SUPPORTING INFORMATION

Distiboranes based on *ortho*–phenylene backbones as bidentate Lewis acids for fluoride anion chelation

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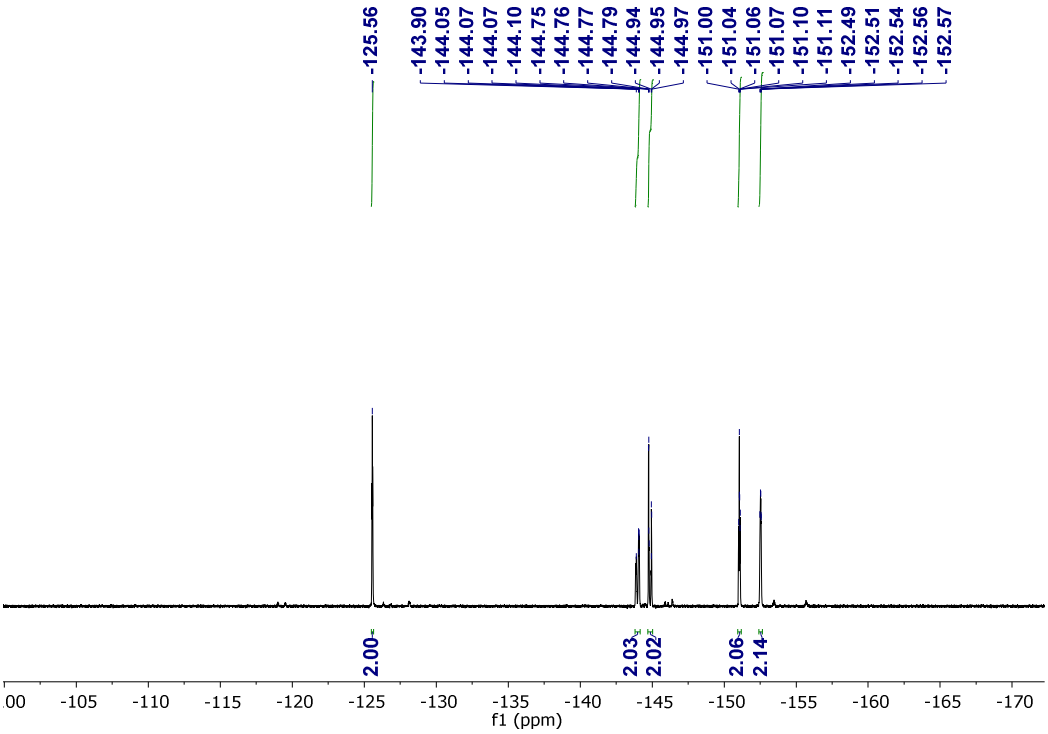


Figure S1: ^{19}F NMR spectrum of decafluorophenanthrene in $CDCl_3$.

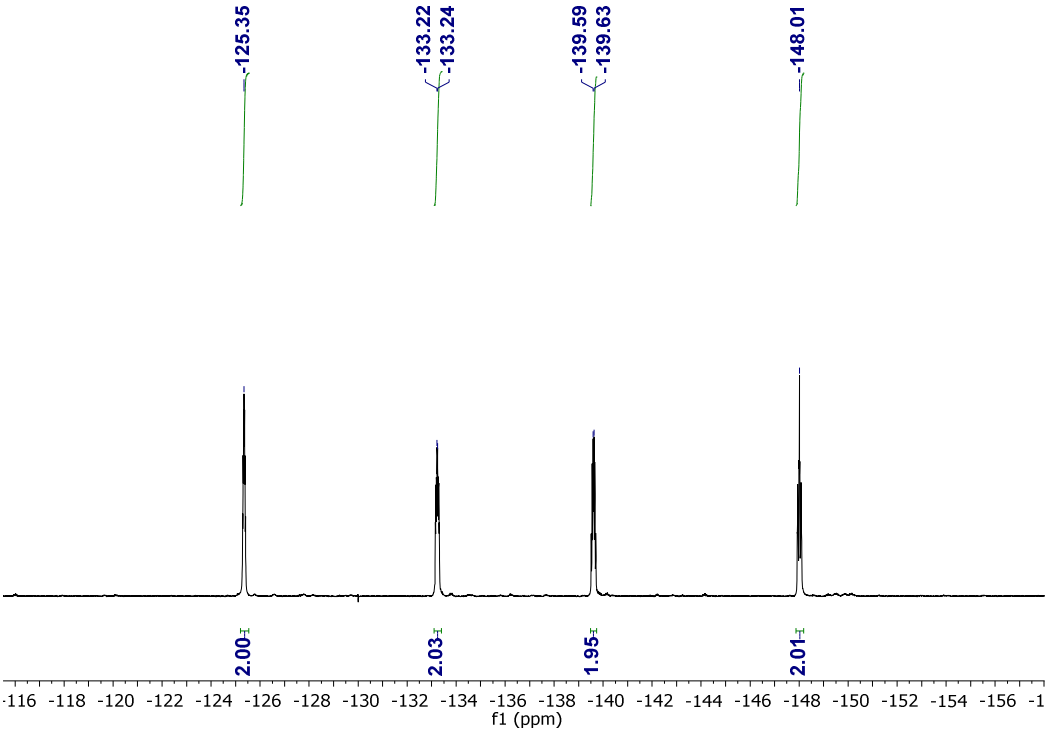


Figure S2: ^{19}F NMR spectrum of octafluorophenanthra-9,10-quinone in $CDCl_3$.

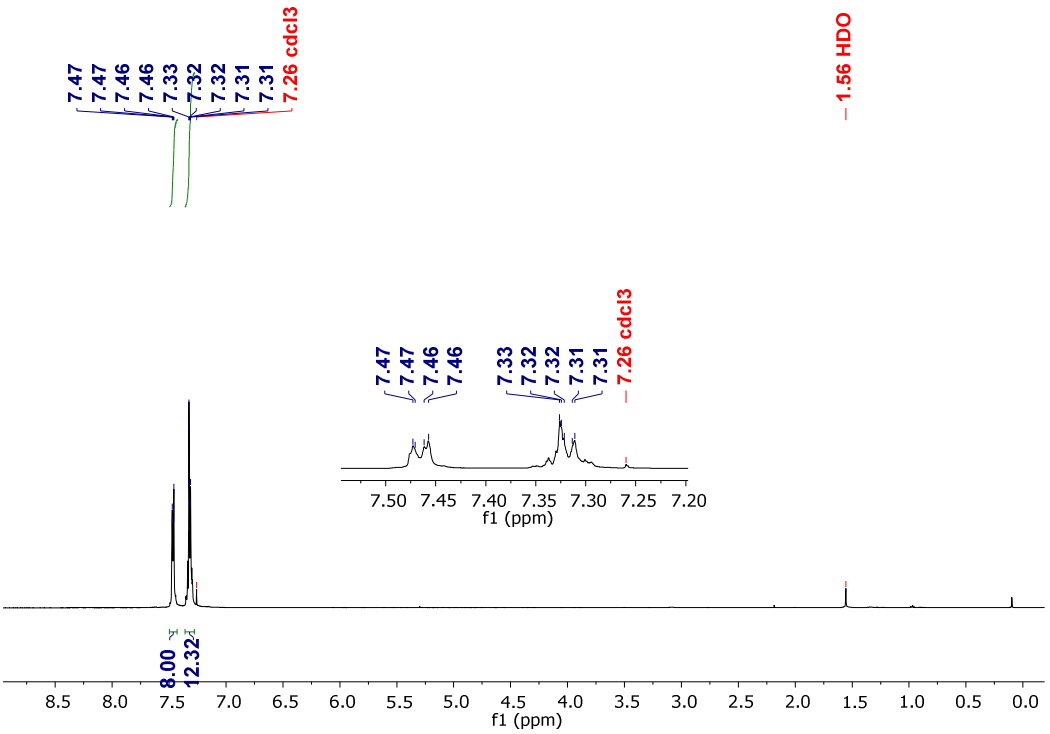


Figure S3: ^{1}H NMR spectrum of **5** in $CDCl_3$.

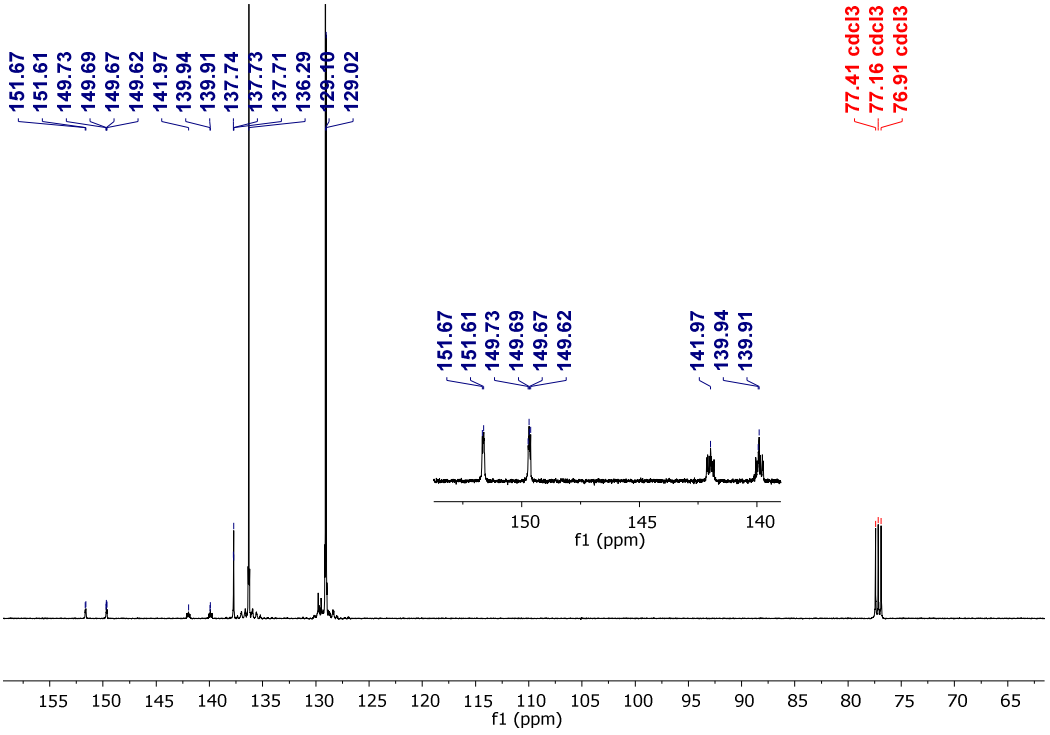


Figure S4: ^{13}C NMR spectrum of **5** in $CDCl_3$.

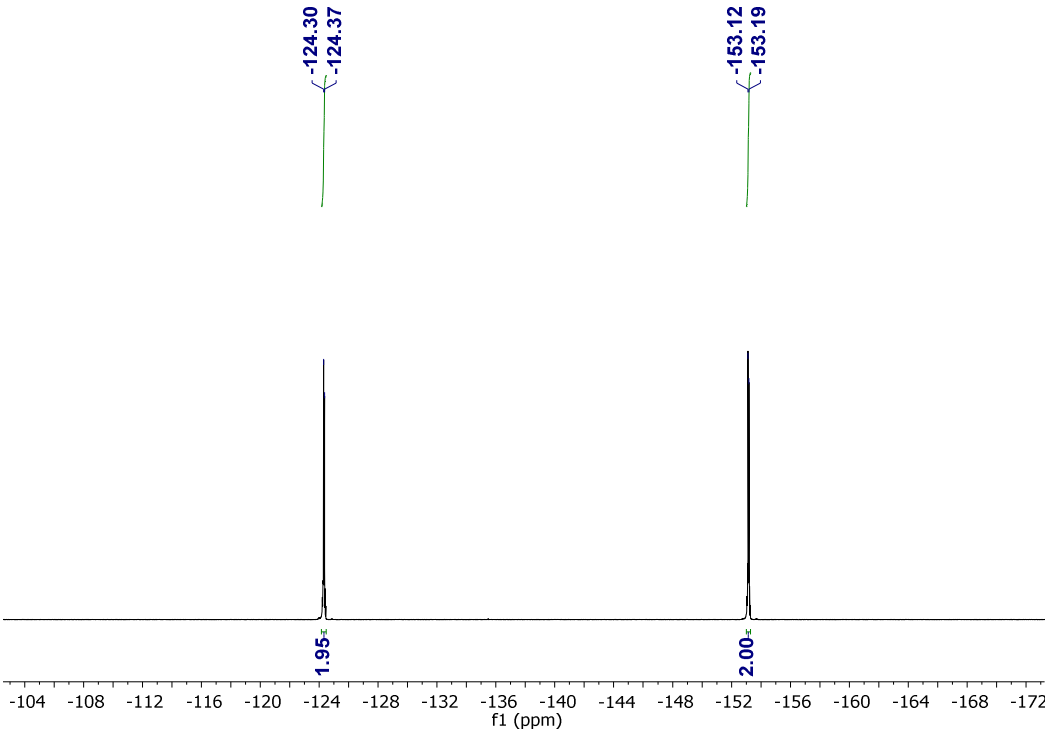


Figure S5: ^{19}F NMR spectrum of **5** in CD_2Cl_2.

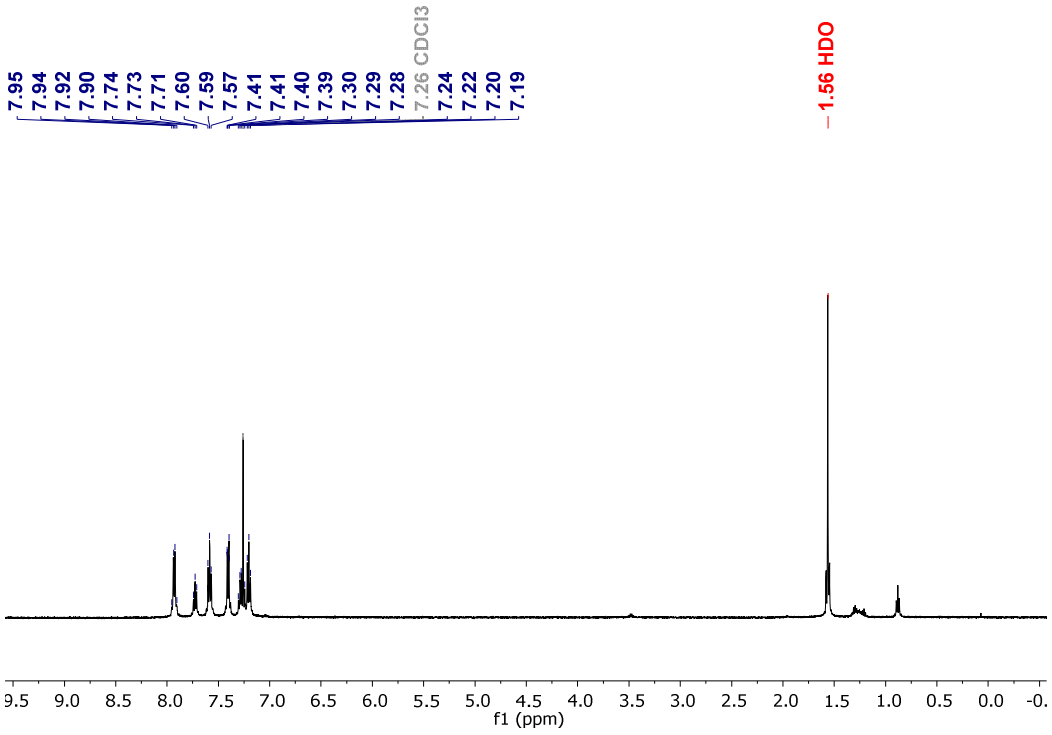


Figure S6: ^{1}H NMR spectrum of **7** in $CDCl_3$.

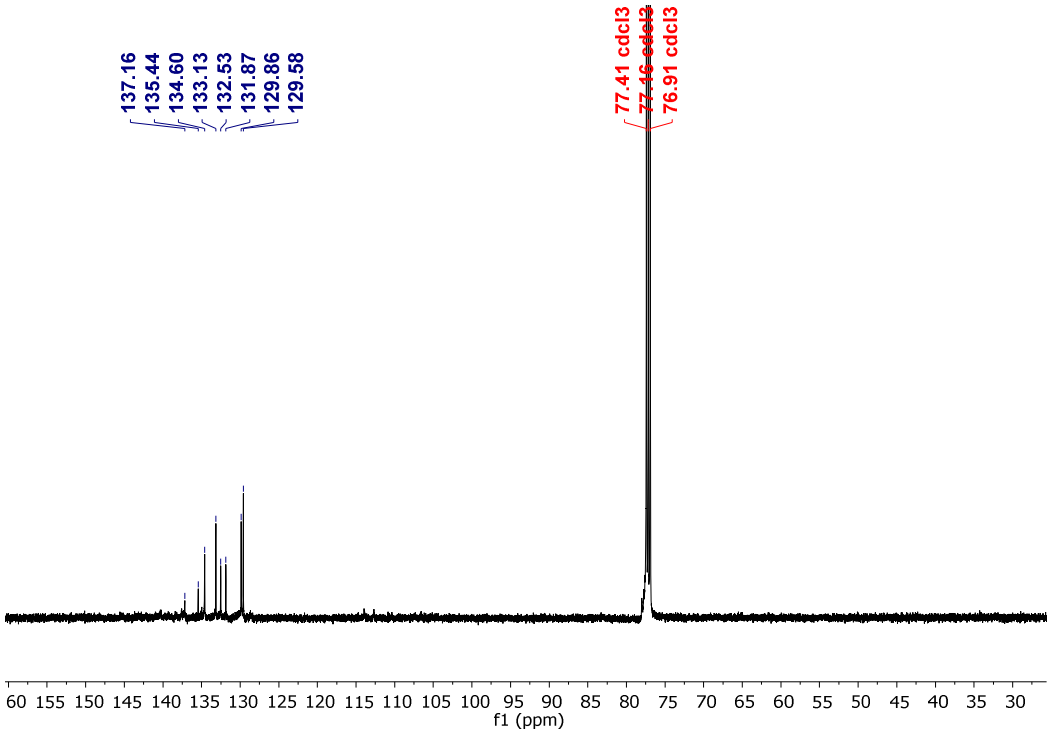


Figure S7: ^{13}C NMR spectrum of **7** in $CDCl_3$.

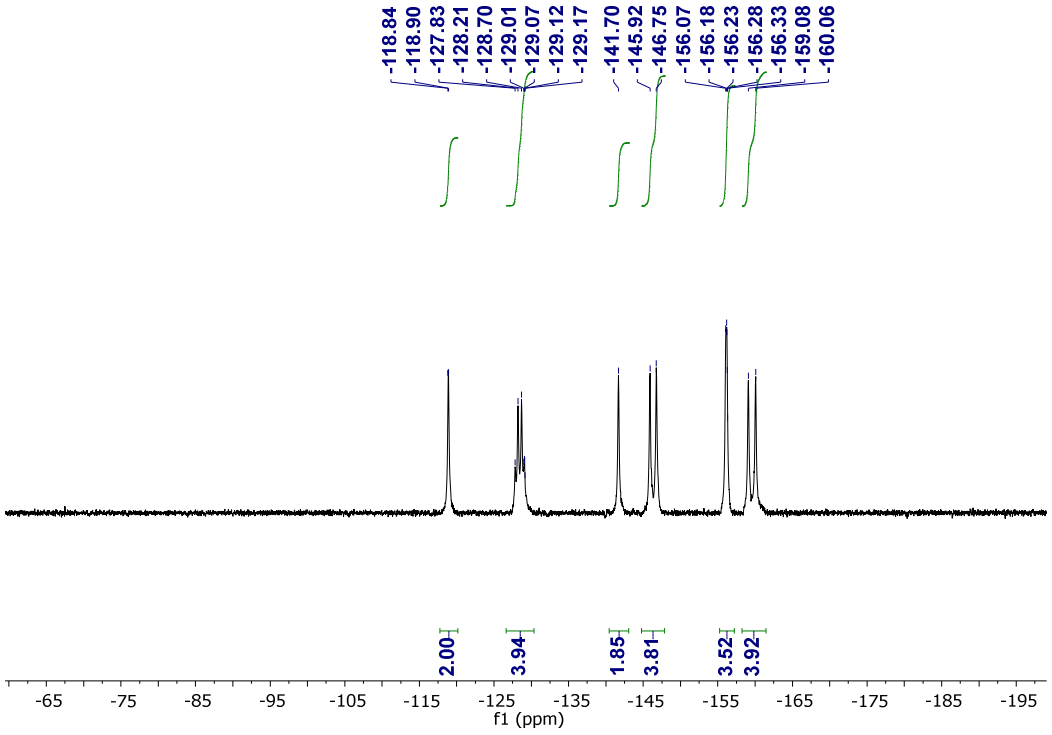


Figure S8: ^{19}F NMR spectrum of **7** in $CDCl_3$.

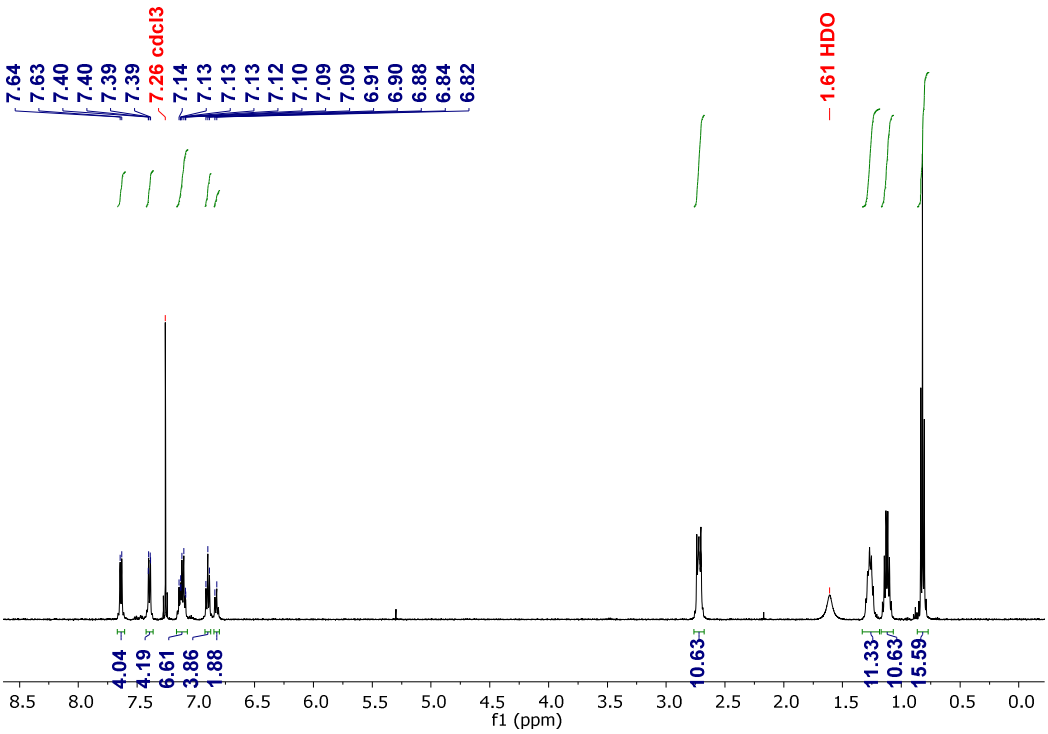


Figure S9: ^{1}H NMR spectrum of [^{n}Bu$_4$N][**7**-μ_2-F] in $CDCl_3$.

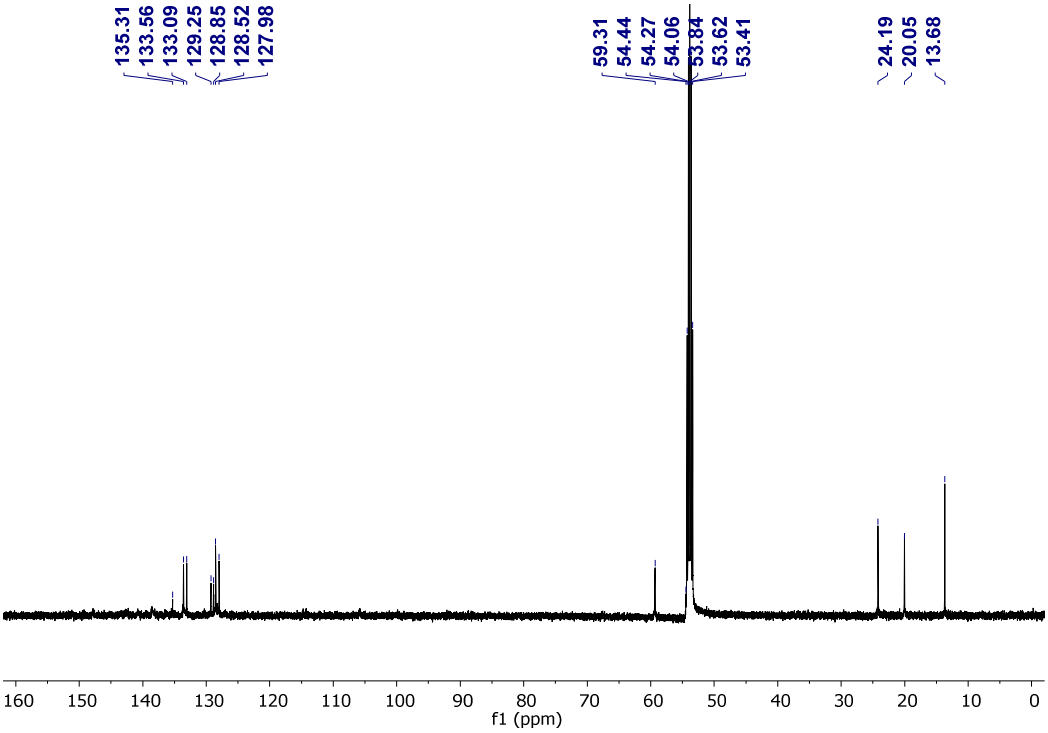


Figure S10: ^{19}F NMR spectrum of [^{n}Bu$_4$N][**7**-μ_2-F] in CD_2Cl_2.

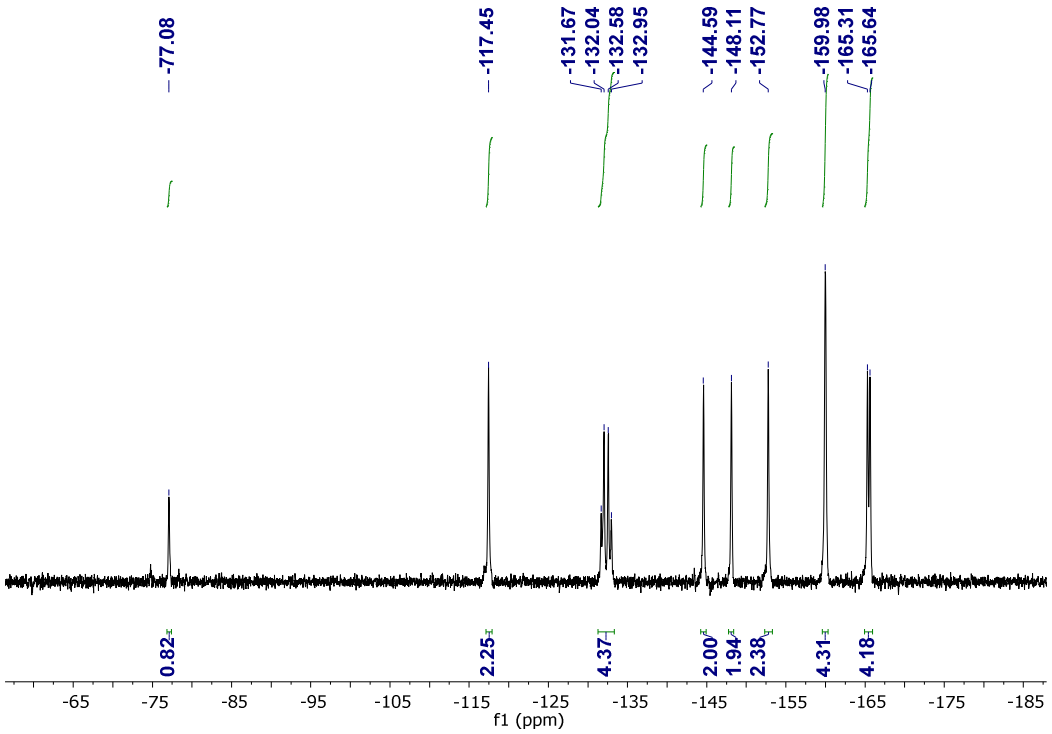


Figure S11: ^{19}F NMR spectrum of [$^{n}Bu_4N$][**7**-μ_2-F] in $CDCl_3$.

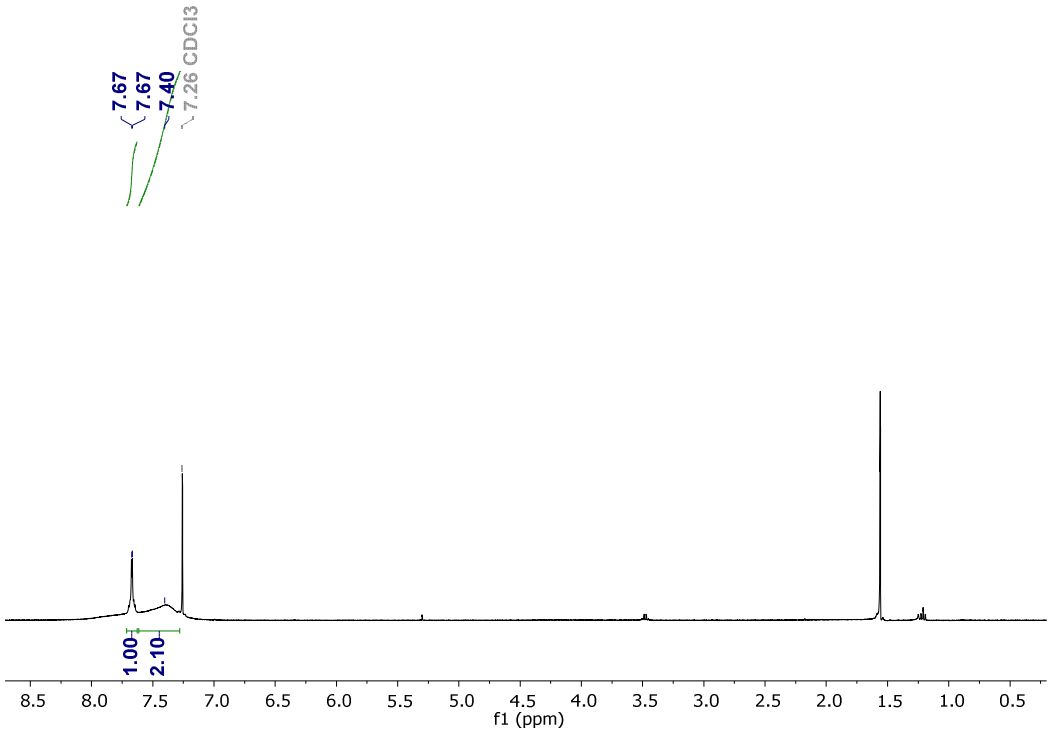


Figure S12: ^{19}F NMR spectrum of **8** in $CDCl_3$.

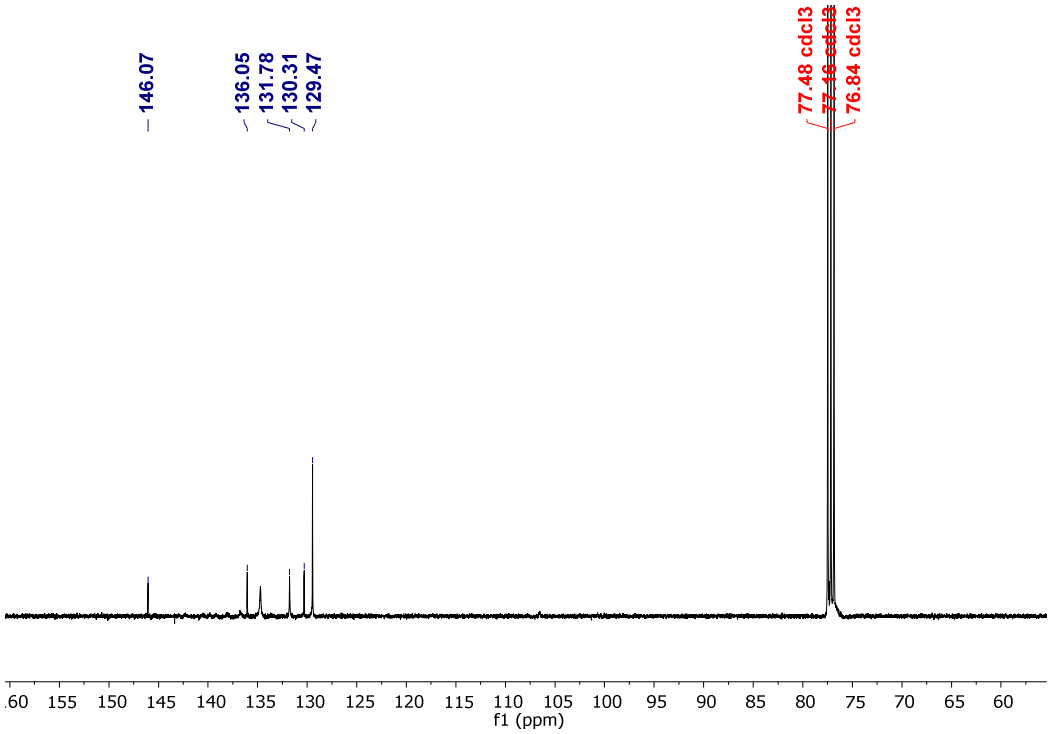


Figure S13: ^{13}C NMR spectrum of **8** in $CDCl_3$.

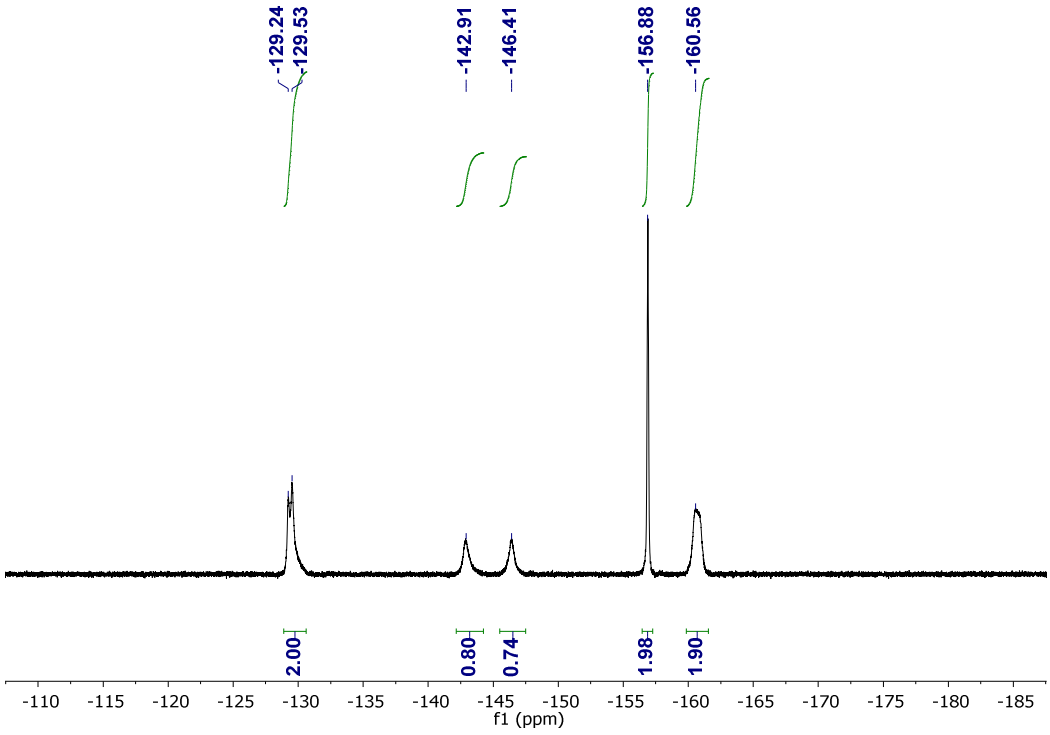


Figure S14: ^{19}F NMR spectrum of **8** in $CDCl_3$.

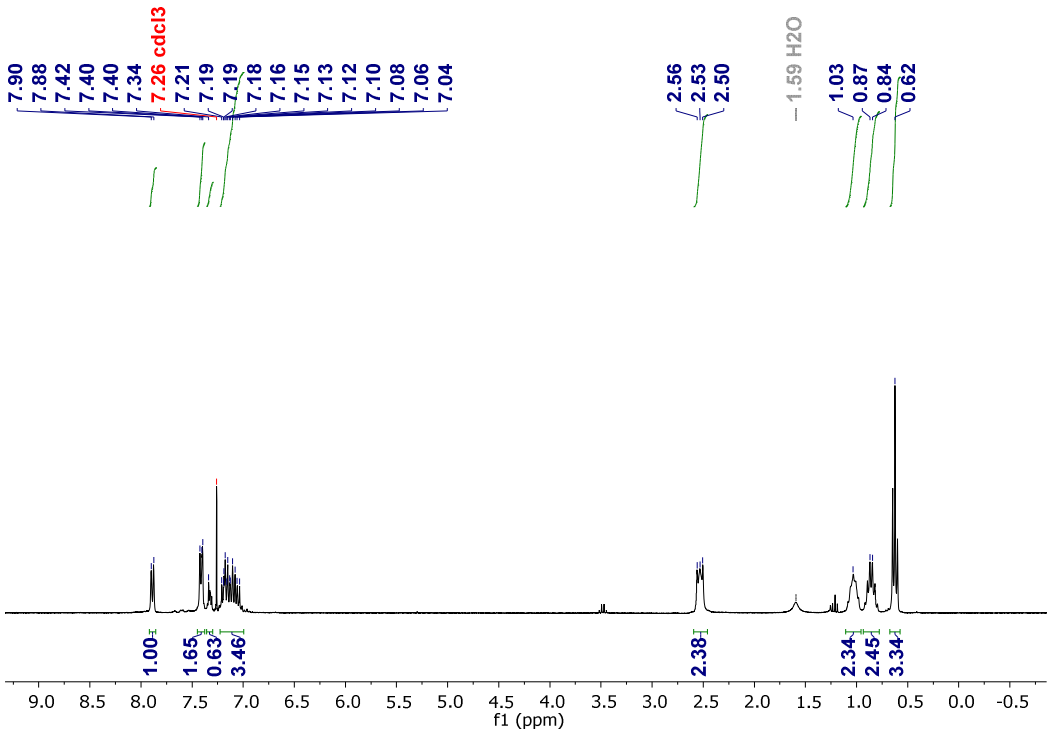


Figure S15: ^{1}H NMR spectrum of [^{n}Bu$_4$N][**8**-μ_2-F] in CDCl$_3$.

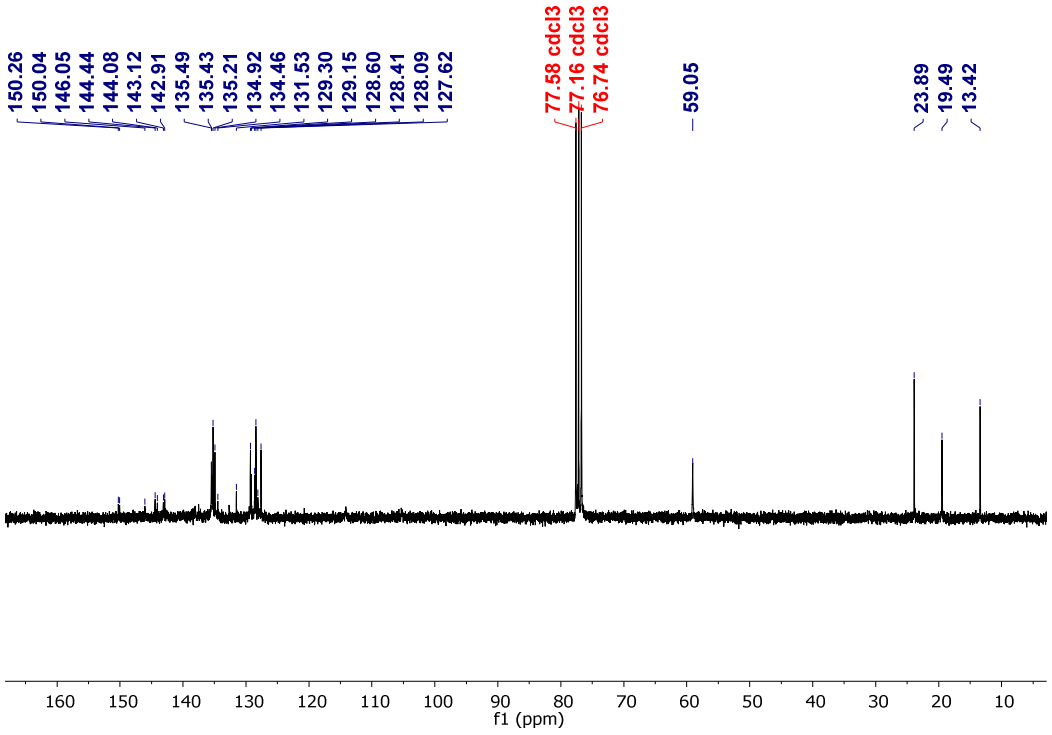


Figure S16: ^{13}C NMR spectrum of [^{n}Bu$_4$N][**8**-μ_2-F] in CDCl$_3$.

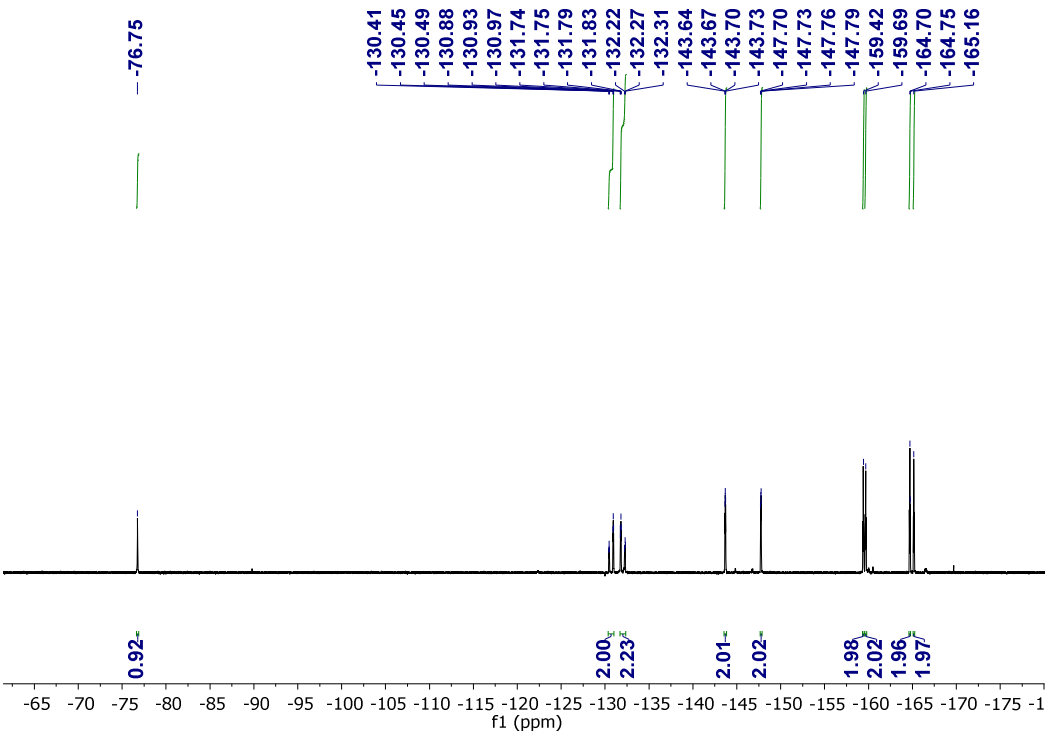
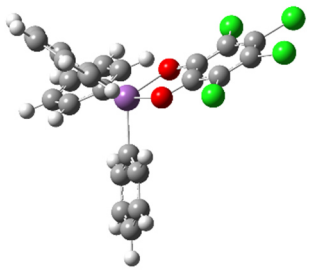


Figure S17: ^{19}F NMR spectrum of **8** in $CDCl_3$.

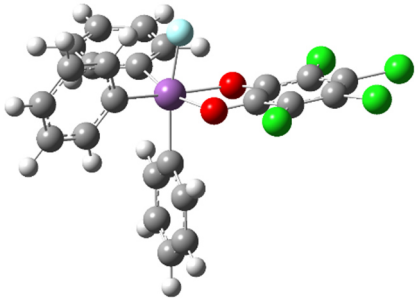
Figure S18: Optimized structure of **A** and atomic coordinates in Å.



A

Sb	3.063011	0.770948	2.401471	C	4.137640	3.834811	-0.586959
Cl	5.918410	-0.019224	6.493429	C	4.041526	2.642493	0.138991
Cl	8.892220	-0.960191	5.779570	C	2.160744	-0.876838	1.377723
Cl	9.731160	-1.292584	2.735835	C	2.780389	-1.424757	0.238559
Cl	7.591541	-0.681963	0.438222	C	2.175070	-2.493094	-0.432350
O	4.916192	0.175600	1.546243	C	0.966256	-3.025832	0.032644
O	4.225589	0.449368	4.054348	C	0.358562	-2.491938	1.174273
C	5.884620	-0.103834	2.459799	C	0.950934	-1.416638	1.848260
C	5.520138	0.041398	3.814308	H	0.075572	1.693526	2.167235
C	6.431869	-0.217951	4.831790	H	-1.784867	2.307119	3.666204
C	7.739605	-0.632097	4.502406	H	-1.469239	2.268260	6.135204
C	8.109429	-0.778798	3.154663	H	0.729436	1.608370	7.092674
C	7.177583	-0.513381	2.130965	H	2.608341	0.988734	5.594813
C	1.479734	1.295897	3.779489	H	1.942605	3.719416	2.619203
C	0.231550	1.670777	3.243078	H	2.139630	5.821438	1.333406
C	-0.827541	2.019978	4.089765	H	3.532923	5.902022	-0.725761
C	-0.648791	1.997712	5.478137	H	4.756891	3.870925	-1.477311
C	0.588338	1.626371	6.016636	H	4.603500	1.769532	-0.167824
C	1.652791	1.275543	5.175262	H	3.733787	-1.038087	-0.098403
C	3.237297	2.592820	1.293381	H	2.653385	-2.913308	-1.311064
C	2.552721	3.742955	1.723458	H	0.504426	-3.858426	-0.488261
C	2.663430	4.933554	0.994309	H	-0.571445	-2.910980	1.544653
C	3.449798	4.978326	-0.162095	H	0.473109	-1.011705	2.733059

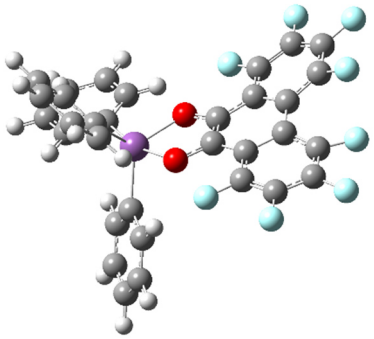
Figure S19: Optimized structure of [**A-**F]$^-$ and atomic coordinates in Å.



[**A-F**]$^-$

Sb	-0.015351	-0.101766	0.006057
Cl	0.086537	0.334943	5.094288
Cl	3.067989	0.314642	6.260311
Cl	5.518419	-0.093851	4.272005
Cl	4.955537	-0.475219	1.143814
F	0.469270	1.825534	0.216529
O	-0.012828	-0.082403	2.126420
O	2.034621	-0.422296	0.466939
C	-2.473094	1.813573	0.264831
H	-1.695890	2.534457	0.487445
C	-2.109127	0.481369	-0.007672
C	-3.120694	-0.451672	-0.297825
H	-2.862116	-1.487105	-0.497468
C	-4.467990	-0.063302	-0.319194
H	-5.237920	-0.796571	-0.544934
C	-4.819250	1.262556	-0.043637
H	-5.863344	1.564172	-0.054915
C	-3.819233	2.198422	0.250225
H	-4.086900	3.228659	0.469579
C	0.509573	0.071364	-2.092831
C	1.856864	0.101467	-2.499367
H	2.637103	0.022490	-1.751189
C	2.183121	0.238940	-3.854622
H	3.227032	0.263450	-4.155884
C	1.173110	0.348293	-4.818903
H	1.430102	0.455836	-5.869445
C	-0.168789	0.322124	-4.422994
H	-0.958714	0.411809	-5.164280
C	-0.497858	0.185807	-3.067072
H	-1.543434	0.176442	-2.771889
C	2.326904	-0.249544	1.773999
C	3.629146	-0.249038	2.277254
C	3.865890	-0.077320	3.657746
C	2.787576	0.102815	4.532596
C	1.468791	0.112194	4.029620
C	1.227296	-0.065964	2.666576
C	-0.744309	-5.065380	0.120547
H	-0.898705	-6.140798	0.147824
C	-0.264378	-4.452724	-1.042380
H	-0.041713	-5.051121	-1.922097
C	-0.063723	-3.065412	-1.075166
H	0.316129	-2.604755	-1.981815
C	-0.337366	-2.271127	0.052945
C	-0.816097	-2.899741	1.219066
H	-1.018887	-2.300555	2.100192
C	-1.019315	-4.285457	1.250841
H	-1.387147	-4.754940	2.159445

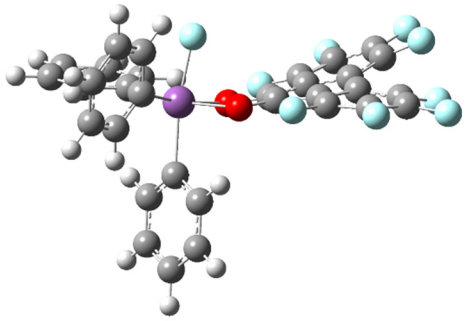
Figure S20: Optimized structure of **B** and atomic coordinates in Å.



B

Sb	-1.975706	-0.110200	0.013104
F	1.232966	-3.462165	0.450551
F	3.637175	-4.647318	0.185698
F	5.854894	-3.167243	-0.432692
F	5.711484	-0.525328	-0.708145
F	5.566447	1.415717	0.663059
F	5.296133	4.049253	0.377186
F	2.867169	5.160170	-0.224314
F	0.675922	3.619819	-0.453429
O	-0.246061	-1.295433	0.256327
O	-0.464092	1.251034	-0.188069
C	-2.501336	-1.359187	-1.645024
C	-3.402208	-0.894765	-2.619280
H	-3.829166	0.099085	-2.546605
C	-3.747533	-1.716705	-3.699377
H	-4.438143	-1.351767	-4.452831
C	-3.200662	-3.000010	-3.807762
H	-3.471185	-3.635938	-4.644647
C	-2.296938	-3.460479	-2.842124
H	-1.863792	-4.451589	-2.930575
C	-1.937937	-2.644547	-1.763260
H	-1.209370	-2.986210	-1.038379
C	-3.334809	1.549133	-0.272083
C	-4.719328	1.286019	-0.264402
H	-5.089504	0.274212	-0.117605
C	-5.639076	2.326166	-0.445727
H	-6.703448	2.112926	-0.438587
C	-5.183532	3.636413	-0.635119
H	-5.895747	4.443392	-0.775506
C	-3.809855	3.903502	-0.642786
H	-3.454241	4.918541	-0.789003
C	-2.882963	2.867773	-0.462650
H	-1.821436	3.078799	-0.469458
C	-2.603360	-0.811460	1.937034
C	-3.532087	-0.071198	2.688969
H	-3.929511	0.863226	2.309252
C	-3.944563	-0.537236	3.943765
H	-4.656252	0.041046	4.524194
C	-3.437525	-1.740167	4.447043
H	-3.760184	-2.100492	5.418651
C	-2.506428	-2.474575	3.701910
H	-2.104391	-3.402517	4.095624
C	-2.079827	-2.013438	2.451509
H	-1.330159	-2.560796	1.893786
C	2.320880	-2.668403	0.244278
C	3.541281	-3.299378	0.101653
C	4.680666	-2.539505	-0.182778
C	4.594623	-1.160272	-0.271413
C	4.359239	1.869805	0.240668
C	4.230586	3.244779	0.145409
C	2.982867	3.814801	-0.128133
C	1.872610	3.002620	-0.249866
C	0.926898	-0.610136	0.130802
C	0.822600	0.746461	-0.094449
C	1.968658	1.594733	-0.140984
C	3.273092	0.991513	0.001029
C	3.388655	-0.461858	-0.011786
C	2.200486	-1.262518	0.149287

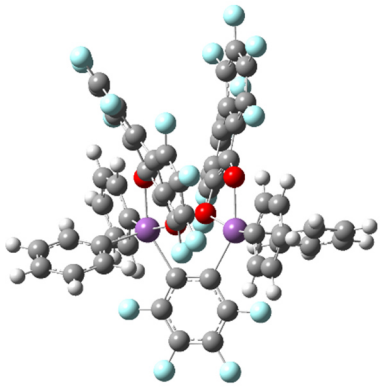
Figure S21: Optimized structure of [**B-**F]$^-$ and atomic coordinates in Å.



[**B-F**]$^-$

Sb	1.873458	0.036902	-0.249316
F	1.208939	0.362359	-2.112097
O	0.246747	-1.309755	-0.159380
O	0.249120	1.281524	0.290919
C	3.049762	-1.915023	-2.391548
H	2.312167	-1.429068	-3.018505
C	3.160357	-1.525544	-1.043351
C	4.121127	-2.156591	-0.232932
H	4.214035	-1.880230	0.812913
C	4.956485	-3.153660	-0.756910
H	5.693626	-3.631881	-0.117096
C	4.835694	-3.535760	-2.097247
H	5.478897	-4.311833	-2.503691
C	3.879571	-2.915576	-2.911763
H	3.778650	-3.211456	-3.952666
C	3.122047	1.799377	-0.465055
C	2.566277	3.090586	-0.388487
H	1.503808	3.201325	-0.205043
C	3.378995	4.219452	-0.554620
H	2.938363	5.211161	-0.495710
C	4.750769	4.076003	-0.798785
H	5.377460	4.954543	-0.928055
C	5.310264	2.795915	-0.879162
H	6.372911	2.675491	-1.073711
C	4.499254	1.664340	-0.714411
H	4.944202	0.675870	-0.788798
C	2.744925	-0.842264	4.614415
H	2.928358	-1.032154	5.668669
C	3.248929	0.314574	4.009650
H	3.823384	1.029205	4.593526
C	3.010861	0.558183	2.649383
H	3.402351	1.463160	2.195013
C	2.264017	-0.347697	1.874927
C	1.757500	-1.506183	2.496338
H	1.168198	-2.205909	1.913253
C	1.998758	-1.751827	3.854224
H	1.600719	-2.650541	4.318321
C	-0.961033	-0.694142	-0.088907
C	-2.188572	-1.421081	-0.158994
C	-0.958469	0.686561	0.128746
C	-2.222122	-2.839276	-0.244131
C	-3.443046	-0.705892	-0.065642
C	-2.173071	1.436621	0.084789
C	-3.404338	-3.542577	-0.141774
C	-4.610397	-1.480088	0.160432
C	-3.429150	0.743967	-0.101781
C	-2.188455	2.855153	0.167965
C	-4.604975	-2.859249	0.090748
C	-4.561724	1.538141	-0.417746
C	-3.345047	3.579730	-0.029745
C	-4.536613	2.917227	-0.351787
F	-1.088650	-3.571463	-0.403557
F	-3.414774	-4.901453	-0.215605
F	-5.745661	-3.568295	0.322054
F	-5.785199	-0.910691	0.554342
F	-5.713891	0.988027	-0.895334
F	-5.643529	3.645637	-0.669737
F	-3.336708	4.938479	0.043574
F	-1.060740	3.571372	0.427844

Figure S22: Optimized structure of **7** and atomic coordinates in Å.

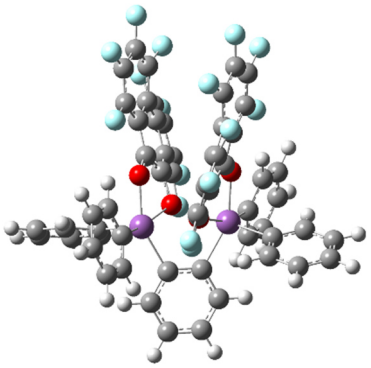


7

F	-1.872608	-3.735752	3.150388
C	-0.944376	-3.150872	-0.349444
F	-2.012135	-6.651183	-0.591571
Sb	-0.599807	-0.997065	1.880337
C	-1.654337	-3.937791	1.814093
C	-1.166722	-2.908080	1.020297
F	-2.423053	-6.184365	2.087324
C	-1.945509	-5.201154	1.292203
F	-1.049348	-4.670648	-2.194940
O	0.993924	-1.258782	0.395281
C	-1.735395	-5.438111	-0.063373
Sb	-0.312959	-1.525248	-1.643461
O	0.217702	0.889113	1.644584
C	-1.240390	-4.406016	-0.865419
O	0.210575	0.459193	-1.879893
O	-1.601072	-0.441363	-0.232918
C	0.701043	-1.661130	3.447701
C	1.741816	-2.569256	3.181523
H	1.920911	-2.919955	2.170745
C	2.565180	-3.009693	4.224433
H	3.368063	-3.709887	4.016370
C	2.358133	-2.546775	5.529662
H	2.999130	-2.890501	6.335261
C	1.326216	-1.639292	5.795448
H	1.164387	-1.277860	6.805926
C	0.497360	-1.195575	4.757948
H	-0.301922	-0.494576	4.975361
C	-3.259081	1.779380	4.029514
H	-3.217655	2.827032	4.309862
C	-4.356610	0.994395	4.400495
H	-5.171535	1.432270	4.967898
C	-4.402650	-0.357223	4.039409
H	-5.251626	-0.969852	4.324422
C	-3.356384	-0.925947	3.304369
H	-3.409173	-1.974402	3.040351
C	-2.256754	-0.136475	2.927934
C	-2.205673	1.222473	3.292605
H	-1.359945	1.834559	3.006557
C	1.424997	-2.095077	-2.754952
C	2.154212	-1.106282	-3.442952
H	1.874618	-0.063649	-3.361899
C	3.251953	-1.480874	-4.228932
H	3.813533	-0.717924	-4.758444
C	3.626021	-2.825884	-4.328250
H	4.481727	-3.109090	-4.932429
C	2.896544	-3.806273	-3.645604
H	3.184144	-4.849882	-3.717909
C	1.796278	-3.445800	-2.859884
H	1.242621	-4.218866	-2.343153
C	-0.771474	1.340135	-1.506382
C	-2.953194	1.625075	-0.432327
C	-2.983728	3.002300	-0.858015
C	-1.780407	3.591271	-1.434981
C	-0.729470	2.720331	-1.896430
C	-1.768188	0.864756	-0.683565
C	-4.124798	1.050654	0.108485
C	-5.296069	1.771168	0.240531
C	-5.352728	3.085476	-0.230754
C	-4.233041	3.665604	-0.804369
C	0.360024	3.273988	-2.605756
C	0.484743	4.639981	-2.784002
C	-0.459361	5.499998	-2.215935
C	-1.547497	4.983865	-1.530590
C	5.428442	0.584760	-0.431575
C	5.865772	-0.612273	-0.973968
C	5.076172	-1.762490	-0.869773
C	3.823444	-1.671919	-0.298509
C	4.681673	2.840274	1.535008
C	4.244787	3.960801	2.221704
C	2.890040	4.113999	2.526746
C	1.997261	3.118845	2.176921
C	-1.884012	-1.570384	-3.095999
C	-1.563650	-1.567341	-4.464356
H	-0.528645	-1.527819	-4.788349

C	-2.583834	-1.619866	-5.421802
H	-2.331957	-1.618123	-6.477461
C	-3.922850	-1.676046	-5.018241
H	-4.712240	-1.717906	-5.761928
C	-4.244524	-1.675993	-3.655355
H	-5.282767	-1.714989	-3.341163
C	-3.230163	-1.621350	-2.692258
H	-3.488616	-1.602729	-1.639096
C	4.208241	0.683858	0.285854
C	3.787513	1.850803	1.053845
C	3.319937	-0.447194	0.195700
C	1.960033	-0.278582	0.595904
C	1.520429	0.870704	1.214661
C	2.413786	1.960059	1.481273
F	3.084473	-2.815476	-0.215166
F	5.534700	-2.939523	-1.354740
F	7.043006	-0.669822	-1.641875
F	6.198239	1.669794	-0.694074
F	6.026970	2.703818	1.431971
F	5.135372	4.882437	2.655854
F	2.471370	5.210980	3.197896
F	0.701977	3.302708	2.548935
F	1.348575	2.493699	-3.119098
F	1.539126	5.152641	-3.458592
F	-0.277062	6.838275	-2.296912
F	-2.329737	5.885623	-0.887450
F	-4.429761	4.869409	-1.397909
F	-6.528246	3.757130	-0.196660
F	-6.406575	1.193980	0.755111
F	-4.167074	-0.266027	0.462489

Figure S23: Optimized structure of **8** and atomic coordinates in Å.



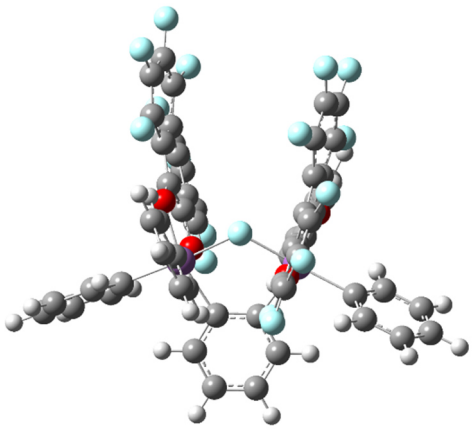
8

Sb	-0.225677	-1.774741	-1.827325	H	-5.659022	-1.956196	-4.440366
Sb	0.226506	-1.774275	1.827369	C	-4.213185	-3.022480	-3.248733
F	3.892064	-1.608075	0.056823	H	-4.815075	-3.924314	-3.176198
F	6.363921	-0.681379	0.454995	C	-2.967453	-2.969739	-2.620004
F	6.980593	1.893185	-0.147248	H	-2.622677	-3.828878	-2.052754
F	5.150112	3.539296	-1.095875	C	1.068915	-2.198620	-3.479378
F	3.299572	4.883478	-0.431916	C	0.572913	-2.191805	-4.789741
F	1.456291	6.380562	-1.590680	H	-0.471076	-1.960269	-4.982309
F	-0.672098	5.258626	-2.846483	C	1.422873	-2.480780	-5.860387
F	-1.000354	2.609752	-2.854576	H	1.034036	-2.472877	-6.875164
F	0.999266	2.610820	2.853999	C	2.766857	-2.776946	-5.625705
F	0.669739	5.259542	2.845533	H	3.427279	-3.000499	-6.459325
F	-1.459237	6.380267	1.589680	C	3.263836	-2.783476	-4.319982
F	-3.301865	4.882137	0.431216	H	4.310752	-3.010097	-4.136357
F	-5.151736	3.537153	1.095316	C	2.420032	-2.495016	-3.245493
F	-6.981416	1.890032	0.146873	H	2.814320	-2.491173	-2.233562
F	-6.363527	-0.684311	-0.454968	C	-1.067883	-2.198214	3.479589
F	-3.891218	-1.609794	-0.056601	C	-2.418856	-2.495309	3.245760
O	1.370360	-1.187957	-0.542809	H	-2.813134	-2.491891	2.233824
O	-0.283469	0.275849	-1.934507	C	-3.262571	-2.783853	4.320297
O	-1.369740	-1.188381	0.542955	H	-4.309365	-3.011058	4.136691
O	0.283462	0.276460	1.934302	C	-2.765651	-2.776679	5.626039
C	-0.097927	-3.610113	-0.692104	H	-3.425995	-3.000300	6.459702
C	0.099657	-3.609927	0.692612	C	-1.421822	-2.479784	5.860677
C	0.181181	-4.825054	1.383238	H	-1.033035	-2.471333	6.875470
H	0.305977	-4.837657	2.463523	C	-0.571947	-2.190769	4.789972
C	0.087766	-6.037310	0.692161	H	0.471933	-1.958722	4.982516
H	0.151099	-6.975455	1.236641	C	2.190970	-1.806516	2.700661
C	-0.084540	-6.037492	-0.691169	C	2.968937	-2.967740	2.620666
H	-0.147284	-6.975777	-1.235478	H	2.624971	-3.827111	2.053262
C	-0.178723	-4.825429	-1.382482	C	4.214415	-3.019769	3.249959
H	-0.303557	-4.838354	-2.462756	H	4.816838	-3.921266	3.177655
C	-2.190225	-1.808044	-2.700338	C	4.687583	-1.913152	3.957187
C	-2.667120	-0.693087	-3.406291	H	5.659111	-1.952715	4.442282
H	-2.082058	0.218304	-3.452986	C	3.915101	-0.752269	4.032613
C	-3.915512	-0.754782	-4.031509	H	4.283891	0.114299	4.574902
H	-4.285071	0.111558	-4.573642	C	2.666951	-0.691293	3.406839
C	-4.687293	-1.916112	-3.955715	H	2.081384	0.219775	3.453306

C	0.114993	3.103576	-2.305931
C	0.258455	4.477988	-2.303689
C	1.370073	5.055060	-1.681414
C	2.348256	4.251433	-1.119162
C	4.728743	2.344863	-0.678429
C	5.714621	1.483396	-0.227211
C	5.401483	0.153310	0.067106
C	4.109131	-0.296751	-0.115259
C	1.757596	0.083794	-0.826125
C	0.858036	0.859311	-1.525449
C	1.090365	2.262423	-1.725229
C	2.303564	2.841007	-1.215377
C	3.371915	1.955132	-0.767153
C	3.074164	0.567927	-0.532426

C	-0.116339	3.104031	2.305333
C	-0.260464	4.478365	2.302897
C	-1.372397	5.054820	1.680602
C	-2.350213	4.250645	1.118508
C	-4.729794	2.342864	0.678048
C	-5.715244	1.480868	0.226932
C	-5.401480	0.150871	-0.067171
C	-4.108929	-0.298551	0.115290
C	-1.757573	0.083247	0.826068
C	-0.858322	0.859288	1.525210
C	-1.091335	2.262326	1.724782
C	-2.304834	2.840244	1.214918
C	-3.372771	1.953788	0.766843
C	-3.074375	0.566690	0.532339

Figure S24: Optimized structure of [**7**-μ_2-F]$^-$ and atomic coordinates in Å.

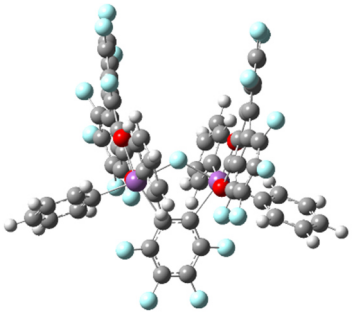


[**7**-μ_2-F]$^-$

Sb	-0.936264	-1.342584	1.701222
Sb	0.936286	-1.342655	-1.701172
F	-4.524924	-2.237475	-1.118714
F	-6.897768	-1.888332	-2.319026
F	-8.294490	0.449178	-1.994713
F	-7.274807	2.469616	-0.588327
F	-5.651370	4.196723	-0.857804
F	-4.567596	6.135814	0.613854
F	-2.670175	5.577355	2.507590
F	-1.778904	3.067077	2.855146
F	1.778888	3.066958	-2.855267
F	2.670108	5.577265	-2.507782
F	4.567509	6.135818	-0.614052
F	5.651314	4.196789	0.857667
F	7.274790	2.469701	0.588244
F	8.294498	0.449326	1.994702
F	6.897810	-1.888192	2.319096
F	4.524976	-2.237413	1.118789
O	-2.606925	-1.315426	0.436318
O	-1.707895	0.568342	2.017971
O	2.606972	-1.315449	-0.436300
O	1.707924	0.568251	-2.018025
C	-0.304571	-3.132361	0.637903
C	0.304608	-3.132385	-0.637771
C	0.585725	-4.361445	-1.261592
H	1.053562	-4.374961	-2.240490
C	0.289109	-5.578740	-0.634632
H	0.516731	-6.514458	-1.136835
C	-0.289016	-5.578716	0.634881
H	-0.516613	-6.514415	1.137131
C	-0.585658	-4.361398	1.261784
H	-1.053486	-4.374879	2.240686
C	0.791360	-0.768219	2.852877
C	0.826739	0.453258	3.550812
H	0.001880	1.149118	3.457791
C	1.934119	0.768264	4.348774
H	1.958048	1.714151	4.882193
C	3.008184	-0.124483	4.453953
H	3.866157	0.126193	5.071246
C	2.980858	-1.333676	3.750311
H	3.822118	-2.017721	3.801144
C	1.876015	-1.655316	2.949666
H	1.882756	-2.580993	2.384074
C	-2.121564	-2.244666	3.287482
C	-1.656149	-2.254077	4.614814
H	-0.689586	-1.822560	4.855174
C	-2.435032	-2.808691	5.639745
H	-2.063687	-2.805396	6.660726
C	-3.687369	-3.361115	5.349473
H	-4.291522	-3.790129	6.143875
C	-4.159895	-3.356802	4.031135
H	-5.132432	-3.782632	3.800392
C	-3.384378	-2.801566	3.005618
H	-3.752990	-2.797009	1.985330
C	2.121553	-2.244815	-3.287419
C	3.384335	-2.801779	-3.005547
H	3.752937	-2.797245	-1.985255
C	4.159826	-3.357068	-4.031055
H	5.132339	-3.782950	-3.800304
C	3.687304	-3.361374	-5.349395
H	4.291435	-3.790431	-6.143789
C	2.434992	-2.808897	-5.639675

H	2.063647	-2.805600	-6.660656
C	1.656134	-2.254234	-4.614751
H	0.689591	-1.822676	-4.855120
C	-0.791355	-0.768346	-2.852830
C	-1.876066	-1.655390	-2.949477
H	-1.882846	-2.580997	-2.383772
C	-2.980914	-1.333782	-3.750128
H	-3.822214	-2.017787	-3.800853
C	-3.008191	-0.124674	-4.453918
H	-3.866169	0.125977	-5.071213
C	-1.934070	0.768023	-4.348880
H	-1.957959	1.713847	-4.882413
C	-0.826685	0.453048	-3.550914
H	-0.001786	1.148874	-3.457999
C	-2.787274	3.263384	1.963484
C	-3.224515	4.561612	1.797315
C	-4.223416	4.843116	0.857949
C	-4.806751	3.816588	0.139409
C	-6.460306	1.401982	-0.812773
C	-7.029639	0.348398	-1.503259
C	-6.333661	-0.858641	-1.633599
C	-5.105480	-1.009653	-1.024549
C	-3.287490	-0.132675	0.434324
C	-2.796107	0.873377	1.257035
C	-3.348018	2.190607	1.224003
C	-4.478519	2.455395	0.364678
C	-5.145083	1.339457	-0.285743
C	-4.490204	0.051341	-0.313646
C	2.787253	3.263312	-1.963611
C	3.224466	4.561554	-1.797476
C	4.223358	4.843105	-0.858114
C	4.806709	3.816609	-0.139541
C	6.460304	1.402062	0.812723
C	7.029651	0.348510	1.503247
C	6.333690	-0.858534	1.633629
C	5.105513	-1.009587	1.024580
C	3.287519	-0.132688	-0.434339
C	2.796126	0.873328	-1.257090
C	3.348014	2.190568	-1.224095
C	4.478504	2.455404	-0.364772
C	5.145084	1.339497	0.285689
C	4.490225	0.051373	0.313634
F	0.000027	-0.329998	0.000004

Figure S25: Optimized structure of [**8-**μ_2-F]$^-$ and atomic coordinates in Å.



[**8-**μ_2-F]$^-$

Sb	-0.812840	-1.010356	1.775847
Sb	0.812385	-1.009196	-1.776194
F	-4.354291	-2.142673	-1.002485
F	-6.765530	-1.941458	-2.160203
F	-8.268463	0.333327	-1.868186
F	-7.317644	2.441768	-0.542388
F	-5.780029	4.228052	-0.911392
F	-4.750670	6.266207	0.461777
F	-2.787006	5.862760	2.326665
F	-1.779836	3.408792	2.746810
F	1.781141	3.409969	-2.745343
F	2.789512	5.863332	-2.324490
F	4.753288	6.265294	-0.459401
F	5.781596	4.226273	0.913238
F	7.318379	2.439366	0.543783
F	8.268213	0.330030	1.868838
F	6.764346	-1.944283	2.159772
F	4.353220	-2.144095	1.001645
O	-2.474919	-1.102793	0.517205
O	-1.624851	0.887804	2.014072
O	2.473984	-1.102619	-0.517033
O	1.624632	0.889001	-2.013007
C	-0.138519	-2.809063	0.695003
C	0.137388	-2.808542	-0.696816
C	0.200075	-4.033663	-1.354308
C	0.086822	-5.256787	-0.689967
C	-0.089337	-5.257327	0.686003
C	-0.201902	-4.034720	1.351417
C	0.943348	-0.370501	2.833966
C	1.021696	0.921597	3.384625
H	0.215682	1.626945	3.221253
C	2.147038	1.288122	4.134219
H	2.207855	2.287671	4.554414
C	3.190481	0.376344	4.337731
H	4.061135	0.666869	4.918365
C	3.115900	-0.906036	3.781992
H	3.930772	-1.610821	3.916313
C	1.995154	-1.278919	3.028048
H	1.961455	-2.265273	2.578564
C	-1.988595	-1.822442	3.401328
C	-1.562090	-1.653947	4.729074
H	-0.627565	-1.144616	4.942260
C	-2.339363	-2.139318	5.788550
H	-2.001261	-2.001763	6.811667
C	-3.546075	-2.799067	5.529860
H	-4.147280	-3.177248	6.351682
C	-3.976543	-2.968867	4.208606
H	-4.913005	-3.479450	4.002605
C	-3.204979	-2.480274	3.146831
H	-3.544867	-2.605867	2.124485
C	1.988706	-1.820422	-3.401678
C	3.204698	-2.478928	-3.147060
H	3.544055	-2.605401	-2.124641
C	3.976604	-2.967028	-4.208813
H	4.912745	-3.478165	-4.002726
C	3.546892	-2.796011	-5.530158
H	4.148364	-3.173808	-6.351961
C	2.340607	-2.135527	-5.788963
H	2.003111	-1.997011	-6.812150
C	1.562987	-1.650661	-4.729512
H	0.628788	-1.140756	-4.942770
C	-0.943459	-0.368533	-2.834406
C	-1.995551	-1.276559	-3.028759
H	-1.962179	-2.263021	-2.579491
C	-3.116124	-0.903132	-3.782685
H	-3.931206	-1.607627	-3.917252
C	-3.190243	0.379395	-4.338145
H	-4.060772	0.670342	-4.918754
C	-2.146508	1.290781	-4.134371
H	-2.206969	2.290441	-4.554354
C	-1.021334	0.923714	-3.384787
H	-0.215088	1.628754	-3.221223
C	-2.816081	3.526825	1.873534
C	-3.313494	4.797995	1.669662

C	-4.344686	5.000157	0.745198
C	-4.898368	3.922811	0.079227
C	-6.460165	1.405388	-0.750693
C	-6.992496	0.305922	-1.397842
C	-6.242022	-0.869866	-1.508574
C	-4.996661	-0.945150	-0.920593
C	-3.200806	0.056614	0.485536
C	-2.738408	1.112718	1.259904
C	-3.346997	2.403814	1.189167
C	-4.505149	2.586842	0.346636
C	-5.133610	1.419470	-0.249555
C	-4.421343	0.162432	-0.248879
C	2.817378	3.527267	-1.871959
C	3.315427	4.798130	-1.667739
C	4.346686	4.999524	-0.743181
C	4.899824	3.921724	-0.077494
C	6.460428	1.403293	0.751676
C	6.992263	0.303346	1.398413
C	6.241315	-0.872191	1.508582
C	4.995979	-0.946732	0.920460
C	3.200434	0.056434	-0.485041
C	2.738440	1.113062	-1.258927
C	3.347715	2.403810	-1.187872
C	4.505961	2.586013	-0.345285
C	5.133897	1.418142	0.250479
C	4.421097	0.161402	0.249285
F	-0.000563	-0.040428	-0.000032
F	-0.366772	-4.098699	2.712084
F	-0.165468	-6.430235	1.364388
F	0.162189	-6.429155	-1.369370
F	0.364686	-4.096528	-2.715064

Table S1: Fluoride anion calculation details.

Compound	HF (Hartree)	H_{corr} (Hartree)	H	FIA (Hartree)	FIA (kJ/mol)
A	-3155.5347259	0.353272	-3155.181454	0.1230609	323.10
[**A**-F]$^-$	-3255.5461819	0.355335	-3255.190847		
B	-2418.5135861	0.427208	-2418.086378	0.1245093	326.90
[**B**-F]$^-$	-2518.5262055	0.428985	-2518.097221		
7	-5001.7648994	0.716896	-5001.0480034	0.1521099	399.36
[**7**-μ_2-F]$^-$	-5101.8047435	0.718297	-5101.0864465		
8	-4604.7092489	0.746627	-4603.9626219	0.1487957	390.66
[**8**-μ_2-F]$^-$	-4704.7464288	0.748678	-4703.9977508		

The enthalpy of the fluoride anion in the gas phase was determined as -99.8863332 Hartree.