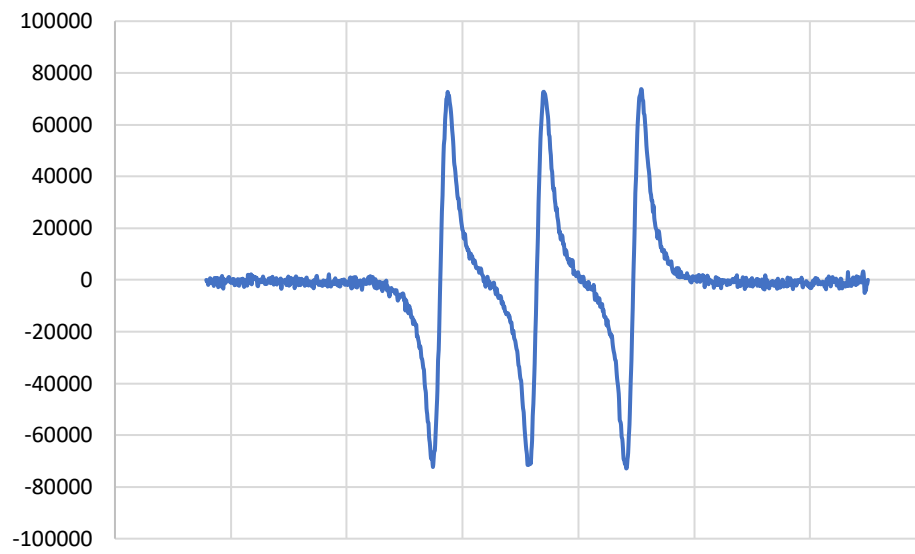
Table S6: Average areas of EPR peaks with potential error margins shown within a 95% confidence interval.

Solvent	I_0/I_{-1}	I_0/I_{+1}
DCM	0.98	0.95
	0.98	0.97
	1.00	0.96
DCM Average	0.98 ± 0.03	0.96 ± 0.02
[Im][BF ₄]	0.75	0.74
	0.80	0.77
	0.70	0.78
[Im][BF₄] Average	0.75 ± 0.09	0.76 ± 0.04
[Im][DCA]	0.79	0.78
	0.88	0.86
	0.90	0.87
[Im][DCA] Average	0.85 ± 0.12	0.83 ± 0.11
[Im][NTf ₂]	0.80	0.76
	0.82	0.79
	0.83	0.81
[Im][NTf₂] Average	0.82 ± 0.03	0.78 ± 0.05
[Im][Trif]	0.71	0.66
	0.73	0.67
	0.73	0.69
[Im][Trif] Average	0.72 ± 0.02	0.67 ± 0.03
Paraffin	0.87	0.85
	0.86	0.87
	0.86	0.85
Paraffin Average	0.86 ± 0.02	0.86 ± 0.02
[Pyr][DCA]	0.85	0.82
	0.87	0.86
	0.77	0.75
[Pyr][DCA] Average	0.83 ± 0.11	0.81 ± 0.12
[Pyr][NTf ₂]	0.83	0.80
	0.78	0.75
	0.76	0.74
[Pyr][NTf₂] Average	0.79 ± 0.07	0.77 ± 0.06
[Pyr][Trif]	0.77	0.72
	0.77	0.73
	0.78	0.74
[Pyr][Trif] Average	0.77 ± 0.02	0.73 ± 0.02

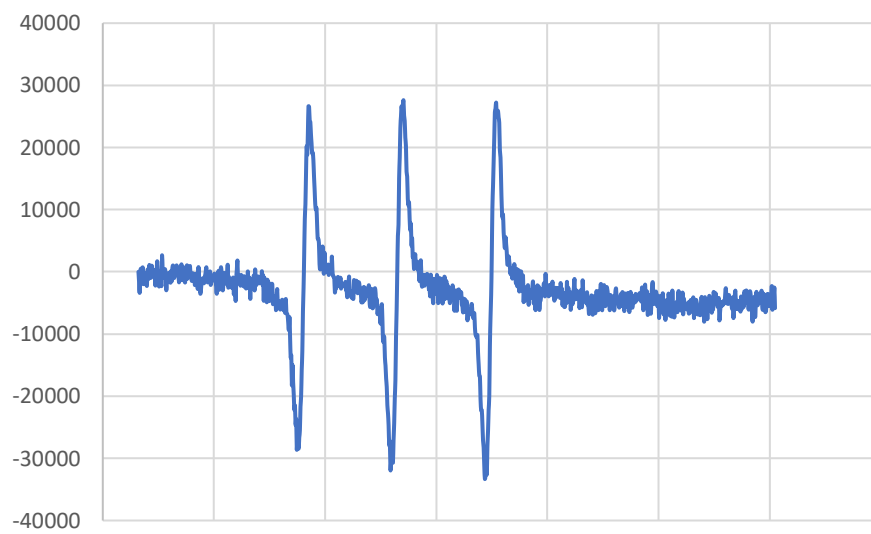
DCM Rep 1:



DCM Rep 2:



DCM Rep 3:



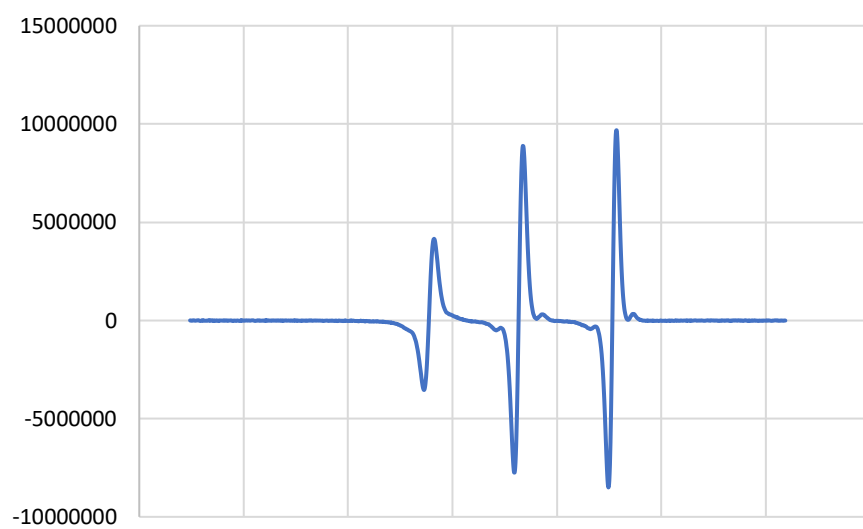
C₂mim BF₄ Rep 1:



C₂mim BF₄ Rep 2:



C₂mim BF₄ Rep 3:



C₂mim N(CN)₂ Rep 1:



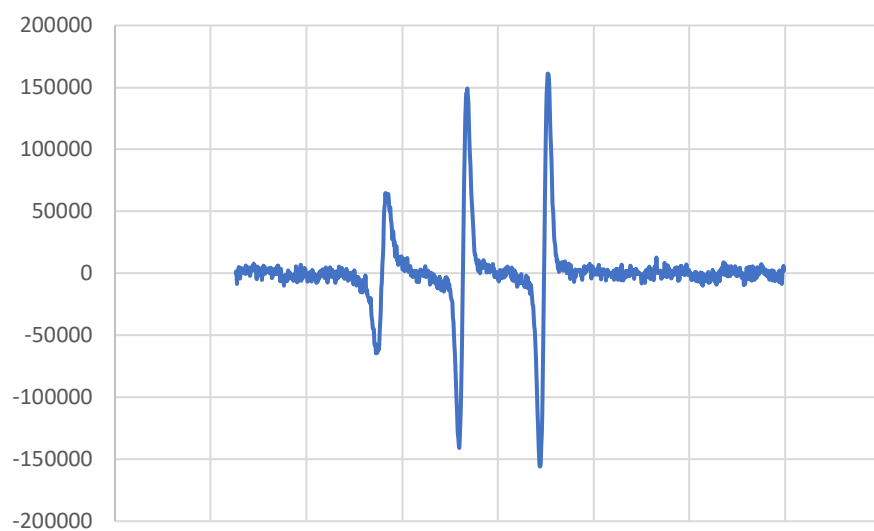
C₂mim N(CN)₂ Rep 2:



C₂mim N(CN)₂ Rep 3:



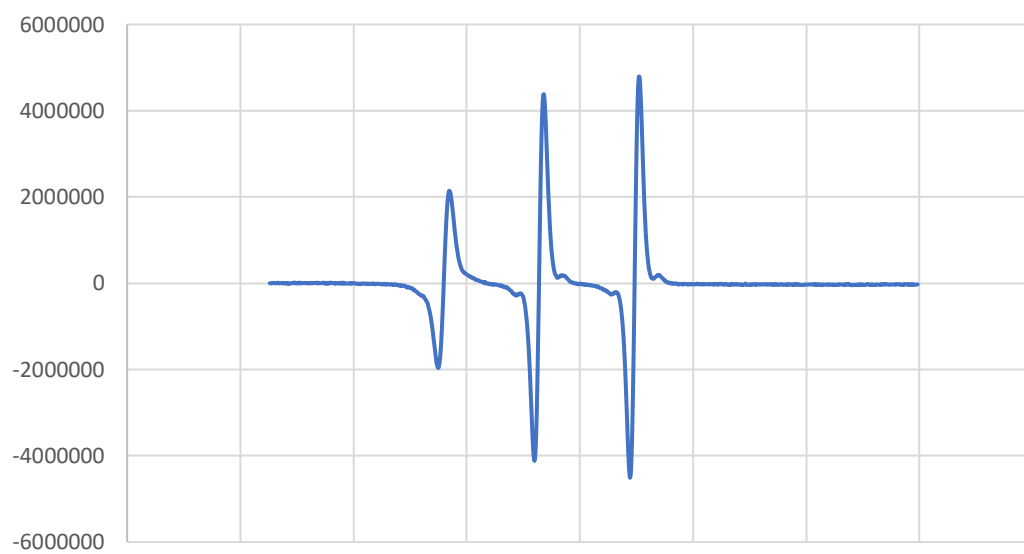
C₂mim N(SO₂CF₃)₂ Rep 1:



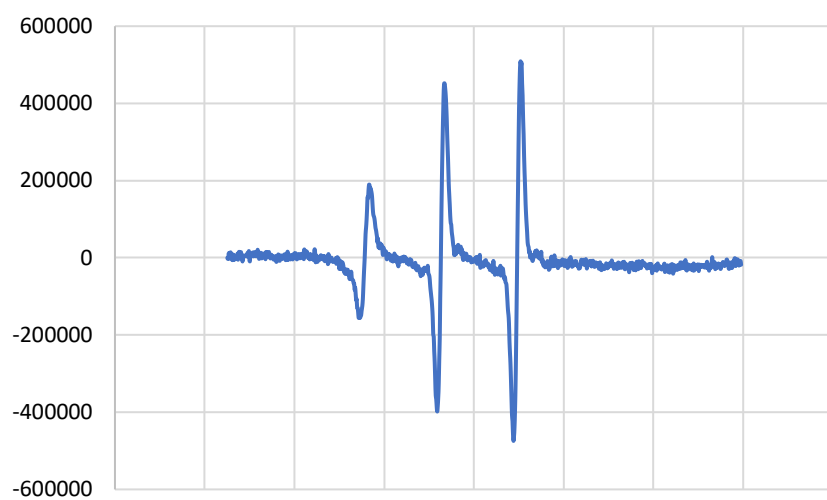
C₂mim N(SO₂CF₃)₂ Rep 2:



C₂mim N(SO₂CF₃)₂ Rep 3:



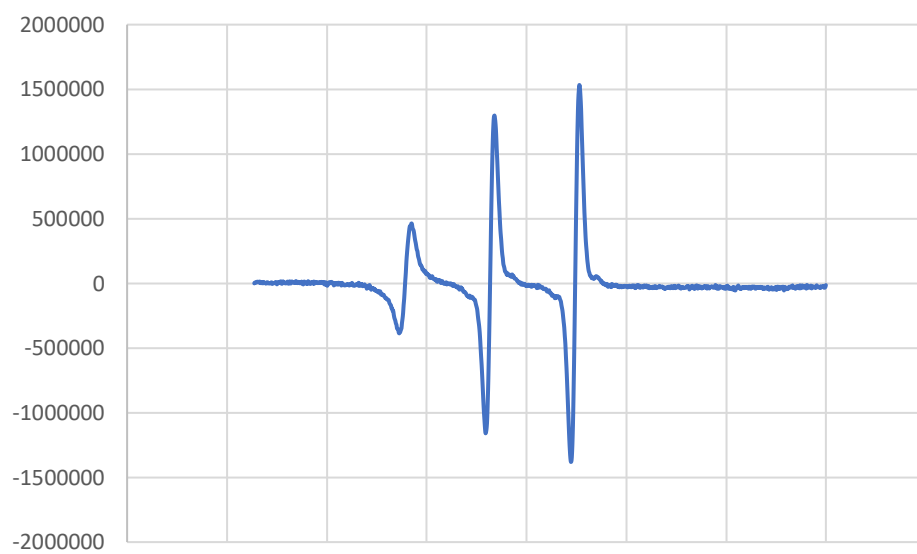
C₂mim SO₃CF₃ Rep 1:



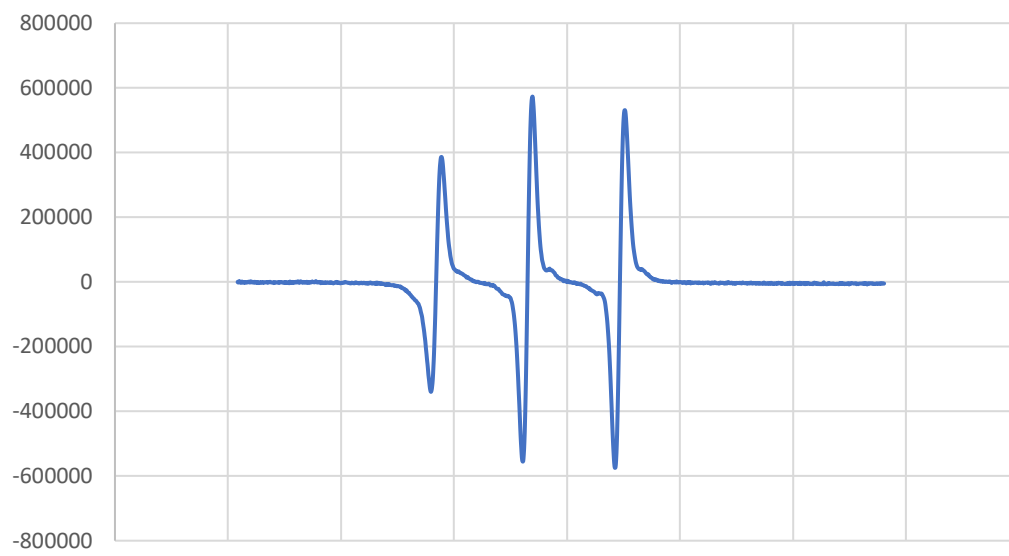
C₂mim SO₃CF₃ Rep 2:



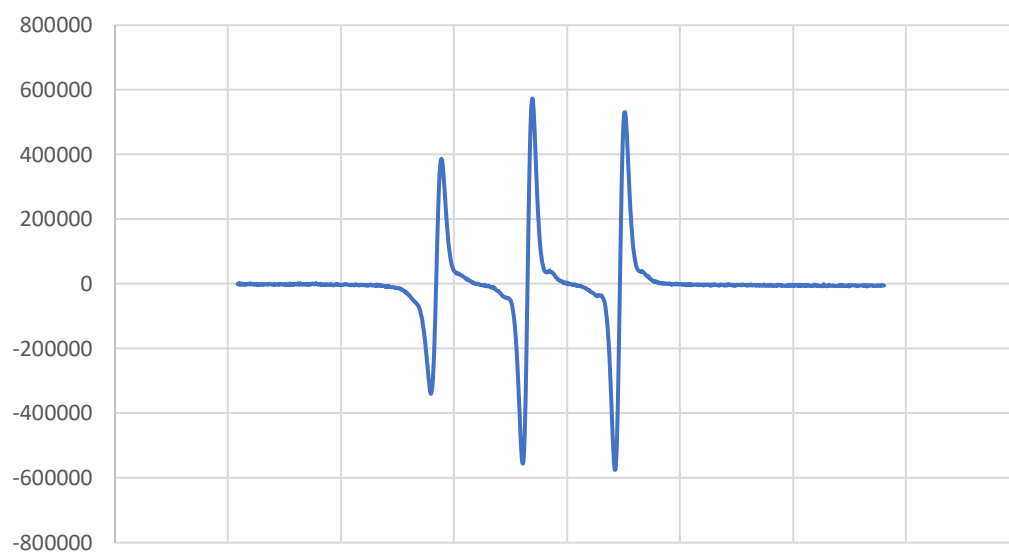
C₂mim SO₃CF₃ Rep 3:



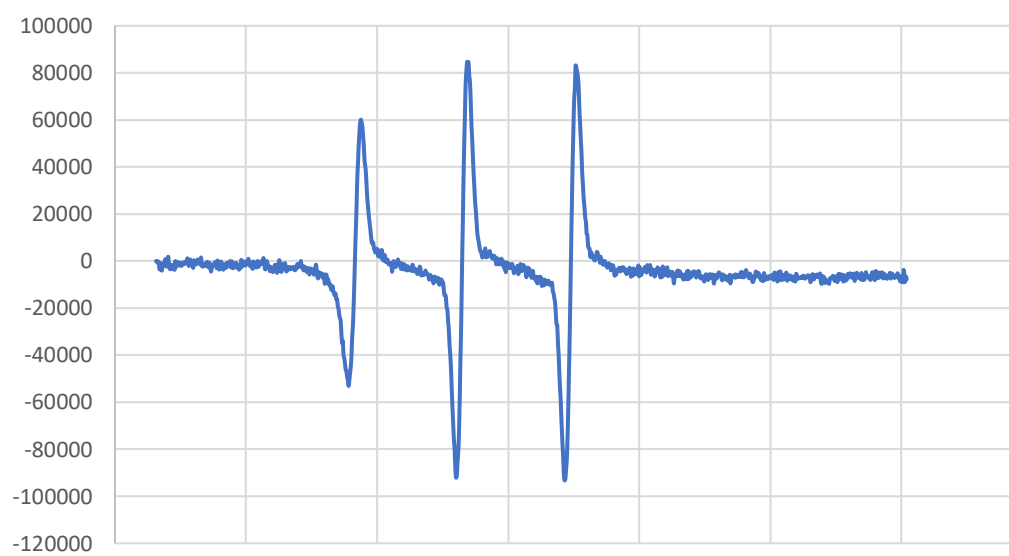
Paraffin oil rep 1:



Paraffin oil rep 2:



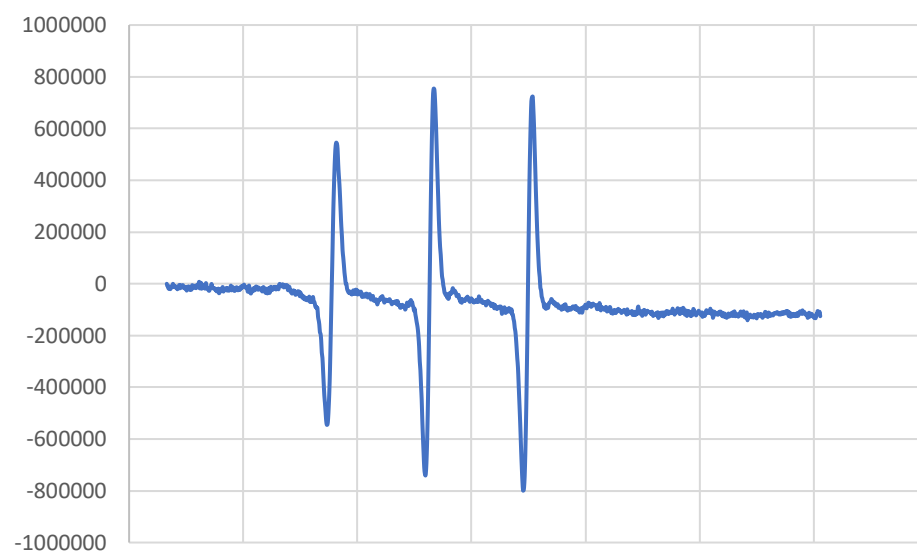
Paraffin oil rep 3:



C₄mpyr N(CN)₂ rep 1:



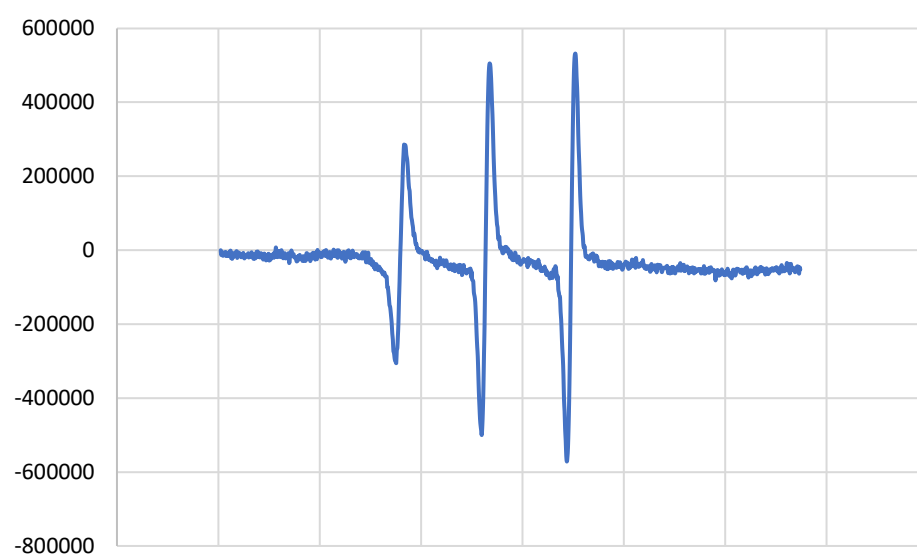
C₄mpyr N(CN)₂ rep 2:



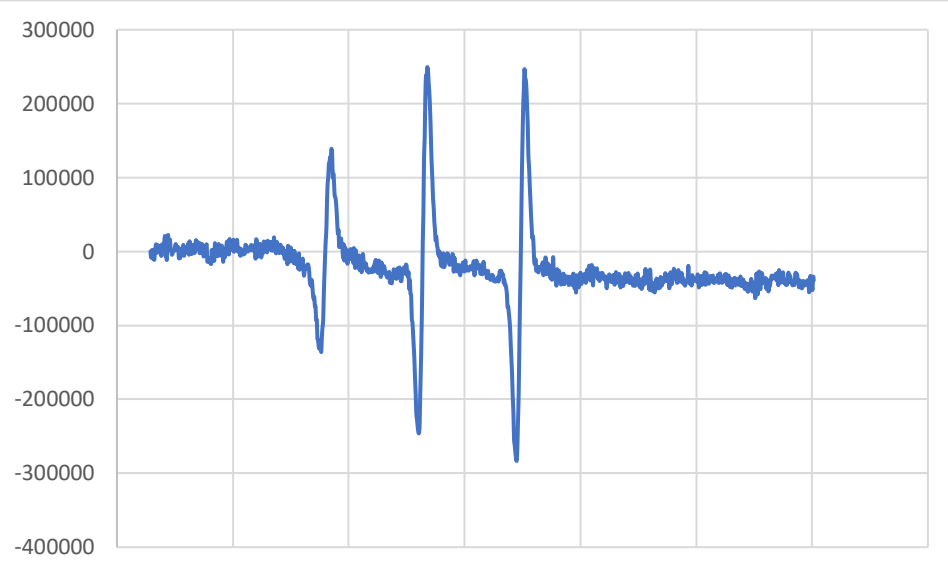
C₄mpyr N(CN)₂ rep 3:



C₃mpyr N(SO₂CF₃)₂ rep 1:



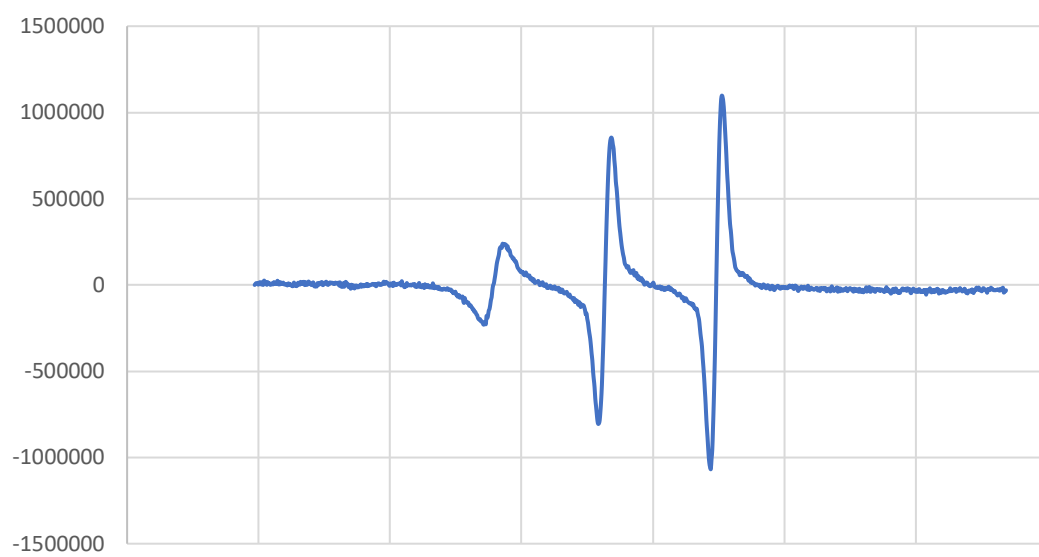
C₃mpyr N(SO₂CF₃)₂ Rep 2:



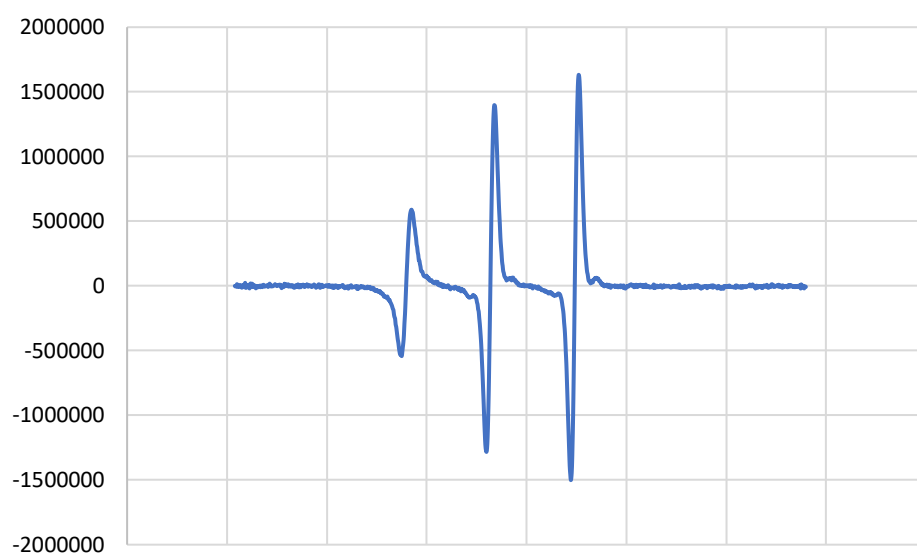
C₃mpyr N(SO₂CF₃)₂ Rep 3:



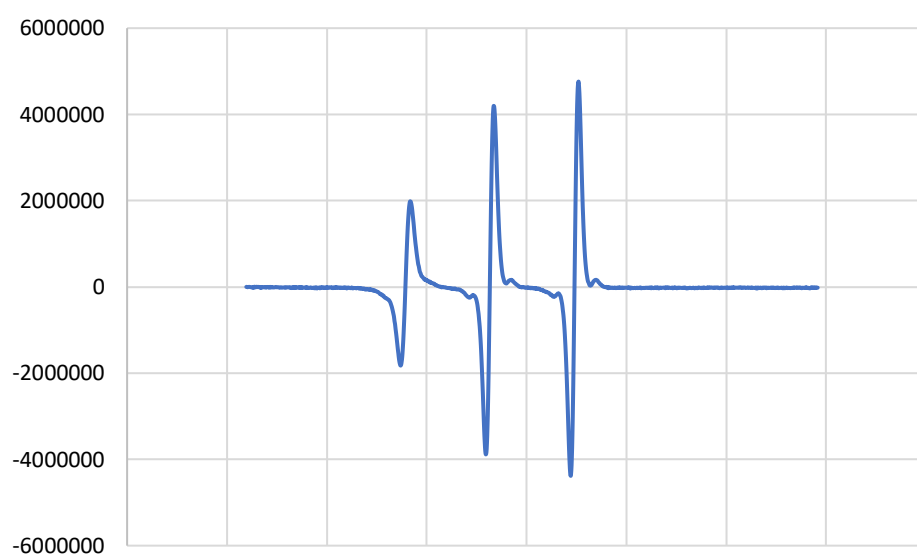
C₄mpyr SO₃CF₃ conf 1:



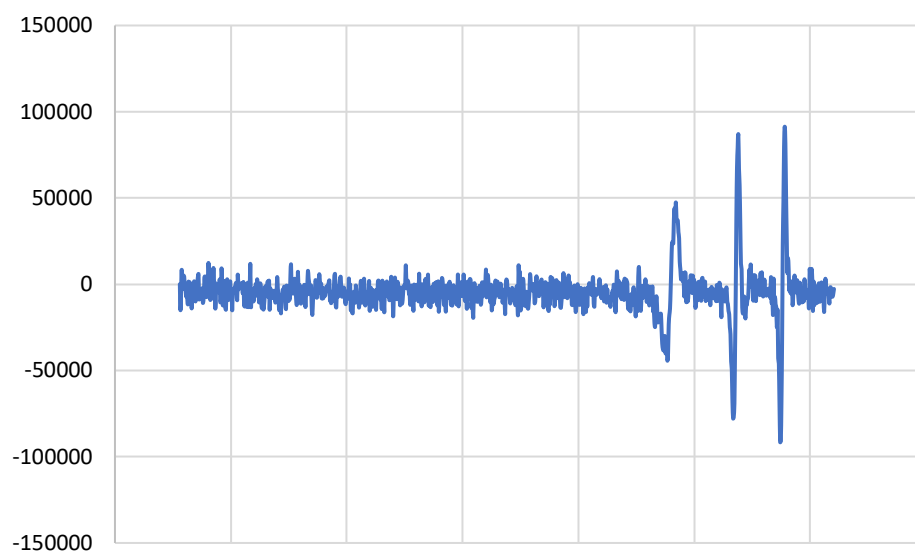
C₄mpyr SO₃CF₃ conf 2:



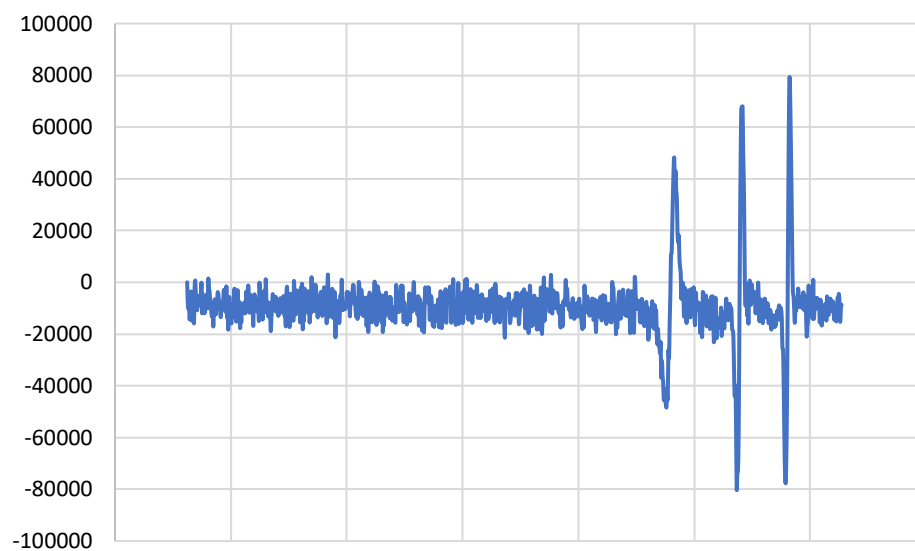
C₄mpyr SO₃CF₃ conf 3:



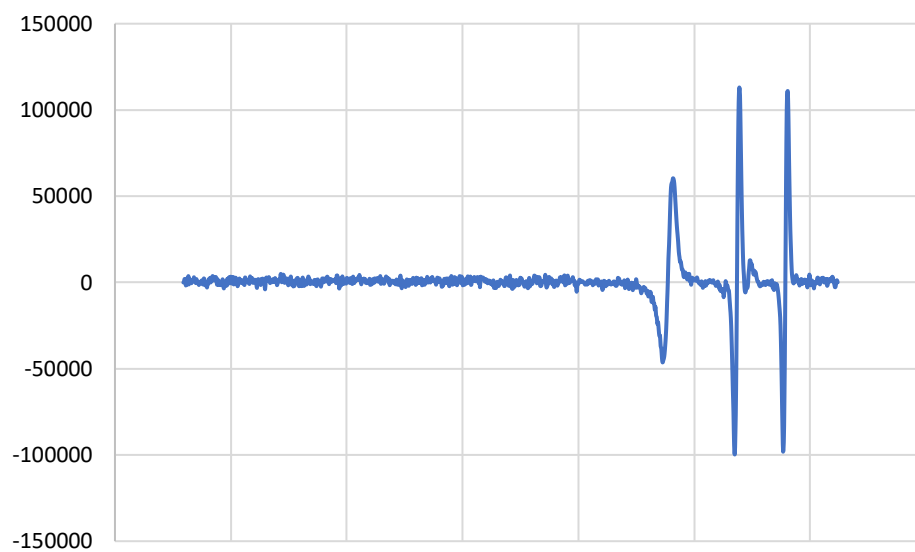
C₂mim BF₄ 80°C:



C₂mim N(CN)₂ 80°C:



C₄mpyr N(CN)₂ 80°C:



C₁mim BF₄ conf 1:

C	-1.050855732	-1.818134436	0.615402419
N	0.177299138	-1.526016822	1.166572087
C	1.081913986	-1.471891847	0.190150839
N	0.481208024	-1.743593289	-0.964207771
C	-0.858327357	-1.952858564	-0.726212652
C	0.444865754	-1.198759553	2.563642532
C	1.099308515	-1.634556977	-2.280142927
F	0.137024836	1.044880648	-0.979118580
B	1.381916680	1.456528154	-0.436453135
F	1.370555326	1.213034610	0.957695931
F	1.590660610	2.811117191	-0.689558002
F	2.408095033	0.681218992	-1.026513953
H	2.125293555	-1.202190960	0.306295064
H	-1.553423183	-2.186393151	-1.523170695
H	-1.960224271	-1.874520975	1.202612183
H	-0.385274129	-1.573151125	3.170410810
H	1.374107198	-1.687561902	2.875065429
H	0.540837317	-0.110949628	2.656349342
H	2.183913982	-1.709591916	-2.165728169
H	0.726538394	-2.445486970	-2.914215100
H	0.844488914	-0.653648821	-2.696790913
H	-5.881989896	1.533504485	-1.006555868
H	-5.286909914	2.003562881	1.595572675
C	-5.225848606	0.997732416	-1.706691062
C	-4.357697604	1.690357603	2.092798231
H	-5.480530254	-0.071232948	-1.685336809
H	-4.514621752	0.702662069	2.548616913
H	-4.106836266	2.419321084	2.874421515
H	-5.392498196	1.386294262	-2.720927917
C	-2.714281576	4.141100609	0.789170482
C	-3.380712667	2.593369094	-1.062631883
C	-3.086664246	2.828295906	0.220858985
C	-3.755113123	1.159484665	-1.311122387
C	-3.207349432	1.596260896	1.087818884
N	-3.539132806	0.595926396	0.043090908
O	-2.624831178	5.102793952	-0.139423195
O	-2.515924629	4.341259631	1.966915152
O	-3.797078660	-0.609128271	0.316712821
H	-2.381188655	5.923787497	0.322650184
H	-3.368046927	3.341405741	-1.855377195
C	-1.900976964	1.212565575	1.780966448
C	-2.834271626	0.473002692	-2.319667004
H	-2.957870734	0.932864647	-3.310637115
H	-1.616630215	2.005477716	2.485931341
H	-2.058439662	0.281910255	2.346468651
H	-3.112987568	-0.588185403	-2.391494736
H	-1.093951662	1.069387892	1.048124086
H	-1.786547770	0.561136003	-2.001066843

C₁mimBF₄ conf 2:

C	0.443164931	-0.825201720	-2.866996782
N	0.064832874	-1.085975513	-1.565927271
C	0.214488225	0.025139898	-0.846916626
N	0.656605314	0.992784718	-1.642351277
C	0.811899950	0.486559456	-2.914671660
C	-0.447930509	-2.347747181	-1.039863919
C	0.853533617	2.373412567	-1.210635895
F	-2.154953682	1.445600235	-0.458129907
B	-2.124869692	1.051103351	0.892506242
F	-2.033853096	-0.365401015	0.960185964
F	-3.257088410	1.495051345	1.568913375
F	-0.950885776	1.590332117	1.489723075

H	0.004352171	0.141513156	0.210411441
H	1.155782760	1.099916526	-3.739492923
H	0.405095013	-1.584441568	-3.639528700
H	0.382940618	-3.016470842	-0.782301494
H	-1.052425776	-2.116061292	-0.156334222
H	-1.075581776	-2.815532373	-1.805338782
H	1.924311441	2.602736420	-1.198222475
H	0.319285243	3.034010079	-1.902260682
H	0.438320892	2.459287483	-0.201853233
H	0.607046452	-1.824478230	1.717703596
H	2.581231460	-1.934843988	-0.672797615
C	0.761066689	-1.108055155	2.537835377
C	3.420531896	-1.225134630	-0.713568404
H	0.139586203	-0.217980940	2.364680652
H	3.113654473	-0.338932124	-1.290519342
H	4.270439906	-1.707249643	-1.213287136
H	0.443242945	-1.581923055	3.477403996
C	5.032391315	-2.973931959	1.434128127
C	3.157823120	-1.887184957	2.695348823
C	4.002933592	-1.937592032	1.659077422
C	2.233701409	-0.703679871	2.627563596
C	3.821986718	-0.787580768	0.695619802
N	2.676313450	-0.105566299	1.344297394
O	5.043639635	-3.912749436	2.389328247
O	5.790468254	-2.981884367	0.489884581
O	2.247249536	1.009225027	0.936976312
H	5.747286242	-4.545269007	2.161445320
H	3.120578827	-2.612363497	3.508436300
C	5.027009251	0.153701461	0.656009014
C	2.456991278	0.296490003	3.763832662
H	2.123361494	-0.133466660	4.718151433
H	5.879760971	-0.359466646	0.193005131
H	4.769941266	1.044302100	0.065975425
H	1.871303880	1.202252497	3.553923897
H	5.305166516	0.469081871	1.671654685
H	3.518978888	0.567274456	3.844186455

C₁mim N(CN)₂ conf 1:

C	-0.963157347	-0.413625192	-0.743481392
N	-2.062889814	-0.454740783	0.008434507
C	-2.566459809	0.822359216	0.125355153
C	-1.746539572	1.639937667	-0.592966774
N	-0.759580146	0.845071937	-1.130486137
C	0.340384172	1.297893901	-1.979031268
C	-2.618216815	-1.642081340	0.651300336
H	1.042272474	0.463058624	-2.085629775
H	-0.054871156	1.595261794	-2.957305648
H	0.824275558	2.145956635	-1.480648560
H	-1.767362523	2.711373628	-0.754123616
H	-3.449995900	1.035328369	0.715735640
H	-3.681974235	-1.716586222	0.400125116
H	-2.092217635	-2.522481914	0.268784535
H	-2.477536054	-1.545931419	1.734394668
N	-1.299645185	-0.020040278	3.166070286
C	-0.405824011	0.411931631	2.541438717
N	0.655506756	0.762278956	1.845187549
C	0.736573547	1.977931343	1.345493998
N	0.913529625	3.019477135	0.836120910
H	-0.308289688	-1.247966214	-0.992233257
H	3.138748234	-4.521347431	-0.818179677
H	4.847698354	-2.304178706	-1.920339089
C	2.255012118	-4.297653207	-0.204677938
C	4.627742525	-1.249253296	-1.702765310
H	1.371364540	-4.250612452	-0.856360265
H	4.020185074	-0.836355131	-2.520078256
H	5.570577991	-0.692107004	-1.631648416

H	2.114502221	-5.103177626	0.529204486
C	5.842442259	-1.502650454	1.257957555
C	3.726337737	-2.842170283	1.242928821
C	4.497909109	-1.863088831	0.758756918
C	2.417206527	-2.956602491	0.513062856
C	3.856702837	-1.117550862	-0.389590628
N	2.583217251	-1.872349441	-0.482974143
O	6.236701694	-2.268383464	2.283738862
O	6.523219399	-0.614688028	0.795775606
O	1.718103395	-1.633038644	-1.372409588
H	7.122823655	-1.962788433	2.545465848
H	3.991303854	-3.498140781	2.072122408
C	3.569161650	0.345986272	-0.049262272
C	1.220599693	-2.657195728	1.419300728
H	1.164357183	-3.402283400	2.225305221
H	4.518190854	0.873025697	0.116016637
H	3.039171057	0.824809210	-0.884817914
H	0.292260111	-2.718472756	0.832365148
H	2.944482506	0.413013334	0.852690857
H	1.305385931	-1.649683535	1.849226557

C₁mim N(CN)₂ conf 2:

C	0.866621493	-1.469205938	0.425406791
N	2.072033744	-1.748432131	-0.066296214
C	3.018668990	-1.075342800	0.671946005
C	2.353374128	-0.390873600	1.645047035
N	1.013073577	-0.658331562	1.475033034
C	-0.066311141	-0.191949613	2.344808575
C	2.332473739	-2.508055981	-1.283393541
H	-1.016633026	-0.491589335	1.889326353
H	0.045242329	-0.657940428	3.330913497
H	0.007528204	0.899227433	2.423072493
H	2.704752654	0.270241385	2.428584075
H	4.075100447	-1.135795914	0.437437078
H	3.206338532	-3.147238892	-1.120444495
H	1.457612418	-3.128688217	-1.500978702
H	2.504176510	-1.796459504	-2.098674528
H	-0.093308076	-1.807620330	0.038739311
N	1.680536012	0.507273842	-1.985254654
C	1.747763484	1.472765767	-1.321455011
N	1.844013418	2.614701672	-0.676011221
C	1.567059487	2.615780347	0.610201431
N	1.341171905	2.711643018	1.757878686
H	-4.165318455	0.589392041	1.787287641
H	-1.912630341	1.912963286	0.502962504
C	-4.619461247	-0.331463125	1.395316341
C	-1.450267119	1.526153993	-0.416889330
H	-4.168526133	-1.196218039	1.902211149
H	-0.580591907	0.906419634	-0.154470204
H	-1.098335986	2.367577180	-1.028829812
H	-5.697651577	-0.317241222	1.606467720
C	-3.836427991	2.616885267	-2.271120075
C	-4.793173676	0.775192210	-0.869769361
C	-3.758063996	1.381168677	-1.462095729
C	-4.379045638	-0.454416609	-0.111133753
C	-2.440605052	0.680245211	-1.217773182
N	-2.923991322	-0.447910049	-0.384895163
O	-5.086753362	3.085621669	-2.380617313
O	-2.881325530	3.156360514	-2.782485280
O	-2.156725785	-1.332740425	0.087817751
H	-5.042611847	3.894129143	-2.920462312
H	-5.827845082	1.115133568	-0.914263425
C	-1.793831466	0.143562123	-2.495147557
C	-5.000067809	-1.736998311	-0.668124085
H	-6.077702787	-1.759961044	-0.455628544
H	-1.525107020	0.987456758	-3.144107324

H	-0.873424158	-0.401329737	-2.242160401
H	-4.521850531	-2.601657367	-0.187223734
H	-2.487497492	-0.520186178	-3.030745124
H	-4.846725517	-1.802928384	-1.754137395

C₁mim SO₃CH₃ conf 1:

C	2.177686212	-2.028999748	1.643399697
N	2.545371243	-0.701788974	1.688264952
C	2.837446972	-0.293079734	0.454430362
N	2.679240072	-1.319792891	-0.380551274
C	2.261243397	-2.417782118	0.339988281
C	2.559538154	0.169143425	2.861543370
C	2.930138863	-1.255633185	-1.818003093
H	3.090304477	0.728837905	0.187735766
H	2.046163794	-3.368962154	-0.132617664
H	1.871053883	-2.572469481	2.529556917
H	1.740951236	-0.128221965	3.525537087
H	3.517933149	0.072745355	3.385085802
H	2.403100253	1.194831146	2.505509335
H	3.992875890	-1.438409259	-2.016302290
H	2.324500116	-2.023186501	-2.309792152
H	2.627230964	-0.258919350	-2.158085477
H	-3.805221242	-2.264897234	-1.437940235
H	-3.910090973	-0.987038066	1.512146957
C	-2.832504524	-2.339256513	-1.944145970
C	-2.954748352	-0.711722213	1.981914350
H	-2.422514524	-3.345625066	-1.777586971
H	-2.585737452	-1.569726858	2.561988544
H	-3.115522585	0.143397827	2.650095734
H	-2.976836536	-2.187455035	-3.022920625
C	-2.874399446	1.969603770	0.236228619
C	-2.404697687	0.093992197	-1.360131044
C	-2.423351740	0.609452834	-0.127134855
C	-1.854724610	-1.305471398	-1.386888854
C	-1.916493489	-0.354469112	0.918761433
N	-1.662221781	-1.538698181	0.063882965
O	-3.233111345	2.699864716	-0.828080889
O	-2.957002550	2.377715614	1.373108573
O	-1.096187943	-2.576745447	0.506206286
H	-3.491664184	3.574635627	-0.491303462
H	-2.717461257	0.619128924	-2.262535313
C	-0.602122506	0.100069628	1.550444294
C	-0.498185153	-1.373314402	-2.093994610
H	-0.629351158	-1.273715755	-3.181455572
H	-0.751168826	1.049190711	2.081691178
H	-0.261255745	-0.677217735	2.250290073
H	-0.046403495	-2.353664369	-1.878448771
H	0.154943019	0.251560673	0.767112769
H	0.160281670	-0.565486323	-1.737501169
O	2.049888227	2.537278457	0.733299329
S	1.153200837	2.592133570	-0.473922701
C	1.722086637	3.998025475	-1.427560972
H	1.612912450	4.894015825	-0.806236110
H	2.772274865	3.831531766	-1.691793829
H	1.099389651	4.069779736	-2.326391477
O	-0.275730905	2.863797936	-0.148057383
O	1.352523981	1.396685950	-1.367069914

C₁mim SO₃CH₃ conf 2:

C	-1.561758481	3.073444376	-0.847113131
N	-1.378919546	1.768493141	-1.253825908
C	-1.557961658	0.966368105	-0.205558676
N	-1.861946105	1.707743390	0.854316927
C	-1.870804230	3.033508537	0.480658074
C	-1.093885961	1.301483831	-2.608274905

C	-2.229264916	1.153087380	2.154143337
H	-1.483161464	-0.116124782	-0.201484196
H	-2.107057726	3.826510766	1.180643722
H	-1.469982604	3.907046424	-1.533701972
H	-0.009844697	1.228553416	-2.763771744
H	-1.581613929	0.325331263	-2.722992159
H	-1.518225455	2.021019320	-3.315974888
H	-1.386044815	1.249442877	2.846107017
H	-3.105533642	1.696243033	2.524356483
H	-2.475680683	0.097022359	1.994700085
H	0.145834814	-1.245850309	-1.584889278
H	1.346225960	1.580709314	-0.824782926
C	0.194083283	-2.071411924	-0.859824035
C	1.756117185	1.719596596	0.186087019
H	-0.768286576	-2.138730013	-0.329314496
H	0.961562698	2.102734106	0.845206631
H	2.574721249	2.449081904	0.140840612
H	0.357064512	-3.007907960	-1.412258588
C	4.424038582	0.189799410	-0.706738576
C	2.649966797	-1.573575672	-0.536896175
C	3.148295365	-0.373342364	-0.217655180
C	1.333840950	-1.848579468	0.135442785
C	2.268810474	0.391567927	0.744178795
N	1.140752187	-0.564937206	0.8544447814
O	5.064185894	-0.628017777	-1.552749725
O	4.855032078	1.273865147	-0.381936893
O	0.195921675	-0.386988091	1.671899455
H	5.886948040	-0.180180739	-1.816474521
H	3.124894259	-2.289999390	-1.207464491
C	2.914908609	0.585734017	2.117168143
C	1.410989944	-2.995557847	1.145955272
H	1.542813108	-3.952886335	0.623386756
H	3.761497074	1.279168863	2.031324148
H	2.170000219	0.999823952	2.810739553
H	0.472480802	-3.024743287	1.716624506
H	3.275068301	-0.373784503	2.514669925
H	2.248409264	-2.849129342	1.842416669
O	-2.939448336	-1.216757636	-1.867741853
S	-3.749870344	-1.224916093	-0.602918431
C	-5.077194272	-2.395339838	-0.877238562
H	-5.671286575	-2.039597332	-1.726450922
H	-4.629428859	-3.371346742	-1.094534424
H	-5.684134148	-2.436926596	0.034041582
O	-4.394985898	0.091088642	-0.308704399
O	-2.964892405	-1.757426847	0.564855744

C₁mim N(SO₂CF₃)₂ conf 1:

C	-0.617895000	2.734933000	0.989637000
N	-1.768610000	2.827061000	0.320737000
C	-2.779524000	2.339744000	1.118534000
C	-2.209906000	1.957439000	2.296588000
N	-0.865360000	2.223181000	2.193092000
C	0.137378000	2.029179000	3.235981000
C	-1.910032000	3.314611000	-1.050421000
H	1.108967000	2.315184000	2.817278000
H	-0.110419000	2.663588000	4.094528000
H	0.138764000	0.970616000	3.515596000
H	-2.640171000	1.518991000	3.189125000
H	-3.808231000	2.301236000	0.779826000
H	-2.923420000	3.711171000	-1.169395000
H	-1.185391000	4.118701000	-1.213850000
H	-1.741543000	2.487775000	-1.751434000
H	0.370779000	3.031307000	0.639776000
H	4.752678000	2.370690000	-1.819682000
H	5.399974000	0.844009000	0.377260000
C	3.736007000	2.712735000	-2.057308000

C	4.673338000	0.524401000	1.137515000
H	3.585369000	3.712199000	-1.624680000
H	4.645677000	1.272013000	1.943037000
H	4.987666000	-0.443518000	1.549592000
H	3.626425000	2.777093000	-3.148822000
C	3.581553000	-1.856947000	-0.751851000
C	2.954048000	0.320105000	-1.820828000
C	3.260450000	-0.413096000	-0.745648000
C	2.688384000	1.759098000	-1.475837000
C	3.273225000	0.391988000	0.533776000
N	2.827490000	1.701437000	-0.000670000
O	3.432349000	-2.414105000	-1.959841000
O	3.943207000	-2.477381000	0.222819000
O	2.488362000	2.660752000	0.749989000
H	3.663686000	-3.355236000	-1.871715000
H	2.898497000	-0.055673000	-2.842449000
C	2.270342000	-0.107951000	1.568508000
C	1.274799000	2.197156000	-1.851815000
H	1.145030000	2.145821000	-2.942141000
H	2.466029000	-1.165877000	1.783077000
H	2.377367000	0.463142000	2.500038000
H	1.123171000	3.239926000	-1.536147000
H	1.242856000	0.005709000	1.194121000
H	0.524016000	1.541224000	-1.387429000
C	-3.660200000	-0.187349000	-1.205489000
F	-4.143253000	-0.411354000	0.007292000
F	-4.355093000	-0.887154000	-2.091018000
F	-3.804703000	1.112763000	-1.478273000
S	-1.847530000	-0.653929000	-1.328761000
O	-1.844712000	-2.096061000	-1.627395000
N	-1.239221000	-0.269597000	0.120785000
S	-1.296348000	-1.429596000	1.263520000
O	-2.535076000	-2.218462000	1.320039000
O	-0.774165000	-0.838152000	2.507528000
C	0.025683000	-2.676100000	0.730930000
F	-0.539973000	-3.792749000	0.307371000
F	0.790426000	-2.178976000	-0.240253000
F	0.796531000	-2.955347000	1.777512000
O	-1.323356000	0.291836000	-2.328957000

C₁mim N(SO₂CF₃)₂ conf 2:

C	2.355761188	-1.171116690	-0.362103561
N	3.508503908	-1.141037052	-1.027666226
C	4.540609655	-1.049892895	-0.121996009
C	3.979171657	-1.041070251	1.119061068
N	2.616334857	-1.118563239	0.942574568
C	1.601304538	-1.017868576	1.989983716
C	3.630354713	-0.972081166	-2.469751569
H	0.663428964	-1.416077154	1.586355012
H	1.924076802	-1.610259498	2.852885099
H	1.486087631	0.039601589	2.261905758
H	4.428097731	-0.981896701	2.103314696
H	5.576702520	-0.999429601	-0.435782013
H	4.505437829	-1.525650536	-2.824504708
H	2.726975348	-1.362707150	-2.948399807
H	3.736323247	0.098908116	-2.683973285
H	1.353793163	-1.232717612	-0.785319514
H	-2.261371776	-1.345180333	2.360888376
H	-0.936765995	0.893901621	1.252679600
C	-2.595194680	-2.204253735	1.762068149
C	-0.792439045	1.086066496	0.179720172
H	-1.811941497	-2.975489316	1.773690201
H	0.259467314	0.890619831	-0.079464587
H	-0.996392873	2.145610011	-0.018039216
H	-3.508504253	-2.619096541	2.210377569
C	-3.843855575	1.779459487	-0.540109092

C	-3.792609098	-0.607154287	0.213713046
C	-3.196324072	0.469360005	-0.310636189
C	-2.862816858	-1.783612358	0.314872110
C	-1.743523460	0.232680508	-0.660149262
N	-1.636925872	-1.192483714	-0.267790739
O	-5.127247336	1.796426550	-0.156468658
O	-3.286081481	2.739581582	-1.022145609
O	-0.562901836	-1.850622773	-0.360512308
H	-5.469444180	2.688402905	-0.341927510
H	-4.831955640	-0.652336655	0.538899548
C	-1.453032994	0.381308406	-2.153965673
C	-3.311863154	-2.974691162	-0.533858592
H	-4.211832821	-3.431594161	-0.099892875
H	-1.580710711	1.431237276	-2.445384119
H	-0.414644631	0.081898468	-2.357803890
H	-2.505656734	-3.721218725	-0.554440652
H	-2.132637267	-0.247410257	-2.746720460
H	-3.530734737	-2.657729487	-1.562850146
O	3.899310051	3.339215803	-1.826317718
S	2.914035602	2.946475914	-0.810861086
O	2.661075337	1.505739813	-0.601780221
C	1.290242500	3.624147928	-1.447570440
F	0.487741454	3.946298779	-0.438464049
F	0.686838352	2.706024364	-2.199348582
F	1.509363188	4.706560847	-2.182079462
N	3.147929253	3.825914133	0.523582815
S	2.594413078	3.279047016	1.942853258
O	1.454504914	2.345025577	1.882607654
C	4.028685523	2.224619496	2.550892530
F	3.556744727	1.159738479	3.203899817
F	4.772162199	1.799005566	1.535559750
F	4.793206658	2.924489555	3.376996415
O	2.541824679	4.404105503	2.883086895

C₁mim SO₃CF₃ conf 1:

C	0.885839000	3.454547000	1.076417000
N	-0.363772000	2.976969000	1.405155000
C	-1.045823000	2.750904000	0.283102000
N	-0.277753000	3.081228000	-0.754979000
C	0.940425000	3.518652000	-0.283247000
C	-0.866394000	2.708125000	2.750767000
C	-0.691628000	2.992109000	-2.153017000
H	-2.038348000	2.316942000	0.232160000
H	1.741805000	3.820631000	-0.947075000
H	1.631049000	3.683941000	1.829034000
H	-0.015930000	2.450041000	3.390163000
H	-1.370123000	3.598838000	3.143743000
H	-1.555616000	1.859209000	2.683557000
H	-1.270561000	3.882505000	-2.424302000
H	0.207224000	2.931278000	-2.774394000
H	-1.288869000	2.081100000	-2.266570000
H	4.724956000	-1.195688000	-1.642488000
H	4.164225000	-1.653127000	1.488651000
C	4.075839000	-0.505210000	-2.198947000
C	3.368607000	-1.051474000	1.951153000
H	4.553220000	0.484734000	-2.227415000
H	3.807570000	-0.121149000	2.339200000
H	2.920877000	-1.619542000	2.776009000
H	3.957207000	-0.873630000	-3.227387000
C	1.193944000	-3.045463000	0.713802000
C	2.065603000	-1.700561000	-1.214784000
C	1.832996000	-1.865953000	0.091158000
C	2.713961000	-0.378130000	-1.517140000
C	2.297001000	-0.693434000	0.922519000
N	2.896324000	0.145679000	-0.142553000
O	0.800078000	-3.956868000	-0.184583000

O	1.066187000	-3.196862000	1.908170000
O	3.304079000	1.319899000	0.078255000
H	0.374387000	-4.675873000	0.313031000
H	1.804610000	-2.417822000	-1.992906000
C	1.132944000	0.059992000	1.564799000
C	1.778699000	0.548977000	-2.297280000
H	1.661265000	0.189378000	-3.329859000
H	0.549970000	-0.621257000	2.198721000
H	1.527479000	0.888622000	2.170825000
H	2.223363000	1.555303000	-2.320287000
H	0.477640000	0.466456000	0.780804000
H	0.789530000	0.582682000	-1.815498000
O	-2.273027000	0.259087000	1.310377000
S	-1.980022000	-0.573372000	0.111100000
C	-3.674130000	-0.965266000	-0.521737000
F	-4.374361000	-1.644771000	0.386207000
F	-4.330395000	0.163979000	-0.799552000
F	-3.607473000	-1.695829000	-1.634817000
O	-1.373894000	-1.894780000	0.378120000
O	-1.388098000	0.189017000	-1.025416000

C₁mim SO₃CF₃ conf 2:

C	-0.238097671	3.513816987	-0.964940796
N	-0.283206167	2.165588195	-1.246614485
C	-0.484249927	1.499913825	-0.110120952
N	-0.585527416	2.373408178	0.886889055
C	-0.432996836	3.644045727	0.378623883
C	-0.174400799	1.542198115	-2.563634670
C	-0.900891353	2.014299648	2.267711117
H	-0.555087768	0.423189026	0.001130473
H	-0.490561885	4.525195052	1.007116991
H	-0.087425889	4.257048297	-1.739171043
H	0.867412490	1.262599872	-2.764566477
H	-0.829434374	0.662947863	-2.567218875
H	-0.513107118	2.263855227	-3.313683985
H	0.013813024	2.032803860	2.869401267
H	-1.635833578	2.731515301	2.648332220
H	-1.325756428	1.004923356	2.255232825
H	0.603938278	-1.175620043	-1.398476336
H	2.392958568	1.396328897	-0.959871508
C	0.535853925	-1.930627407	-0.601568922
C	2.901623672	1.527830948	0.006140113
H	-0.379118767	-1.756385030	-0.015151926
H	2.260899666	2.127740870	0.671146616
H	3.848572076	2.056883771	-0.160099583
H	0.466231208	-2.922494042	-1.070173689
C	5.138972498	-0.589726201	-0.868060201
C	3.059306939	-1.926546398	-0.451133394
C	3.810313053	-0.834160360	-0.268416726
C	1.763589043	-1.868312218	0.308842498
C	3.170350689	0.171944869	0.660118890
N	1.882541631	-0.518543064	0.913643987
O	5.544206559	-1.590068151	-1.660935077
O	5.799370724	0.405349610	-0.668139384
O	1.045912276	-0.081545283	1.751514457
H	6.421286765	-1.346047038	-2.004876898
H	3.333889611	-2.777754126	-1.074340988
C	3.933027331	0.339309018	1.975591980
C	1.676843048	-2.920335276	1.417185597
H	1.576097555	-3.923344096	0.980559124
H	4.895511836	0.830605224	1.782717879
H	3.337155997	0.956452113	2.662273987
H	0.793738194	-2.707563237	2.035526144
H	4.115770329	-0.638050309	2.444222209
H	2.573006530	-2.894609168	2.052663403
O	-2.445323846	-0.484486789	-1.426600813

S	-3.080238691	-0.210918467	-0.108759394
C	-4.659041508	-1.172780376	-0.187357836
F	-5.418824083	-0.743045951	-1.195091651
F	-4.408219321	-2.468783759	-0.372320089
F	-5.346619480	-1.034749431	0.946425675
O	-3.520678311	1.188177169	0.101417794
O	-2.364467300	-0.818787799	1.047616513

P_{1,1,1} BF₄ conf 1:

P	0.246236743	-2.018523965	-0.084030835
C	0.101269623	-0.847348693	-1.446949814
C	1.882699235	-2.780040072	-0.191878018
C	0.102179961	-1.253907570	1.541415163
C	-1.025079274	-3.289429034	-0.263893219
B	-2.625407496	0.794661185	0.179278182
F	-2.579345968	-0.629669875	0.154379936
F	-3.907608295	1.219357573	0.525305920
F	-2.269499727	1.275860763	-1.097226614
F	-1.681019630	1.251470175	1.126429337
H	-1.998486726	-2.787210496	-0.201920434
H	-0.921292213	-4.026904112	0.542273633
H	-0.908142686	-3.781009896	-1.238270157
H	0.918281096	-0.526714227	1.634474041
H	0.197681550	-2.045826444	2.296508990
H	-0.868891626	-0.752220942	1.609983790
H	2.624416613	-1.977104602	-0.079220360
H	1.997192512	-3.268241504	-1.168245413
H	1.997224361	-3.518795257	0.611838624
H	0.938008391	-0.142590728	-1.366402266
H	-0.857864386	-0.318896394	-1.384100472
H	0.167851883	-1.416800269	-2.384237348
H	1.990692886	2.567711065	2.634726121
H	4.778396652	1.808631370	2.027997030
C	1.204260848	2.649404018	1.871539001
C	5.076861836	1.460224057	1.029044780
H	0.540819549	1.775090237	1.913671928
H	5.009327730	0.363760557	0.999509975
H	6.112483981	1.767727269	0.835347283
H	0.596952798	3.542187657	2.078588989
C	5.157961476	4.454665760	-0.129035637
C	2.752720334	3.925447607	0.338893491
C	4.006006542	3.548724667	0.062364941
C	1.811539268	2.760564193	0.470923878
C	4.158174627	2.049190914	-0.042319077
N	2.757979662	1.644980068	0.228633450
O	4.830853306	5.746655000	0.003303763
O	6.281856649	4.079274192	-0.378735284
O	2.410338684	0.431027020	0.258834556
H	5.643224273	6.263792007	-0.137074264
H	2.420225811	4.956732996	0.458032524
C	4.565539176	1.580240885	-1.439910483
C	0.711355188	2.774076130	-0.593353890
H	0.099278741	3.680074817	-0.474077175
H	5.595057319	1.898157784	-1.649076945
H	4.506442035	0.483630209	-1.485214460
H	0.048133748	1.908414435	-0.464483231
H	3.895776759	2.005141747	-2.201051175
H	1.145416181	2.771357727	-1.603522756

P_{1,1,1} BF₄ conf 2:

P	3.373687238	-1.027349107	-0.380112674
C	2.528268886	-1.032230011	1.208515769
C	3.653404026	-2.748001621	-0.865645854
C	2.322243878	-0.266862652	-1.627175720
C	4.965345334	-0.184168423	-0.265362226

B	1.650087431	2.515311833	0.490995097
F	2.962064709	1.965008841	0.549476975
F	1.604449192	3.709401391	1.208859897
F	0.754940820	1.570298750	1.049285253
F	1.310999481	2.730032629	-0.858510278
H	4.766609965	0.856294495	0.016789131
H	5.468734544	-0.231542893	-1.239829008
H	5.578909123	-0.681182454	0.497264491
H	1.360254283	-0.798185638	-1.587288355
H	2.790670889	-0.384730738	-2.613155459
H	2.175107990	0.795169327	-1.391035636
H	2.678879197	-3.249224181	-0.943009482
H	4.268109066	-3.246422442	-0.104712097
H	4.165068196	-2.778203988	-1.836478439
H	1.570860304	-1.548803463	1.050937952
H	2.344992456	0.007282315	1.505271333
H	3.145192819	-1.560503117	1.947015625
H	-0.399803341	0.044031715	2.185711313
H	-0.606866714	1.204214072	-0.791935378
C	-0.855094702	-0.920184503	2.447562604
C	-1.165699694	0.662373060	-1.566158107
H	-0.064186608	-1.674368529	2.567451460
H	-0.451938544	0.231681603	-2.282598277
H	-1.818669246	1.356775354	-2.111851216
H	-1.386106132	-0.831907309	3.406340378
C	-4.165365776	0.977324378	-0.501114759
C	-2.996515650	-0.422692161	1.211088416
C	-3.097826938	0.069319345	-0.028023918
C	-1.836396963	-1.365192265	1.362636778
C	-2.021870355	-0.447169822	-0.956576006
N	-1.226217430	-1.240286138	0.015740129
O	-4.995097670	1.356398379	0.480323000
O	-4.294883843	1.338924624	-1.649187560
O	-0.218755613	-1.920110589	-0.332051506
H	-5.666757526	1.934582730	0.078552853
H	-3.676117574	-0.198014775	2.033323645
C	-2.580931921	-1.373603833	-2.039436988
C	-2.290891269	-2.809893464	1.591141633
H	-2.721506907	-2.916097580	2.596659312
H	-3.150757501	-0.782434826	-2.768272977
H	-1.745660616	-1.874466173	-2.548825763
H	-1.418022128	-3.472479084	1.505002344
H	-3.241878910	-2.136342512	-1.602942554
H	-3.042339258	-3.109650550	0.847227848

P_{1,1,1,1} N(CN)₂ conf 1:

P	-1.936337361	0.309415112	-0.004547301
C	-0.664704015	0.734204852	1.198640499
C	-3.119580261	1.675910637	-0.064590784
C	-1.221118047	0.129098393	-1.651155365
C	-2.797221986	-1.198661479	0.483821140
N	0.569744593	-3.087091368	-2.157448422
C	0.503834651	-2.809941238	-1.021109105
N	0.288390728	-2.482150028	0.240132887
C	1.321692807	-2.099627635	0.964746879
N	2.160023560	-1.710600921	1.686024546
H	-3.542267375	-1.450661167	-0.281715861
H	-3.292435378	-1.030179744	1.448857995
H	-2.044342509	-1.994268516	0.571481945
H	-2.031859892	0.175378853	-2.390366446
H	-0.702355832	-0.835426641	-1.733265871
H	-0.509673010	0.955412799	-1.796755755
H	0.061728878	-0.084815668	1.277518414
H	-1.141369186	0.912051395	2.171762865
H	-0.156246367	1.637344434	0.834713363
H	-3.916787195	1.432687456	-0.778741607

H	-2.594907990	2.584437098	-0.388814158
H	-3.547974181	1.830900296	0.933876133
H	3.421187794	2.908367319	-3.053242072
H	3.518993054	4.444572819	-0.596390536
C	3.019362467	1.886432202	-3.097492883
C	3.131656682	4.058237619	0.357266062
H	1.963032896	1.931280671	-3.397347164
H	2.086838589	4.378282181	0.472507791
H	3.732807914	4.465202566	1.180484197
H	3.578634584	1.313813604	-3.850123801
C	5.754400293	2.249728140	0.790511841
C	4.505281055	1.276987243	-1.148797255
C	4.542904264	1.984447968	-0.014585427
C	3.123455084	1.200861812	-1.733762926
C	3.191300008	2.530425002	0.386033439
N	2.370408854	1.980599898	-0.721703896
O	6.849802602	1.666480585	0.286217597
O	5.769200443	2.923733882	1.796353853
O	1.150820236	2.277828664	-0.868689666
H	7.591717446	1.895455999	0.872860740
H	5.364487537	0.796886667	-1.617189561
C	2.702517737	1.979840580	1.727252975
C	2.597325330	-0.234098172	-1.789126358
H	3.191355632	-0.828169342	-2.498276237
H	3.397148738	2.292503690	2.518333621
H	1.707890923	2.389978857	1.954714218
H	1.553796877	-0.235292518	-2.132513390
H	2.644888274	0.881011392	1.704160773
H	2.650990056	-0.702366243	-0.795751927

P_{1,1,1,1} N(CN)₂ conf 2:

P	-2.319824579	-0.325284338	-0.196462167
C	-1.286570743	-0.467153963	-1.666546425
C	-3.778703345	-1.371329370	-0.425496545
C	-1.449924774	-0.897029962	1.275998382
C	-2.876944477	1.377204229	0.019274948
N	1.543297024	1.157662430	2.469084446
C	1.019914877	1.542021343	1.493804648
N	0.305442701	1.990816718	0.478698903
C	0.877286928	2.085009738	-0.704237193
N	1.271433535	2.205357631	-1.802292179
H	-3.587120842	1.412368173	0.855781183
H	-3.370812369	1.709013654	-0.903379675
H	-1.994523351	1.994436065	0.236242756
H	-2.071281607	-0.681090754	2.155384872
H	-0.476364976	-0.394966796	1.340068787
H	-1.298136111	-1.980725564	1.183298707
H	-0.416558924	0.195556556	-1.572076314
H	-1.893372554	-0.197327195	-2.541204847
H	-0.937580058	-1.504680250	-1.748226203
H	-4.410149538	-1.308863531	0.470303795
H	-3.456731771	-2.409344103	-0.580447178
H	-4.341091580	-1.022463564	-1.301325633
H	1.828747695	-3.879576491	-1.187707197
H	3.096255128	-1.677559329	-2.654501284
C	1.569414295	-3.794743283	-0.123071564
C	3.412228850	-0.740078418	-2.173698039
H	0.530045737	-3.447326186	-0.038015164
H	2.640556931	0.029198127	-2.321211633
H	4.354507082	-0.404865768	-2.627057235
H	1.654365900	-4.784376971	0.346751897
C	5.970743767	-2.079373974	-0.739120790
C	3.943865425	-3.076862076	0.334620285
C	4.546693101	-2.091824073	-0.340595394
C	2.488745346	-2.793444166	0.579627007
C	3.617542345	-0.946003903	-0.672615572

N	2.367712054	-1.466234503	-0.065745246
O	6.630015229	-3.177327185	-0.342153195
O	6.498998884	-1.183807919	-1.359203450
O	1.252559421	-0.895288918	-0.211631635
H	7.549415062	-3.082553524	-0.646434850
H	4.429362217	-3.990670075	0.677490117
C	4.027828711	0.362748020	0.004807502
C	2.150767486	-2.684008506	2.068064007
H	2.249939445	-3.664821549	2.554108326
H	5.002662591	0.682573307	-0.387645129
H	3.277537624	1.133965840	-0.217794465
H	1.113909257	-2.335239112	2.177313515
H	4.092817203	0.234846961	1.094055755
H	2.814579750	-1.964023474	2.565446362

P_{1,1,1} SO₃CH₃ conf 1:

P	3.089474259	-1.592014354	-0.311436739
C	3.072039771	-3.402686668	-0.289513334
C	1.942261266	-1.059918775	-1.591509281
C	2.551563665	-1.039024620	1.316109992
C	4.766463566	-1.024618982	-0.662411049
S	2.020632673	2.334858749	0.033586471
O	3.217009325	1.632103438	-0.545317405
O	2.008714127	2.309315829	1.528692241
C	2.192830602	4.056130106	-0.435723335
O	0.736161921	1.865713379	-0.581388416
H	4.734295654	0.072472210	-0.669917092
H	5.079264978	-1.415220189	-1.639723298
H	5.441919620	-1.393921072	0.120365247
H	0.958772956	-1.465955268	-1.317876185
H	2.278394489	-1.463395968	-2.556291716
H	1.910080052	0.036675902	-1.599524591
H	2.048062847	-3.734455638	-0.068653089
H	3.757143854	-3.769492139	0.485751876
H	3.382666187	-3.783857533	-1.271013897
H	1.515467207	-1.387066604	1.437760803
H	2.597764778	0.057084183	1.378768053
H	3.204215496	-1.497884689	2.071318219
H	2.200226761	4.110100848	-1.530106588
H	3.134981366	4.428735618	-0.018104090
H	1.338462536	4.604748304	-0.023061043
H	-0.292581525	1.083449453	1.429969086
H	-0.898737975	0.541313678	-1.547278434
C	-0.699889879	0.445164677	2.225535876
C	-1.543889555	-0.282611578	-1.886109144
H	0.113049380	-0.172072610	2.634133389
H	-0.920827363	-1.058699930	-2.353724235
H	-2.258157785	0.081102703	-2.637047415
H	-1.086099557	1.073885025	3.041670122
C	-4.406212805	0.689766246	-0.826800982
C	-3.005331297	0.331631543	1.213741450
C	-3.276656654	0.102190446	-0.075358261
C	-1.821160112	-0.452534468	1.702719834
C	-2.321675726	-0.881142052	-0.712513388
N	-1.416319465	-1.120244038	0.440795099
O	-5.119752778	1.556602003	-0.095165590
O	-4.676222412	0.420030076	-1.976279497
O	-0.473579883	-1.961401892	0.394078695
H	-5.841094000	1.882247562	-0.661231345
H	-3.574746118	0.996161607	1.864025809
C	-3.002041952	-2.192568848	-1.109453106
C	-2.217372812	-1.507484031	2.739410707
H	-2.495296963	-1.019709844	3.684377321
H	-3.651764527	-2.021575034	-1.977820378
H	-2.229536080	-2.929986374	-1.369504813
H	-1.357761465	-2.168429468	2.919784757

H	-3.607089757	-2.586922483	-0.280183697
H	-3.064815892	-2.111947437	2.386257387

P_{1,1,1} N(SO₂CF₃)₂ conf 1:

P	-3.293466768	-0.997965463	-0.126549239
C	-1.789891785	-0.924134524	-1.111225400
C	-3.792357261	-2.732051557	0.006768609
C	-2.952922959	-0.371779002	1.530429546
C	-4.641720630	-0.069809146	-0.889487191
H	-5.550110404	-0.205133410	-0.288097278
H	-4.805743907	-0.451733028	-1.905591914
H	-4.354132417	0.987631851	-0.920677032
H	-3.796438200	-0.606853432	2.191847321
H	-2.806457201	0.713225006	1.454157109
H	-2.028750158	-0.854784692	1.880878009
H	-1.424634615	0.112162612	-1.131704525
H	-1.999440004	-1.284715937	-2.126610740
H	-1.053585166	-1.565525237	-0.609072349
H	-4.704163420	-2.804592394	0.613331713
H	-2.981602710	-3.297160016	0.485285063
H	-3.980097194	-3.132481090	-0.998069404
H	2.544172590	-0.674102379	3.239345750
H	3.317809218	-2.432401429	1.323421932
C	1.702780360	0.025655202	3.138057064
C	2.857755489	-2.527926514	0.329465232
H	0.793869254	-0.449952518	3.532283959
H	2.085979511	-3.309117192	0.368300527
H	3.630365448	-2.811009908	-0.397175271
H	1.916573795	0.928951207	3.726016687
C	4.364944303	0.105810073	-0.765093846
C	2.738024193	0.836488251	0.991357075
C	3.138013034	-0.024282263	0.049383670
C	1.471941305	0.397982909	1.670585306
C	2.211085900	-1.209300318	-0.098844618
N	1.167040647	-0.824896202	0.887270361
O	5.037015966	1.237040284	-0.513389249
O	4.738361683	-0.717894953	-1.570447960
O	0.217502552	-1.599617669	1.198157447
H	5.825727994	1.233940543	-1.083393495
H	3.260541856	1.753018613	1.265470592
C	1.608853095	-1.320526149	-1.500496113
C	0.341207864	1.414877242	1.528573009
H	0.622780412	2.353796704	2.026783660
H	2.416657686	-1.506288868	-2.220698010
H	0.908526673	-2.167617749	-1.536469893
H	-0.563928188	1.026510621	2.015545948
H	1.081354786	-0.395272405	-1.774327221
H	0.124512244	1.617683349	0.470938138
O	0.225124058	3.307347423	-3.874242024
S	-0.574289263	2.645025010	-2.839324574
O	0.111336022	1.816618449	-1.826873238
C	-1.642284593	1.431088303	-3.771444062
F	-2.740904539	1.144458183	-3.069374170
F	-0.964722361	0.304634804	-3.974395929
F	-2.003688214	1.939376975	-4.939281206
N	-1.670760716	3.695463509	-2.281217073
S	-2.386987460	3.451767732	-0.855049634
O	-2.354568738	2.064372516	-0.337545949
C	-1.283621854	4.393010228	0.314764715
F	-1.535341778	4.007312133	1.562144169
F	-0.006892942	4.154198345	0.038084121
F	-1.514168124	5.693635636	0.205690474
O	-3.666894370	4.168231730	-0.831338603

P_{1,1,1} N(SO₂CF₃)₂ conf 2:

P	1.286400501	2.895667595	-1.265020147
C	0.656552508	1.704559974	-2.463417678
C	1.083722547	4.556783888	-1.950902639
C	0.322096065	2.793508370	0.250573752
C	3.038741312	2.620104145	-0.934865992
H	3.381697528	3.362511718	-0.202303126
H	3.599524111	2.726970777	-1.872468509
H	3.160270860	1.602903120	-0.546546745
H	0.700452020	3.527851911	0.974155189
H	0.393897381	1.779130854	0.663765400
H	-0.722607955	3.002286210	-0.017610430
H	0.975647249	0.700598350	-2.158935637
H	1.063752161	1.941864015	-3.454833492
H	-0.440814321	1.782369089	-2.457868667
H	1.432998265	5.295281005	-1.217731684
H	0.020768341	4.723826789	-2.169269830
H	1.671506304	4.641738224	-2.874001533
H	-5.507434964	2.110436681	-0.053524645
H	-4.864601979	0.163505592	-2.015127914
C	-4.766658521	2.514960838	0.650193409
C	-3.863215357	-0.275317925	-2.131558568
H	-4.324842100	3.424032870	0.219077352
H	-3.311118952	0.294726441	-2.891775026
H	-3.963978467	-1.318285145	-2.458543654
H	-5.270684242	2.773478286	1.591684177
C	-4.272535887	-2.209387499	0.406755208
C	-4.179543009	0.139589134	1.270228959
C	-3.881902470	-0.784405964	0.350773970
C	-3.651198839	1.499932943	0.910721272
C	-3.093033800	-0.227362606	-0.811258974
N	-2.959493012	1.181160220	-0.362222875
O	-4.943763645	-2.519784002	1.523795396
O	-4.022474594	-3.017427288	-0.459501457
O	-2.437610894	2.073374177	-1.089771574
H	-5.160304290	-3.467182211	1.473341081
H	-4.743091093	-0.044280975	2.184994265
C	-1.708727735	-0.857048855	-0.949905792
C	-2.656284250	2.025377651	1.948250925
H	-3.161566113	2.133935393	2.918741716
H	-1.810588226	-1.922501705	-1.195047390
H	-1.160291942	-0.360187928	-1.761594019
H	-2.289210313	3.015689123	1.642400417
H	-1.138800226	-0.746360139	-0.016590251
H	-1.804740170	1.338447082	2.057577628
O	0.129435273	-0.084964794	2.005651667
S	1.391356499	-0.747277347	1.624797053
O	1.628459792	-2.134822494	2.039265603
C	2.695562395	0.264890652	2.476126483
F	3.900312345	-0.082252925	2.042287773
F	2.628944099	0.078982908	3.787310021
F	2.502193792	1.556795129	2.209999538
N	1.688446213	-0.384460434	0.071913441
S	2.688068753	-1.312273136	-0.809828207
O	3.666900418	-2.117405900	-0.069242602
C	1.503958081	-2.539377686	-1.554342705
F	2.182899797	-3.530014507	-2.117556269
F	0.704241100	-3.035028832	-0.617609805
F	0.761904460	-1.940241813	-2.481745520
O	3.133958199	-0.495732043	-1.952059337

P_{1,1,1} SO₃CF₃ conf 1:

P	3.08947	-1.59201	-0.31144
C	3.07204	-3.40269	-0.28951
C	1.94226	-1.05992	-1.59151
C	2.55156	-1.03902	1.31611
C	4.76646	-1.02462	-0.66241

S	2.02063	2.33486	0.03359
O	3.21701	1.63210	-0.54532
O	2.00871	2.30932	1.52869
C	2.19283	4.05613	-0.43572
O	0.73616	1.86571	-0.58139
H	4.73430	0.07247	-0.66992
H	5.07926	-1.41522	-1.63972
H	5.44192	-1.39392	0.12037
H	0.95877	-1.46596	-1.31788
H	2.27839	-1.46340	-2.55629
H	1.91008	0.03668	-1.59952
H	2.04806	-3.73446	-0.06865
H	3.75714	-3.76949	0.48575
H	3.38267	-3.78386	-1.27101
H	1.51547	-1.38707	1.43776
H	2.59776	0.05708	1.37877
H	3.20422	-1.49788	2.07132
F	2.20023	4.11010	-1.53011
F	3.13498	4.42874	-0.01810
F	1.33846	4.60475	-0.02306
H	-0.29258	1.08345	1.42997
H	-0.89874	0.54131	-1.54728
C	-0.69989	0.44516	2.22554
C	-1.54389	-0.28261	-1.88611
H	0.11305	-0.17207	2.63413
H	-0.92083	-1.05870	-2.35372
H	-2.25816	0.08110	-2.63705
H	-1.08610	1.07389	3.04167
C	-4.40621	0.68977	-0.82680
C	-3.00533	0.33163	1.21374
C	-3.27666	0.10219	-0.07536
C	-1.82116	-0.45253	1.70272
C	-2.32168	-0.88114	-0.71251
N	-1.41632	-1.12024	0.44080
O	-5.11975	1.55660	-0.09517
O	-4.67622	0.42003	-1.97628
O	-0.47358	-1.96140	0.39408
H	-5.84109	1.88225	-0.66123
H	-3.57475	0.99616	1.86403
C	-3.00204	-2.19257	-1.10945
C	-2.21737	-1.50748	2.73941
H	-2.49530	-1.01971	3.68438
H	-3.65176	-2.02158	-1.97782
H	-2.22954	-2.92999	-1.36950
H	-1.35776	-2.16843	2.91978
H	-3.60709	-2.58692	-0.28018
H	-3.06482	-2.11195	2.38626

C₁mpyr BF₄ conf 1:

C	0.501567092	-0.950499340	-0.278512978
C	0.765665628	-0.404543349	-1.682444820
C	1.727044510	0.793961011	-1.493790175
C	1.924837327	0.920074274	0.014224395
N	1.660200161	-0.461995763	0.557783890
C	2.845168585	-1.338150882	0.351579279
C	1.305947901	-0.410518357	2.001567662
F	-1.001645196	1.661521574	-0.497610665
B	-1.515032124	1.821483550	0.811440019
F	-1.930367383	0.548721784	1.289378905
F	-2.584843076	2.710209531	0.812294070
F	-0.477781951	2.288528217	1.652424590
H	3.081433474	-1.373071283	-0.717561028
H	3.690569646	-0.923778691	0.911765497
H	2.602717561	-2.343091623	0.713912843
H	0.434712223	0.245448958	2.114395754
H	1.079928299	-1.427736024	2.340669459

H	2.163751943	-0.011163605	2.555378378
H	1.168182987	1.570434259	0.465437524
H	2.928016999	1.230005747	0.330203010
H	2.681601615	0.622833980	-2.007724071
H	1.295702010	1.723571299	-1.880758399
H	1.205898034	-1.170055958	-2.333879001
H	-0.184240737	-0.082402038	-2.120861481
H	0.440567594	-2.042704276	-0.206814769
H	-0.398174721	-0.502884123	0.158638010
H	-1.595691067	-1.543081958	1.990116492
H	-2.520378530	-0.331527205	-0.809741741
C	-1.650066130	-2.628853187	2.148635041
C	-2.920104742	-1.007506886	-1.578599303
H	-0.676967630	-3.090097154	1.920945282
H	-2.118023334	-1.275057022	-2.282006239
H	-3.723574538	-0.500156362	-2.128513733
H	-1.893331737	-2.831694114	3.201337571
C	-5.719498321	-1.334563422	-0.060503916
C	-4.043636553	-2.559821164	1.341007634
C	-4.445321551	-2.046496022	0.172878671
C	-2.709999787	-3.245487898	1.236098956
C	-3.460927975	-2.288878202	-0.947621672
N	-2.381223294	-2.957220949	-0.180212732
O	-6.444905174	-1.187078062	1.056354761
O	-6.082515463	-0.928233462	-1.141801301
O	-1.347049177	-3.418727638	-0.738073982
H	-7.258209934	-0.713864268	0.808356518
H	-4.604169542	-2.507190270	2.274380650
C	-3.999803576	-3.245074513	-2.014043061
C	-2.807174642	-4.759361845	1.444708295
H	-3.028421507	-4.985221086	2.496986978
H	-4.796691504	-2.750261673	-2.584313282
H	-3.180563939	-3.521746111	-2.692346045
H	-1.844683895	-5.215740361	1.173998014
H	-4.402900952	-4.158072280	-1.552772538
H	-3.595563908	-5.192175759	0.813228786

C1mpyr BF₄ conf 2:

C	-2.787690000	-0.936140000	-0.587680000
C	-2.423000000	-1.434690000	0.810320000
C	-3.367160000	-0.671120000	1.772610000
C	-4.214350000	0.229880000	0.875390000
N	-4.212590000	-0.455860000	-0.468520000
C	-5.151920000	-1.610460000	-0.466880000
C	-4.566360000	0.483820000	-1.565570000
F	-1.385340000	1.295880000	0.997100000
B	-1.240010000	2.203150000	-0.076960000
F	-0.655510000	1.521440000	-1.173070000
F	-0.449800000	3.285320000	0.301090000
F	-2.531000000	2.647250000	-0.462750000
H	-4.876260000	-2.297510000	0.339850000
H	-6.168100000	-1.233000000	-0.309210000
H	-5.081080000	-2.118780000	-1.434650000
H	-3.871090000	1.329030000	-1.522380000
H	-4.482130000	-0.049570000	-2.519330000
H	-5.597650000	0.822350000	-1.412820000
H	-3.727250000	1.197650000	0.713030000
H	-5.254200000	0.370250000	1.193100000
H	-3.994600000	-1.363740000	2.348080000
H	-2.804860000	-0.049390000	2.476480000
H	-2.569460000	-2.520150000	0.891820000
H	-1.367760000	-1.219390000	1.014370000
H	-2.743990000	-1.689560000	-1.383740000
H	-2.191670000	-0.060110000	-0.870370000
H	0.212740000	-0.600920000	-1.393340000
H	1.184200000	1.353040000	0.324400000

C	0.522450000	-1.656150000	-1.413190000
C	1.804760000	1.131220000	1.201920000
H	-0.248070000	-2.268970000	-0.922170000
H	1.140320000	0.973770000	2.062590000
H	2.470020000	1.981840000	1.401970000
H	0.623130000	-1.990070000	-2.455840000
C	4.465850000	0.895960000	-0.587100000
C	2.955560000	-0.997310000	-1.223840000
C	3.388200000	-0.086230000	-0.344790000
C	1.846520000	-1.846400000	-0.668330000
C	2.637830000	-0.128390000	0.966550000
N	1.739540000	-1.276070000	0.692660000
O	5.002240000	0.788440000	-1.811020000
O	4.835550000	1.714960000	0.224240000
O	0.883700000	-1.681090000	1.526270000
H	5.693760000	1.469540000	-1.879440000
H	3.347680000	-1.131350000	-2.232070000
C	3.521510000	-0.455000000	2.169790000
C	2.222410000	-3.326680000	-0.578260000
H	2.264660000	-3.772070000	-1.581960000
H	4.183750000	0.392670000	2.387090000
H	2.877710000	-0.649850000	3.039070000
H	1.457700000	-3.849130000	0.013690000
H	4.131170000	-1.348690000	1.972870000
H	3.197980000	-3.451600000	-0.088040000

C₁mpyr N(CN)₂ conf 1:

C	1.436606586	1.493713156	-1.312883743
C	0.883112714	0.074100133	-1.589975958
C	1.566933107	-0.830185579	-0.566331084
C	2.417575121	1.325988578	-0.151342107
N	2.851543804	-0.117730390	-0.216933010
C	3.865430775	-0.309230063	-1.288923390
C	3.394057690	-0.584621302	1.087053336
H	3.451125160	0.036517964	-2.241811859
H	4.109604728	-1.375447632	-1.349790610
H	4.758878330	0.270988551	-1.033182498
H	4.295363263	-0.004449903	1.316410868
H	3.644426586	-1.647802783	0.995343704
H	2.619719701	-0.426358577	1.846980921
H	1.810775250	-1.839788574	-0.918275096
H	0.986060607	-0.889127639	0.361217620
H	1.107002096	-0.243781415	-2.616713135
H	-0.201894807	0.024799113	-1.441724386
H	1.938919019	1.906811432	-2.197036826
H	0.632362598	2.184220364	-1.030813436
H	3.309638880	1.962007222	-0.193475449
H	1.921083762	1.438162866	0.820246358
N	0.496973276	0.356818784	2.465120784
C	-0.542841568	0.678351640	2.021341925
N	-1.740927924	1.031330584	1.622001061
C	-1.845605260	1.441037589	0.373427210
N	-2.021756786	1.829514768	-0.719145605
H	-2.803996404	-3.832399299	-1.741526809
H	-1.150586070	-4.791342333	0.445660974
C	-3.268903728	-2.836444673	-1.733646702
C	-0.956761331	-4.198303889	1.351165757
H	-2.604788812	-2.128675377	-2.249036081
H	-0.008628368	-3.656555989	1.225551490
H	-0.880276681	-4.873284454	2.213378729
H	-4.226164594	-2.883907426	-2.271096553
C	-3.872668975	-4.821253306	2.555267702
C	-4.210614912	-3.365620018	0.546358466
C	-3.456187289	-3.815998569	1.555078752
C	-3.492451357	-2.352236382	-0.299205097
C	-2.081137046	-3.189072172	1.587428635

N	-2.195599950	-2.288552083	0.414646822
O	-5.132722921	-5.242227728	2.376389883
O	-3.161593922	-5.233117233	3.444857314
O	-1.214245174	-1.634093805	-0.031661314
H	-5.315412341	-5.897687953	3.071980564
H	-5.233464419	-3.680823906	0.339228131
C	-1.828778238	-2.368605742	2.852560702
C	-4.173005257	-0.982466893	-0.280402801
H	-5.157194076	-1.045952061	-0.766520695
H	-1.818090909	-3.035590997	3.725037407
H	-0.861357744	-1.854224453	2.769278013
H	-3.548877354	-0.255634161	-0.818874795
H	-2.614014577	-1.609987006	2.980891953
H	-4.302434260	-0.630470981	0.752733956

C₁mpyr N(CN)₂ conf 2:

C	-2.241828262	1.587385658	-0.008333900
C	-1.562152250	1.157636653	1.311422759
C	-0.880945301	-0.155067171	0.961696841
C	-2.226634589	0.345514133	-0.916030698
N	-1.818003480	-0.805740722	-0.025314476
C	-3.008563117	-1.361485479	0.675704959
C	-1.140437250	-1.884374971	-0.797194895
H	-3.537952367	-0.552418020	1.189071741
H	-2.670055265	-2.112882953	1.397669796
H	-3.665334565	-1.821125260	-0.070500730
H	-1.860634653	-2.294871143	-1.514662702
H	-0.810557336	-2.655593859	-0.092350530
H	-0.274993731	-1.447140385	-1.307207520
H	-0.715607133	-0.846889007	1.796784072
H	0.071092756	-0.012935343	0.430915756
H	-2.296087797	1.018355335	2.115981911
H	-0.818928307	1.891926819	1.641414500
H	-3.261516867	1.952655486	0.162352723
H	-1.670401727	2.392471461	-0.487977055
H	-3.190065577	0.096184888	-1.375312509
H	-1.455756983	0.413554845	-1.692732985
N	0.737415008	0.303537628	-2.616351828
C	1.323519752	0.882651585	-1.779028853
N	2.062862256	1.478746386	-0.872291039
C	1.472781963	2.337027519	-0.065621291
N	1.037469096	3.108668436	0.702909715
H	4.151460895	-0.068499483	-1.387738586
H	3.358822876	0.932619823	1.394515179
C	4.042097863	-1.124015208	-1.670226145
C	2.905479649	0.251942858	2.127202159
H	3.100411154	-1.234023776	-2.226900845
H	1.811968477	0.348948085	2.053694601
H	3.225629910	0.527977148	3.140480559
H	4.879411493	-1.426768846	-2.314969732
C	5.725525928	-1.086242492	2.822251939
C	5.170518219	-1.800815229	0.486782380
C	4.806839720	-1.368313607	1.699407305
C	3.993985709	-2.009456751	-0.424510126
C	3.311895035	-1.192977230	1.838391603
N	2.893800522	-1.573425958	0.467323851
O	7.012997584	-1.274254146	2.500869452
O	5.366581754	-0.727156026	3.921654900
O	1.680875813	-1.700338932	0.145106799
H	7.537855780	-1.070020589	3.294425551
H	6.196424798	-1.992809081	0.172060094
C	2.688606447	-2.157459993	2.848711171
C	3.798865872	-3.480848163	-0.799812901
H	4.603494125	-3.811151721	-1.471240022
H	3.008956633	-1.887231841	3.863160917
H	1.593719141	-2.091298102	2.779915994

H	2.834729324	-3.589904153	-1.315489168
H	2.994599465	-3.192428618	2.638401994
H	3.797371540	-4.116800489	0.096697318

C₁mpyr SO₃CH₃ conf 1:

C	-1.877219871	-1.199309155	0.487259833
C	-2.300237688	-0.920839145	1.929464226
C	-3.721405384	-0.313873584	1.843701770
C	-4.042714244	-0.235070324	0.353411329
N	-3.169134977	-1.282628082	-0.292250028
C	-3.774469180	-2.631639932	-0.129550014
C	-2.957486261	-0.989084163	-1.735057090
H	-3.912828019	-2.833737646	0.938282380
H	-4.741096551	-2.648258171	-0.645090031
H	-3.096530580	-3.373155302	-0.566172151
H	-2.523680243	0.014787802	-1.820760484
H	-2.281342677	-1.746945202	-2.146859865
H	-3.928305029	-1.035262528	-2.242738297
H	-3.734833233	0.726561907	-0.074473421
H	-5.085426003	-0.448733534	0.088534210
H	-4.453343097	-0.932597865	2.379061390
H	-3.744763052	0.697037726	2.264670328
H	-2.292394392	-1.837081630	2.534132514
H	-1.598761258	-0.202267888	2.365368256
H	-1.311030402	-2.126416367	0.338262435
H	-1.315394436	-0.355564869	0.067134472
H	0.194842083	-0.542984200	-1.823284090
H	0.568469662	0.711716207	1.039567839
C	0.715788180	-1.478580222	-2.075307343
C	1.255326563	0.238521424	1.756569007
H	0.058609436	-2.340334112	-1.881838521
H	0.682423416	-0.413348477	2.432596730
H	1.759064541	1.013508340	2.349856270
H	0.979256248	-1.476818409	-3.142965536
C	3.855456934	1.323559182	0.232626096
C	2.860639089	-0.415565764	-1.268703853
C	3.032359400	0.132027277	-0.060295125
C	1.978114503	-1.631383593	-1.226187425
C	2.299515457	-0.609963460	1.033279539
N	1.618268989	-1.640338237	0.211594813
O	4.408285251	1.857587377	-0.865680923
O	4.025468860	1.777803859	1.342304117
O	0.932082494	-2.565738088	0.727776288
H	4.929496481	2.626764635	-0.576806999
H	3.302257998	-0.044172108	-2.193463906
C	3.245880527	-1.290137660	2.024929075
C	2.731466767	-2.917939772	-1.575102304
H	2.989555176	-2.930125179	-2.643097242
H	3.749932502	-0.529489844	2.635291949
H	2.662375368	-1.955520517	2.676506258
H	2.084626971	-3.778172918	-1.352522842
H	4.003831297	-1.886053340	1.496202591
H	3.653733300	-3.004847956	-0.983571158
O	-2.770134038	2.412435627	-1.230320868
S	-1.516582859	2.320039350	-0.411991315
C	-0.822200646	3.970519370	-0.371041117
H	-0.615681667	4.275321510	-1.402910646
H	-1.559429022	4.634548515	0.093785816
H	0.100284772	3.935805687	0.219506397
O	-0.475982886	1.451132140	-1.060682947
O	-1.779195570	1.936362310	1.013256613

C₁mpyr SO₃CH₃ conf 2:

C	-4.179120064	-1.442814470	0.367932021
C	-2.739222623	-1.774053674	-0.093022974

C	-2.105613270	-0.433400428	-0.477014111
C	-4.217968836	0.078557302	0.446771767
N	-3.253064619	0.534959243	-0.617624566
C	-3.857084245	0.411046238	-1.970712708
C	-2.787159291	1.929944506	-0.393313960
H	-4.126879687	-0.635410677	-2.149043032
H	-3.115461589	0.736663597	-2.708805588
H	-4.748555185	1.046305448	-2.020013839
H	-3.628762861	2.612868445	-0.558216473
H	-1.975607311	2.126193041	-1.106145131
H	-2.418847303	1.986840295	0.638695867
H	-1.538531395	-0.413574359	-1.412595127
H	-1.469624344	-0.044003082	0.328259662
H	-2.739850552	-2.477955214	-0.935249345
H	-2.160371126	-2.205165726	0.732577929
H	-4.927185139	-1.825529895	-0.339134475
H	-4.381418796	-1.857392310	1.360921271
H	-5.195206931	0.540051155	0.259265013
H	-3.795993830	0.426679694	1.397942113
H	0.317268025	1.283560368	1.422933399
H	0.416914886	-1.567618528	0.234109015
C	0.735656115	2.137394267	0.872283584
C	0.884528257	-1.774853878	-0.740681621
H	-0.082138204	2.679754279	0.376416702
H	0.106403883	-1.898332363	-1.508338808
H	1.460637610	-2.708123246	-0.681377637
H	1.225460058	2.824963289	1.577552721
C	3.897743135	-1.418381464	0.244042489
C	2.851468944	0.848221883	0.408747343
C	2.901148621	-0.384622826	-0.106987639
C	1.742353686	1.672994127	-0.178804531
C	1.825962204	-0.636554173	-1.139623683
N	1.117954625	0.669667332	-1.077250629
O	4.743828662	-1.018789429	1.203580121
O	3.960543473	-2.510519058	-0.275474313
O	0.210984491	0.984580416	-1.899198952
H	5.361749156	-1.753456000	1.362608750
H	3.533101379	1.239159012	1.164251396
C	2.387557102	-0.846195077	-2.546626323
C	2.268666030	2.847552620	-1.007750506
H	2.720105253	3.602248517	-0.348914789
H	2.907171219	-1.811930562	-2.595276520
H	1.558126174	-0.838500220	-3.267339594
H	1.429552197	3.303049376	-1.551598519
H	3.093476278	-0.045034589	-2.809025532
H	3.021999358	2.510344688	-1.733655706
O	-2.728073478	-1.263641845	3.058941281
S	-1.564031767	-0.324379599	3.033670683
C	-1.022446871	-0.149362687	4.732765093
H	-1.863233253	0.242652667	5.315849528
H	-0.723645935	-1.139484617	5.094741615
H	-0.175718333	0.545816573	4.751198046
O	-1.946569316	1.059824363	2.586091277
O	-0.383704669	-0.863712744	2.279887947

C₁mpyr N(SO₂CF₃)₂ conf 1:

C	-1.998103848	1.846839816	-2.448611108
C	-0.479195103	1.734754931	-2.169538162
C	-0.245628251	2.537812036	-0.895283912
C	-2.551848498	2.746829294	-1.342845243
N	-1.366263351	3.547821328	-0.859674310
C	-1.081586359	4.668447661	-1.796826572
C	-1.582327077	4.076935967	0.512926733
H	-0.930132864	4.263974855	-2.803154241
H	-0.176774302	5.185659189	-1.458784777
H	-1.935421035	5.354690066	-1.791737741

H	-2.426214956	4.776193698	0.487488570
H	-0.671649204	4.597299982	0.831390725
H	-1.806901412	3.231719594	1.173117035
H	0.707737797	3.077105318	-0.843756117
H	-0.365269700	1.900033578	-0.012121789
H	0.110563629	2.131956360	-3.006823991
H	-0.181246277	0.696929172	-1.984639391
H	-2.193685902	2.270588050	-3.442116615
H	-2.477828624	0.862794306	-2.391723321
H	-3.337091311	3.446313928	-1.653748746
H	-2.888745108	2.160715807	-0.480028992
H	2.421094579	0.048084901	-2.917161568
H	3.232640605	2.038398792	-0.683766880
C	2.141217242	-0.988881552	-2.681186821
C	3.199566572	1.732967464	0.372594355
H	1.045566122	-1.081055968	-2.671781645
H	2.243425588	2.053095269	0.811012187
H	4.026431601	2.211886063	0.912590268
H	2.550512561	-1.654263760	-3.454730894
C	5.890898181	-0.005230937	0.163933381
C	4.170198308	-1.228567385	-1.185781320
C	4.510760034	-0.366583969	-0.220202880
C	2.681572135	-1.394599180	-1.308919960
C	3.313152909	0.214084761	0.496171923
N	2.230205567	-0.428508627	-0.282219110
O	6.817748318	-0.617499124	-0.585895601
O	6.169151809	0.760398120	1.060255790
O	1.010862463	-0.185956922	-0.067975650
H	7.686905602	-0.324147517	-0.261263942
H	4.874364807	-1.771176822	-1.816904449
C	3.225832481	-0.220427912	1.961052758
C	2.211835697	-2.803884266	-0.935766307
H	2.502508522	-3.520547497	-1.717023133
H	4.037619132	0.245664284	2.535077410
H	2.256048947	0.095448075	2.368002685
H	1.117457502	-2.793721536	-0.835199784
H	3.306467248	-1.313629187	2.045977288
H	2.653213537	-3.120709624	0.020098650
O	-2.928044760	1.366736697	1.741009398
S	-2.373942986	0.010142740	1.549988469
O	-3.122046606	-1.150836729	2.061484446
C	-0.817969780	0.071098560	2.569875429
F	-0.084086428	-1.016369887	2.419454724
F	-1.167706681	0.184179721	3.850654362
F	-0.099128352	1.143253927	2.236353211
N	-1.887436515	-0.111147753	0.020963345
S	-1.683141237	-1.597429071	-0.605840847
O	-1.047973624	-2.593728615	0.269902511
C	-3.447542339	-2.234276110	-0.829432707
F	-3.540078673	-2.809878325	-2.024199541
F	-3.747340862	-3.129001442	0.098111873
F	-4.321122547	-1.233241218	-0.772457741
O	-1.203224921	-1.432333374	-1.988661722

C1mpyr N(SO₂CF₃)₂ conf 2:

C	-4.528660277	-1.410627013	0.156144552
C	-3.395775492	-1.909754257	-0.776827324
C	-2.477738389	-0.703757049	-0.966141228
C	-4.228091460	0.070674535	0.393737866
N	-3.384446542	0.488561262	-0.783608086
C	-4.230680032	0.686338378	-1.992287635
C	-2.618654759	1.734084376	-0.504195503
H	-4.789038813	-0.232350063	-2.198972965
H	-3.576826089	0.928816882	-2.837133152
H	-4.925482559	1.511300214	-1.800374446
H	-3.332712797	2.558844366	-0.396679700

H	-1.930036408	1.909185042	-1.338352036
H	-2.051768439	1.582065899	0.420387379
H	-1.976319779	-0.622110686	-1.936749864
H	-1.731744938	-0.631467303	-0.166089070
H	-3.797788841	-2.257619290	-1.737147275
H	-2.833187803	-2.740810455	-0.337184822
H	-5.513416221	-1.553921323	-0.306382018
H	-4.526645730	-1.927816671	1.121734285
H	-5.105978529	0.725292128	0.447510189
H	-3.599468087	0.200623940	1.283284434
H	0.770465679	1.906560849	1.372491599
H	0.868680759	-1.074713023	0.895718637
C	0.970446922	2.611981135	0.555978042
C	1.157837608	-1.514060028	-0.068076837
H	0.019052525	2.925877828	0.102662712
H	0.249800891	-1.791008737	-0.623275118
H	1.759582130	-2.416230624	0.104017532
H	1.471882382	3.501617003	0.963349682
C	4.267048862	-0.847293804	0.296556706
C	3.097904875	1.354842206	0.062183683
C	3.162206675	0.033934161	-0.137692905
C	1.849922716	1.962746533	-0.513747229
C	1.966896320	-0.508634167	-0.887041031
N	1.192185698	0.746540789	-1.048609081
O	5.226070345	-0.188833133	0.961155805
O	4.314008423	-2.037170102	0.077073362
O	0.125456580	0.797270531	-1.722534749
H	5.905748586	-0.841745896	1.203548201
H	3.852170715	1.947713420	0.579669412
C	2.326835310	-1.070766902	-2.262850746
C	2.142213628	2.935479205	-1.658612974
H	2.626230491	3.842457973	-1.270963379
H	2.901700183	-1.998052976	-2.142738680
H	1.401724426	-1.281960549	-2.817099808
H	1.194754852	3.213985315	-2.140694623
H	2.926222293	-0.347613601	-2.834356385
H	2.799186274	2.471319203	-2.407428160
O	-2.840197842	-2.682977266	5.067227125
S	-2.502874407	-1.920164999	3.861802676
O	-3.553555359	-1.132860723	3.191586414
C	-2.026326927	-3.216235753	2.610425229
F	-1.335926690	-2.675249778	1.607634657
F	-3.129307328	-3.771729261	2.110155944
F	-1.289104377	-4.155799799	3.182642206
N	-1.097511488	-1.154602962	4.120682213
S	-0.647905388	0.059217373	3.159856791
O	-1.282390591	0.109351491	1.824027736
C	-1.323379378	1.567903032	4.003757390
F	-1.078389647	2.629460891	3.238222951
F	-2.633984170	1.451218940	4.172042498
F	-0.742377819	1.737947565	5.182171727
O	0.812507245	0.213665727	3.236977194

C1mpyr SO₃CF₃ conf 1:

C	-2.311770000	-1.208290000	0.537790000
C	-2.710670000	-0.728660000	1.933520000
C	-3.846250000	0.300690000	1.714670000
C	-4.047530000	0.369500000	0.202890000
N	-3.527280000	-0.944820000	-0.322610000
C	-4.541670000	-2.015840000	-0.120150000
C	-3.177520000	-0.845320000	-1.764640000
H	-4.794580000	-2.072090000	0.943990000
H	-5.433190000	-1.770340000	-0.707640000
H	-4.114070000	-2.966950000	-0.455100000
H	-2.401740000	-0.078050000	-1.876530000
H	-2.803240000	-1.819090000	-2.100150000

H	-4.081300000	-0.575530000	-2.323080000
H	-3.428230000	1.154010000	-0.248370000
H	-5.086250000	0.487210000	-0.127900000
H	-4.768630000	-0.007350000	2.223260000
H	-3.560680000	1.292250000	2.081110000
H	-3.045210000	-1.562880000	2.563510000
H	-1.842590000	-0.260100000	2.408990000
H	-2.039150000	-2.268280000	0.462130000
H	-1.503700000	-0.596040000	0.119190000
H	-0.277190000	-1.194220000	-1.904460000
H	0.353690000	0.053890000	1.310270000
C	0.151120000	-2.186390000	-2.093550000
C	0.976730000	-0.605770000	1.928230000
H	-0.584160000	-2.969990000	-1.855330000
H	0.332480000	-1.244730000	2.550530000
H	1.609920000	0.010940000	2.579910000
H	0.422050000	-2.271060000	-3.155620000
C	3.520330000	0.351190000	0.290170000
C	2.343900000	-1.236010000	-1.250230000
C	2.596810000	-0.756540000	-0.027720000
C	1.385390000	-2.394900000	-1.220180000
C	1.854610000	-1.499550000	1.058650000
N	0.998380000	-2.367900000	0.211740000
O	3.934000000	1.012860000	-0.799630000
O	3.879990000	0.636230000	1.410690000
O	0.204070000	-3.215210000	0.706540000
H	4.535620000	1.713950000	-0.494390000
H	2.776670000	-0.854830000	-2.175100000
C	2.776200000	-2.365890000	1.922300000
C	2.066070000	-3.729600000	-1.544900000
H	2.345720000	-3.764970000	-2.606990000
H	3.414830000	-1.719290000	2.538220000
H	2.162250000	-3.003770000	2.573980000
H	1.361320000	-4.546270000	-1.332820000
H	3.415410000	-3.006190000	1.297950000
H	2.969220000	-3.872120000	-0.935620000
O	-1.686910000	2.941400000	-1.225260000
S	-0.819510000	2.067050000	-0.404310000
C	0.736480000	3.038310000	-0.154290000
F	1.344000000	3.262600000	-1.318110000
F	0.475400000	4.211140000	0.420880000
F	1.577520000	2.362550000	0.634310000
O	-0.321260000	0.847190000	-1.101300000
O	-1.300690000	1.825040000	0.981720000

C1mpyr SO₃CF₃ conf 2:

C	3.865219164	-0.520358798	-1.660934397
C	2.352482835	-0.591341654	-1.983709391
C	1.684749706	-1.178576769	-0.736813138
C	3.967825744	-0.883630731	-0.183383025
N	2.798859228	-1.803009325	0.065959711
C	3.085500971	-3.169652288	-0.448365441
C	2.434151835	-1.866932190	1.507701224
H	3.282819991	-3.113099838	-1.524385528
H	2.207821986	-3.798290181	-0.261452270
H	3.959799833	-3.568953321	0.077446131
H	3.233125477	-2.385848650	2.049684250
H	1.483085360	-2.408455437	1.588569693
H	2.319093756	-0.835653621	1.861968398
H	0.927315374	-1.948854852	-0.910644339
H	1.244893896	-0.399565042	-0.101876284
H	2.163885164	-1.210529561	-2.869765839
H	1.938719242	0.407979324	-2.166788144
H	4.440102868	-1.218554455	-2.283054785
H	4.259592239	0.490325581	-1.812810519
H	4.890008328	-1.396386984	0.114610524

H	3.797455995	-0.005163992	0.450245652
H	-0.308250245	0.943502179	1.483436830
H	-0.724878326	0.335526837	-1.484090857
C	-0.733671407	0.279510703	2.246937047
C	-1.388528067	-0.466761905	-1.840577659
H	0.033109686	-0.447316674	2.551629628
H	-0.785373439	-1.321335126	-2.181019978
H	-1.980616586	-0.102463948	-2.690739821
H	-1.019781308	0.872586784	3.127896176
C	-4.144564763	0.940355864	-1.048460134
C	-2.973731179	0.453360888	1.109300699
C	-3.182767790	0.216515545	-0.190162998
C	-1.949533241	-0.470150030	1.704500232
C	-2.337624304	-0.916083929	-0.727563892
N	-1.569730986	-1.250959728	0.500139669
O	-4.779738927	1.925596291	-0.399542035
O	-4.351237198	0.677936535	-2.212508622
O	-0.829312633	-2.272612918	0.572768738
H	-5.389444139	2.339292108	-1.035190897
H	-3.478986464	1.221248321	1.695258441
C	-3.167370600	-2.126140993	-1.158307745
C	-2.546800144	-1.407835672	2.756169760
H	-2.830204787	-0.838467689	3.652061473
H	-3.729944386	-1.881077667	-2.068424144
H	-2.492630887	-2.969795922	-1.358732991
H	-1.794571799	-2.159384003	3.032908002
H	-3.873183748	-2.416032026	-0.366627877
H	-3.435244225	-1.921943207	2.363176274
O	3.125245814	2.435947884	-0.709773912
S	1.964576265	2.228206483	0.187721234
C	1.656384314	3.888284237	0.943483805
F	2.730437991	4.309510442	1.610852324
F	1.365782638	4.785760799	0.002335052
F	0.631011509	3.822168504	1.794188422
O	2.242355184	1.375343381	1.377932114
O	0.677979185	1.932490438	-0.497414835