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Does hydrohalic acid HX (X = F, Cl) form true N-protonated twisted amide salts? Effects of anions on the ion-pair interactions and on the amide moiety in N-protonated tricyclic twisted amide salts

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Supporting Information

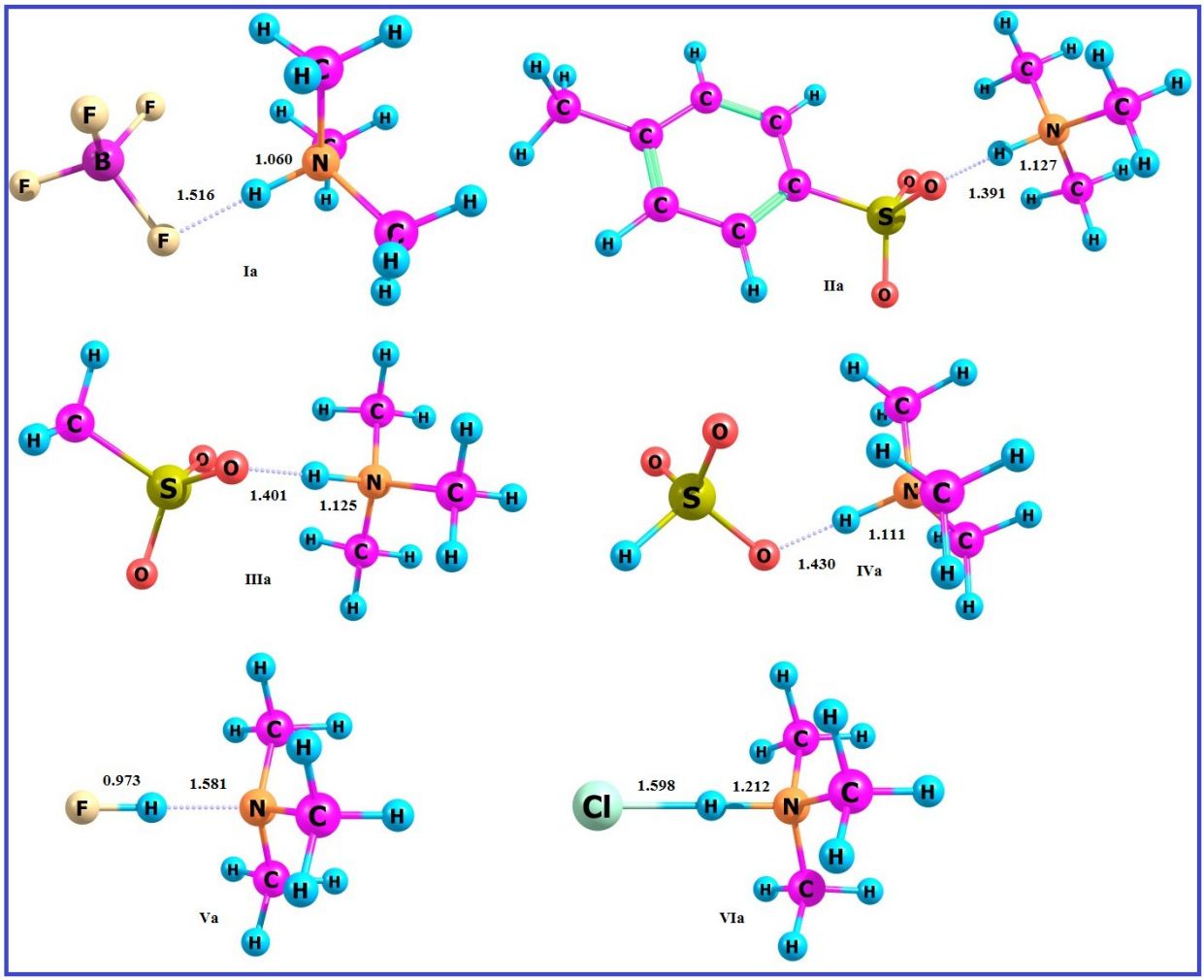
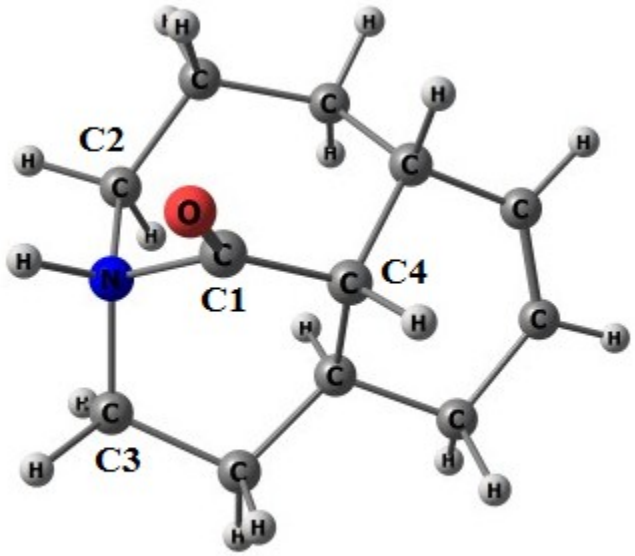


Fig. S1. Optimized structure of the $[Me_3NH]^+[X]^-$ salts (**Ia-VIa**).

Cartesian coordinates for optimized structures of the tricyclic twisted amide salts (**I-VI**) at DFT-D3(BJ)/def2-TZVPP level of theory with PBE and PBE0 functionals and $[Me_3NH]^+[X]^-$ salts (**Ia-VIa**) at DFT-D3(BJ)/def2-TZVPP level of theory with PBE0 functional.

PBE0-D3(BJ)



$\mathbf{I}^+$

C	-0.257998	-1.899028	-1.631908
C	-1.668068	-2.444672	-1.412314
C	-0.112288	-0.394453	-1.448899
C	-2.130769	-2.583508	0.044737
C	-3.617606	-2.792962	0.130805
C	-0.697826	1.358984	0.325863
C	-4.474931	-1.865085	0.546954
C	-2.669185	-0.171210	0.495898
C	-4.089334	-0.468499	0.940732
C	-1.810803	-1.362856	0.922254
C	-0.366086	-1.047305	0.958625
C	-2.034628	1.105074	1.017667
H	0.020682	-2.086139	-2.671543
H	-2.375869	-1.819811	-1.963969
H	-1.732988	-3.431786	-1.873112
H	-0.970708	0.126449	-1.867310
H	0.780981	-0.026153	-1.951726
H	0.485391	-2.437659	-1.035470
H	-0.826924	1.879721	-0.621772
H	-2.692112	-0.125603	-0.597472
H	-3.985974	-3.769397	-0.163639
H	1.018636	0.192268	0.182090
H	-1.623459	-3.447947	0.484238

H	-5.528964	-2.112362	0.603689
H	-2.669885	1.974840	0.843799
H	-0.026416	1.946395	0.949833
H	-2.059653	-1.634029	1.953171
H	-4.188876	-0.340234	2.025990
H	-1.893616	1.030222	2.099950
N	0.025844	0.064248	-0.005309
O	0.503518	-1.505369	1.615875
H	-4.784552	0.244757	0.489706

1^+ BF_4^-

C	-0.017497	-2.005368	-1.560167
C	-1.465312	-2.468167	-1.413054
C	0.221451	-0.520483	-1.328201
C	-1.996384	-2.590520	0.022668
C	-3.494838	-2.704702	0.042398
C	-0.298882	1.210898	0.463969
C	-4.307489	-1.727490	0.436878
C	-2.389425	-0.157983	0.494528
C	-3.843636	-0.367491	0.873334
C	-1.626591	-1.407988	0.924809
C	-0.154651	-1.190119	1.015072
C	-1.688551	1.054489	1.075674
H	0.295151	-2.186232	-2.590920
H	-2.107767	-1.787637	-1.979610
H	-1.578046	-3.443791	-1.891626
H	-0.581079	0.069789	-1.766828
H	1.161997	-0.209880	-1.780136
H	0.664186	-2.603458	-0.947515
H	-0.314411	1.774107	-0.465369
H	-2.358376	-0.082479	-0.596454
H	-3.917213	-3.647384	-0.290587
H	1.382952	0.004210	0.316509
H	-1.564248	-3.492929	0.467528
H	-5.378087	-1.903828	0.439175
H	-2.246775	1.973801	0.889130
H	0.390905	1.723031	1.131330
H	-1.930371	-1.671860	1.942981
H	-3.977531	-0.253500	1.957154
H	-1.619182	0.943934	2.162879
N	0.344906	-0.113907	0.128088
O	0.611368	-1.773602	1.709694
H	-4.471950	0.400418	0.412430
B	3.181460	1.147604	-0.778496
F	4.339273	1.833683	-0.584556
F	3.259347	0.212705	-1.807959
F	2.084146	1.996958	-1.011411
F	2.845265	0.407886	0.435796

1^+ OTs^- (OTs^- = p-$MeC_6H_4SO_3^-$]

C	-0.202537	-2.517054	-1.133465
C	-1.715468	-2.731443	-1.165644
C	0.243735	-1.062541	-1.082509
C	5.528416	0.132835	-1.027747
C	6.898263	-0.075669	-1.022785
C	4.919842	0.700921	0.079307
C	7.674385	0.273850	0.078065
C	9.150316	0.018705	0.090197
C	-2.465268	-2.521140	0.159154
C	-3.947784	-2.418776	-0.066155
C	5.675394	1.069666	1.182651
C	7.042033	0.853180	1.176086
C	-0.234350	1.003063	0.298434
C	-4.634682	-1.282863	0.031115
C	-2.510450	-0.015017	0.182573
C	-4.018672	0.053459	0.332600
C	-2.039102	-1.263182	0.922516
C	-0.575157	-1.250610	1.216941
C	-1.703927	1.168059	0.680619
H	0.213970	-2.918661	-2.059998
H	-2.142027	-2.073849	-1.928780
H	-1.924416	-3.748988	-1.505212
H	-0.373146	-0.458535	-1.747199
H	1.277351	-0.947756	-1.408521
H	4.925249	-0.122797	-1.889133
H	7.375601	-0.511270	-1.893925
H	0.268438	-3.091556	-0.330059
H	9.566526	0.042411	-0.917914
H	-0.026009	1.386941	-0.698462
H	-2.308596	-0.141197	-0.885552
H	-4.468761	-3.335823	-0.323454
H	9.676813	0.758170	0.695158
H	1.298812	-0.408098	0.625988
H	-2.261284	-3.383178	0.802921
H	-5.708182	-1.304054	-0.126321
H	5.188212	1.536650	2.028927
H	9.370945	-0.966090	0.512135
H	7.633268	1.147042	2.036556
H	-2.062711	2.110838	0.263341
H	0.430882	1.531535	0.981409
H	-2.526979	-1.297502	1.902018
H	-4.288299	0.371827	1.348211
H	-1.810148	1.245037	1.767778
N	0.214253	-0.434014	0.286966
O	2.708780	0.902821	-1.277806
O	2.923709	2.192804	0.796874
O	2.650764	-0.221818	0.863195
O	-0.035260	-1.835196	2.101410
S	3.172814	0.955176	0.097919
H	-4.436232	0.809802	-0.338737

1^+ $[MeSO_3]^-$

C	-0.183129	-2.490014	-1.152621
C	-1.693960	-2.720468	-1.170889
C	0.248120	-1.030890	-1.103202
C	-2.433981	-2.519245	0.160915
C	-3.919315	-2.430964	-0.050936
C	-0.236905	1.027046	0.285853
C	-4.616675	-1.302203	0.055228
C	-2.503899	-0.013593	0.189721
C	-4.011153	0.039461	0.354157
C	-2.013214	-1.258363	0.922533
C	-0.546914	-1.231802	1.203425
C	-1.704254	1.176396	0.682507
H	0.228796	-2.885577	-2.083841
H	-2.134282	-2.066372	-1.929266
H	-1.895583	-3.739619	-1.509841
H	-0.383964	-0.432800	-1.758631
H	1.276400	-0.902269	-1.440583
H	0.301526	-3.061249	-0.354941
H	-0.043754	1.413438	-0.713174
H	-2.311000	-0.135708	-0.880538
H	-4.433480	-3.352511	-0.305785
H	1.311659	-0.370254	0.600258
H	-2.215719	-3.380104	0.801589
H	-5.691264	-1.333666	-0.092625
H	-2.076690	2.116378	0.271096
H	0.430674	1.562350	0.960919
H	-2.491607	-1.299540	1.906461
H	-4.274496	0.352964	1.372987
H	-1.800969	1.249980	1.770852
N	0.226171	-0.405754	0.268397
O	2.726608	0.902379	-1.338187
O	2.886398	2.252362	0.697252
O	2.666060	-0.172957	0.832867
O	0.006882	-1.813594	2.081301
S	3.170113	0.996656	0.043018
H	-4.442544	0.793429	-0.311116
C	4.922987	0.776918	0.055241
H	5.265028	0.797970	1.087770
H	5.159735	-0.177193	-0.410574
H	5.362323	1.597801	-0.508249

1^+ $[HSO_3]^-$

C	-0.196651	-2.508044	-1.131242
C	-1.708497	-2.728619	-1.167112
C	0.243265	-1.051902	-1.077791
C	-2.462230	-2.523012	0.156209
C	-3.944413	-2.423504	-0.072200
C	-0.241937	1.010965	0.308802

C	-4.634537	-1.289705	0.026576
C	-2.514219	-0.016477	0.185482
C	-4.022832	0.047459	0.332825
C	-2.041454	-1.265387	0.923642
C	-0.579772	-1.248731	1.224243
C	-1.712745	1.168447	0.687960
H	0.223958	-2.906014	-2.057479
H	-2.135958	-2.071921	-1.930543
H	-1.912450	-3.746415	-1.508433
H	-0.377958	-0.448133	-1.737927
H	1.275882	-0.928904	-1.403333
H	0.275620	-3.082294	-0.328318
H	-0.032263	1.397191	-0.686852
H	-2.310358	-0.139784	-0.882566
H	-4.462239	-3.341246	-0.333029
H	1.271246	-0.400090	0.634483
H	-2.257644	-3.385662	0.798929
H	-5.707553	-1.313130	-0.133253
H	-2.074232	2.110686	0.272176
H	0.419974	1.538006	0.995791
H	-2.532055	-1.303706	1.901610
H	-4.295596	0.362762	1.348576
H	-1.821540	1.242600	1.775017
N	0.210650	-0.426573	0.295058
O	2.716027	0.890558	-1.304280
O	2.966688	2.234717	0.729811
O	2.669588	-0.184083	0.868037
O	-0.037169	-1.828680	2.109261
S	3.167332	0.970754	0.071358
H	-4.440860	0.804588	-0.337277
H	4.500412	0.750425	0.051496

1^{+} F^{-}

C	-0.241533	-1.932763	-1.613477
C	-1.689658	-2.381400	-1.404863
C	0.033227	-0.445855	-1.400430
C	-2.162218	-2.550856	0.049546
C	-3.647398	-2.773726	0.113748
C	-0.761254	1.282126	0.252741
C	-4.515575	-1.867337	0.558069
C	-2.716841	-0.174994	0.553660
C	-4.132865	-0.482891	0.998855
C	-1.839993	-1.354039	0.949953
C	-0.373175	-1.047943	0.885610
C	-2.051293	1.088439	1.051310
H	0.025478	-2.130832	-2.654862
H	-2.353163	-1.681427	-1.921675
H	-1.834019	-3.342639	-1.905514
H	-0.699110	0.127009	-1.977366
H	1.020929	-0.208090	-1.802154
H	0.445367	-2.534178	-1.011993

H	-1.005304	1.711244	-0.721353
H	-2.738970	-0.116604	-0.540889
H	-4.013849	-3.739086	-0.222951
H	1.537793	0.497061	0.296345
H	-1.652885	-3.426690	0.465183
H	-5.569606	-2.123827	0.595678
H	-2.679451	1.972758	0.921688
H	-0.095618	1.987342	0.754633
H	-2.064308	-1.643148	1.981838
H	-4.222022	-0.394841	2.089651
H	-1.840198	1.002773	2.122844
N	-0.010152	0.029369	0.010403
F	2.383033	0.947776	0.372485
O	0.461141	-1.704162	1.440143
H	-4.836915	0.242930	0.579941

1^{+} Cl^{-}

C	-0.245619	-1.918123	-1.603720
C	-1.676608	-2.417475	-1.401505
C	-0.034559	-0.423053	-1.390165
C	-2.155082	-2.567015	0.051933
C	-3.641532	-2.781310	0.112196
C	-0.709389	1.290066	0.326213
C	-4.506456	-1.860792	0.532423
C	-2.695234	-0.174360	0.526302
C	-4.119199	-0.472292	0.954706
C	-1.832948	-1.360781	0.939130
C	-0.366789	-1.052681	0.922747
C	-2.041455	1.086937	1.050463
H	0.033480	-2.108017	-2.643005
H	-2.358496	-1.751730	-1.939111
H	-1.781667	-3.393470	-1.882369
H	-0.824226	0.127283	-1.907392
H	0.922168	-0.124245	-1.826275
H	0.464617	-2.490423	-1.000126
H	-0.873925	1.790426	-0.628623
H	-2.703053	-0.114719	-0.567661
H	-4.011284	-3.750188	-0.209680
H	1.360980	0.383953	0.197526
H	-1.651481	-3.438938	0.482424
H	-5.562492	-2.108915	0.566069
H	-2.663290	1.971182	0.894974
H	-0.031618	1.920658	0.904833
H	-2.074926	-1.637636	1.970459
H	-4.223056	-0.366355	2.042665
H	-1.884900	0.997063	2.130727
N	0.012202	0.025642	0.030934
Cl	2.692156	0.953378	0.170487
O	0.456266	-1.654340	1.542909
H	-4.812988	0.251766	0.516309

PBE-D3(BJ)

1+

C	-0.249059	-1.905200	-1.644162
C	-1.669298	-2.449981	-1.423849
C	-0.094790	-0.392664	-1.464594
C	-2.135321	-2.596750	0.041923
C	-3.628917	-2.806165	0.133209
C	-0.695917	1.380548	0.325604
C	-4.492697	-1.871064	0.553606
C	-2.673719	-0.167296	0.502986
C	-4.103724	-0.467905	0.947162
C	-1.809252	-1.367855	0.933389
C	-0.359704	-1.061522	0.979086
C	-2.037174	1.119399	1.024363
H	0.032431	-2.097407	-2.690101
H	-2.380870	-1.815987	-1.974739
H	-1.739750	-3.441695	-1.891828
H	-0.955350	0.136104	-1.888674
H	0.809193	-0.027918	-1.966974
H	0.497114	-2.449776	-1.043329
H	-0.829079	1.901130	-0.630125
H	-2.694379	-0.123587	-0.597963
H	-3.997783	-3.791348	-0.159683
H	1.039574	0.206103	0.185145
H	-1.621256	-3.467030	0.480898
H	-5.553606	-2.119594	0.615106
H	-2.681621	1.991200	0.846933
H	-0.019148	1.973698	0.950977
H	-2.067580	-1.650102	1.967430
H	-4.207944	-0.334191	2.039152
H	-1.894488	1.048049	2.113853
N	0.039573	0.076291	-0.008898
O	0.521849	-1.521687	1.640409
H	-4.801776	0.251092	0.491125

1^{+} BF_4^{-}

C	-0.012699	-2.014788	-1.570957
C	-1.470152	-2.478242	-1.423467
C	0.232761	-0.522273	-1.339061
C	-2.006178	-2.604388	0.021269
C	-3.511606	-2.719057	0.043597
C	-0.298592	1.226552	0.468438
C	-4.331055	-1.734376	0.441690
C	-2.399847	-0.155116	0.501035
C	-3.864128	-0.367794	0.878894
C	-1.630746	-1.413872	0.934234
C	-0.152256	-1.202106	1.029958
C	-1.696024	1.066591	1.083722
H	0.302098	-2.198658	-2.608570
H	-2.115980	-1.790208	-1.991298

H	-1.586942	-3.459170	-1.907016
H	-0.572826	0.074998	-1.781327
H	1.184740	-0.213539	-1.788452
H	0.672156	-2.618842	-0.954788
H	-0.314263	1.791302	-0.468704
H	-2.366649	-0.080052	-0.597411
H	-3.935089	-3.669235	-0.290803
H	1.409012	0.014481	0.324308
H	-1.568641	-3.512710	0.467407
H	-5.408831	-1.911500	0.446128
H	-2.260659	1.989966	0.893131
H	0.396151	1.742396	1.139597
H	-1.942187	-1.685518	1.956417
H	-4.001435	-0.249510	1.969737
H	-1.627236	0.958114	2.178401
N	0.355523	-0.108389	0.130273
O	0.623206	-1.794201	1.729246
H	-4.495664	0.405979	0.414052
B	3.209689	1.165965	-0.789448
F	3.263617	0.217362	-1.829864
F	2.116330	2.045610	-1.013778
F	2.863763	0.416500	0.447581
F	4.394754	1.830445	-0.595035

1^{+} OTs^{-} (OTs^{-} = p-$MeC_6H_4SO_3^{-}$]

C	-0.243615	-2.503258	-1.209819
C	-1.765903	-2.722788	-1.201463
C	0.205065	-1.040548	-1.150662
C	5.603410	0.082311	-1.035641
C	6.982093	-0.122269	-0.984875
C	4.960460	0.697313	0.038787
C	7.734278	0.276365	0.128682
C	9.216843	0.024956	0.190872
C	-2.484758	-2.537005	0.156245
C	-3.980983	-2.439954	-0.023351
C	5.689934	1.115896	1.153875
C	7.065945	0.902039	1.192037
C	-0.258787	1.022354	0.277637
C	-4.677921	-1.301504	0.113423
C	-2.544138	-0.014534	0.223895
C	-4.057652	0.040296	0.417813
C	-2.038463	-1.279039	0.934748
C	-0.559782	-1.267995	1.188096
C	-1.723594	1.173222	0.716394
H	0.149490	-2.894135	-2.159915
H	-2.219081	-2.047911	-1.944635
H	-1.984929	-3.741266	-1.555079
H	-0.435778	-0.426502	-1.796028
H	1.238142	-0.918959	-1.502489
H	5.019680	-0.211824	-1.907223

H	7.486735	-0.594279	-1.830479
H	0.254755	-3.092621	-0.423987
H	9.661863	-0.003898	-0.812485
H	-0.094281	1.417454	-0.731375
H	-2.370601	-0.124863	-0.858751
H	-4.505863	-3.363535	-0.280336
H	9.731467	0.799697	0.774711
H	1.339610	-0.389670	0.562341
H	-2.252777	-3.413240	0.784063
H	-5.762866	-1.326867	-0.012037
H	5.175784	1.618965	1.972197
H	9.431220	-0.942204	0.672230
H	7.637203	1.235155	2.060995
H	-2.105547	2.125972	0.323470
H	0.433152	1.556080	0.941751
H	-2.504002	-1.336391	1.932619
H	-4.302586	0.346858	1.451750
H	-1.794105	1.233690	1.814823
N	0.208302	-0.421485	0.238020
O	2.763228	0.856670	-1.408496
O	2.918503	2.223533	0.668100
O	2.660043	-0.230519	0.797963
O	0.015688	-1.877806	2.051438
S	3.196165	0.954041	-0.004693
H	-4.501720	0.810115	-0.233472

1^+ $[MeSO_3]^-$

C	-0.185298	-2.490183	-1.180081
C	-1.705295	-2.725973	-1.184951
C	0.247171	-1.022121	-1.133205
C	-2.440777	-2.531272	0.162699
C	-3.935902	-2.452374	-0.034147
C	-0.254179	1.052062	0.263718
C	-4.646413	-1.319982	0.081833
C	-2.527809	-0.009013	0.199660
C	-4.043729	0.031824	0.377275
C	-2.016070	-1.259414	0.930660
C	-0.539915	-1.230045	1.198020
C	-1.724760	1.193026	0.686257
H	0.221677	-2.887635	-2.121586
H	-2.157463	-2.064866	-1.941002
H	-1.909973	-3.750889	-1.528502
H	-0.394443	-0.423400	-1.792219
H	1.282209	-0.892631	-1.476964
H	0.310635	-3.065432	-0.382325
H	-0.084665	1.435504	-0.749013
H	-2.341683	-0.130277	-0.879743
H	-4.448130	-3.384411	-0.286171
H	1.361990	-0.336967	0.587780
H	-2.206580	-3.397405	0.803614

H	-5.729601	-1.358503	-0.055048
H	-2.112635	2.137142	0.278517
H	0.425401	1.603180	0.926414
H	-2.491190	-1.310040	1.924385
H	-4.302693	0.347267	1.405123
H	-1.806892	1.265489	1.783189
N	0.229212	-0.386487	0.248014
O	2.813908	0.857805	-1.396646
O	2.901985	2.294575	0.631186
O	2.668371	-0.164315	0.842747
O	0.032255	-1.827015	2.072961
S	3.207178	1.003140	0.014696
H	-4.489227	0.789430	-0.287231
C	4.976402	0.764678	0.112353
H	5.274941	0.814377	1.164589
H	5.224589	-0.210979	-0.317866
H	5.448125	1.570946	-0.459643

1^{+} $[HSO_3]^{-}$

C	-0.189936	-2.510364	-1.146879
C	-1.711113	-2.734697	-1.179111
C	0.251494	-1.045725	-1.093712
C	-2.468777	-2.533773	0.155165
C	-3.959349	-2.439563	-0.067710
C	-0.250139	1.034386	0.301446
C	-4.660396	-1.300236	0.036329
C	-2.531555	-0.009965	0.192384
C	-4.049988	0.045526	0.342912
C	-2.046162	-1.266113	0.932316
C	-0.577470	-1.249885	1.231699
C	-1.727450	1.185658	0.693798
H	0.231620	-2.911132	-2.080438
H	-2.144856	-2.071095	-1.943663
H	-1.917076	-3.758296	-1.525460
H	-0.376632	-0.439623	-1.758227
H	1.292428	-0.919665	-1.420241
H	0.288066	-3.088648	-0.340401
H	-0.052598	1.418878	-0.705630
H	-2.327936	-0.133160	-0.883542
H	-4.476034	-3.366535	-0.328807
H	1.309379	-0.377758	0.638996
H	-2.254537	-3.402254	0.799801
H	-5.741308	-1.327900	-0.119273
H	-2.099606	2.132061	0.277101
H	0.421336	1.572089	0.982933
H	-2.541467	-1.313407	1.916234
H	-4.324469	0.363767	1.365808
H	-1.830649	1.260279	1.788667
N	0.217982	-0.411653	0.290027
O	2.818752	0.827800	-1.337095

O	2.973303	2.263650	0.690706
O	2.676474	-0.189172	0.904793
O	-0.023074	-1.842034	2.119619
S	3.207128	0.962453	0.073446
H	-4.475572	0.807378	-0.329641
H	4.553666	0.735871	0.131360

1^{+} F^{-}

C	-0.206712	-1.961777	-1.633224
C	-1.697843	-2.302818	-1.434345
C	0.205916	-0.500271	-1.395484
C	-2.177394	-2.527842	0.024116
C	-3.669642	-2.755650	0.095410
C	-0.837316	1.269147	0.127246
C	-4.543076	-1.875978	0.612127
C	-2.754828	-0.173326	0.617199
C	-4.158702	-0.502398	1.111223
C	-1.849114	-1.354273	0.976733
C	-0.375782	-1.059759	0.874429
C	-2.057073	1.107817	1.044873
H	0.057425	-2.169897	-2.681625
H	-2.315241	-1.521839	-1.905997
H	-1.921457	-3.225953	-1.990441
H	-0.365792	0.148888	-2.075770
H	1.269998	-0.381931	-1.646272
H	0.422602	-2.631450	-1.028547
H	-1.187556	1.557574	-0.875767
H	-2.831002	-0.127740	-0.483419
H	-4.037946	-3.711102	-0.288276
H	1.469505	0.571118	0.400499
H	-1.660161	-3.424106	0.405369
H	-5.601031	-2.145315	0.658458
H	-2.695248	1.996738	0.933873
H	-0.174461	2.070460	0.485305
H	-2.058309	-1.686562	2.006385
H	-4.210964	-0.462213	2.214779
H	-1.756929	1.055836	2.104467
N	-0.020607	0.025685	-0.004232
F	2.306873	1.063424	0.512244
O	0.478859	-1.773184	1.358103
H	-4.887397	0.240192	0.747360

1^{+} Cl^{-}

C	-0.233915	-1.930684	-1.616461
C	-1.679328	-2.417736	-1.412800
C	-0.000522	-0.430156	-1.402042
C	-2.161515	-2.574904	0.050160
C	-3.654722	-2.791350	0.113944
C	-0.715503	1.305807	0.314668
C	-4.527255	-1.866584	0.543303

C	-2.706179	-0.169094	0.538127
C	-4.138297	-0.472103	0.970015
C	-1.834500	-1.361963	0.949977
C	-0.359172	-1.063975	0.927958
C	-2.046021	1.101166	1.058389
H	0.044834	-2.123264	-2.663379
H	-2.359646	-1.735704	-1.947107
H	-1.798210	-3.395492	-1.903455
H	-0.778161	0.136815	-1.934971
H	0.976461	-0.143928	-1.820616
H	0.474361	-2.516954	-1.011072
H	-0.894565	1.790971	-0.653907
H	-2.716283	-0.110170	-0.563533
H	-4.024676	-3.766950	-0.212212
H	1.364701	0.400540	0.213289
H	-1.650916	-3.453034	0.479057
H	-5.589982	-2.117628	0.580285
H	-2.674573	1.990164	0.904366
H	-0.029836	1.953421	0.879255
H	-2.078829	-1.648301	1.986392
H	-4.242182	-0.365814	2.065855
H	-1.878424	1.014542	2.144563
N	0.025430	0.032543	0.031877
Cl	2.708107	0.995806	0.195039
O	0.476880	-1.692777	1.529480
H	-4.837965	0.258288	0.532353

Ia

C	0.143514	-0.379813	-1.344824
F	4.451191	1.480989	-0.580382
C	-0.424944	1.259205	0.372559
H	-0.905203	-0.587265	-1.557720
H	0.515685	0.442275	-1.949312
H	0.005565	2.035190	-0.255094
H	1.304249	0.164997	0.274157
H	-0.270301	1.512865	1.419451
N	0.276278	-0.005562	0.079280
F	3.190754	-0.135623	-1.625864
F	2.236681	1.863876	-1.079413
F	2.777391	0.377966	0.562174
B	3.222706	0.920534	-0.726116
H	0.758755	-1.255368	-1.535184
H	-1.489029	1.136559	0.170857
C	-0.150213	-1.096634	0.971429
H	-1.208869	-1.302300	0.815428
H	0.437998	-1.983921	0.747252
H	0.022409	-0.799765	2.003828

IIa

C	0.589632	-1.004237	-1.140244
C	5.254660	0.188077	-0.834931
C	6.581113	-0.196687	-0.940263

C	4.835136	0.906835	0.273312
C	7.503958	0.125873	0.050814
C	8.931176	-0.316414	-0.053879
C	5.740690	1.251732	1.265185
C	7.063402	0.859662	1.149477
C	-0.425091	0.876793	0.016967
H	-0.347932	-1.252151	-1.641389
H	1.170601	-0.296010	-1.727187
H	4.543773	-0.043479	-1.617577
H	6.910102	-0.749019	-1.813868
H	9.233281	-0.443641	-1.094176
H	0.162191	1.538583	-0.616122
H	9.605496	0.402892	0.412949
H	1.310989	-0.119634	0.617798
H	5.402523	1.838706	2.109330
H	9.078830	-1.276035	0.450092
H	7.771629	1.137085	1.922649
H	-0.537877	1.333456	0.998671
N	0.312922	-0.387556	0.165050
O	2.577277	1.428231	-0.901306
O	3.107650	2.601322	1.193387
O	2.524144	0.238556	1.196245
S	3.138972	1.377865	0.440002
H	1.174401	-1.909395	-0.984972
H	-1.406068	0.683905	-0.420730
C	-0.355183	-1.311449	1.085702
H	-1.331166	-1.598452	0.690068
H	0.264078	-2.197671	1.212797
H	-0.479179	-0.822887	2.050420

IIIa

C	0.233005	-0.985090	-1.127609
C	-0.335729	1.034484	0.100020
H	-0.773404	-1.051199	-1.544839
H	0.884237	-0.391650	-1.766505
H	0.284954	1.587417	-0.602118
H	1.252481	-0.245236	0.542680
H	-0.263093	1.504118	1.079297
N	0.187472	-0.338658	0.191707
O	2.628128	1.094773	-1.146554
O	3.116042	2.276572	0.943604
O	2.585160	-0.105682	0.953272
S	3.181467	1.045785	0.199142
C	4.886673	0.606951	0.046507
H	5.308707	0.513097	1.044953
H	4.963175	-0.333418	-0.495056
H	5.384147	1.404979	-0.501381
H	0.651775	-1.983806	-1.015817
H	-1.375402	1.012312	-0.230925
C	-0.538639	-1.138633	1.182065
H	-1.582802	-1.250576	0.884762
H	-0.072272	-2.119252	1.259052

H	-0.483258	-0.640770	2.148459

Iva

C	0.192815	-0.997887	-1.111100
C	-0.377924	1.022341	0.116898
H	-0.813144	-1.064663	-1.528404
H	0.842686	-0.402514	-1.749069
H	0.263568	1.580671	-0.561825
H	1.190078	-0.266613	0.568325
H	-0.337178	1.479504	1.103777
N	0.142083	-0.352105	0.209664
O	2.576255	1.063791	-1.057725
O	3.585916	2.069210	0.944602
O	2.532414	-0.133827	1.042035
S	3.248076	0.881716	0.217271
H	4.413256	0.255884	-0.064858
H	0.612658	-1.995798	-0.998153
H	-1.407216	1.002771	-0.244250
C	-0.592998	-1.153996	1.194407
H	-1.637517	-1.251079	0.895457
H	-0.136867	-2.139704	1.261585
H	-0.531411	-0.665144	2.164635

Va

C	-0.085412	-0.413023	-1.404269
C	-0.719866	1.320018	0.128416
H	-1.118425	-0.605131	-1.728211
H	0.354075	0.335382	-2.063952
H	-0.279416	2.063031	-0.536885
H	1.493531	0.297041	0.326151
H	-0.610520	1.670242	1.155055
N	-0.026944	0.053412	-0.030056
F	2.429960	0.445349	0.546844
H	0.487865	-1.335390	-1.501453
H	-1.791481	1.232993	-0.102194
C	-0.538628	-0.947720	0.889454
H	-1.598364	-1.172995	0.701095
H	0.038108	-1.867142	0.786451
H	-0.433866	-0.590515	1.914235

VIa

C	-0.239555	-0.408762	-1.418789
C	-0.773882	1.321565	0.200328
H	-1.281108	-0.560610	-1.714143
H	0.216089	0.352123	-2.050244
H	-0.311242	2.052384	-0.460908
H	1.030685	0.166124	0.206762
H	-0.593534	1.623930	1.230598
N	-0.149460	0.020335	-0.025178
Cl	2.586995	0.364067	0.508441
H	-1.849369	1.276820	0.009788
H	0.317231	-1.336764	-1.537057

C	-0.628479	-0.998146	0.905721
H	-1.694769	-1.190310	0.760364
H	-0.063343	-1.914845	0.745651
H	-0.450861	-0.655535	1.923761