Electronic Supplementary Material (ESI) for Dalton Transactions.

Design considerations for chiral frustrated Lewis pairs: B/N FLPs derived from 3,5-bicyclic aryl piperidines

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Supporting Information

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General Considerations

All manipulations were carried out under dry, O_2-free N_2 using an MBraun glovebox and a Schlenk vacuum-line. Pentane and dichloromethane were collected from a Grubbs-type column system manufactured by Innovative Technology and into thick-walled glass Schlenk bombs with Young-type Teflon valve stopcocks. Chloroform-d was obtained from Cambridge Isotope Laboratories, dried over CaH_2, and vacuum-transferred into Young bombs, Toluene-d_8 and benzene-d_6 was obtained from Sigma-Aldrich, dried over Na/benzophenone and vacuum-transferred into Young bombs. All solvents were degassed after purification and stored over 4 Å molecular sieves. $B(C_6F_5)_3$ was purchased from Boulder Scientific and used without further purification for the synthesis of bis(perfluorophenyl)borane. (E)-N-tert-butyl-1-phenylmethanimine and triethylsilane were purchased from Sigma-Aldrich, and dried and stored over 4 Å molecular sieves. Commercial reagents were purchased from Sigma-Aldrich, TCI Chemicals, Strem Chemicals or Alfa Aesar, and used without further purification unless indicated otherwise. Hydrogen gas (Grade 5.0) was obtained from Linde and purified through a Matheson Nanochem WeldAssure™ gas purifier column prior to use. Deuterium hydride (extent of labeling: 96 mol% HD, 98 atom % D) and carbon ^{13}C dioxide (99 atom % ^{13}C, <3 atom % ^{18}O) were purchased from Sigma Aldrich. (1R,3s,5S)-7,8-difluoro-3-isopropyl-2,3,4,5-tetrahydro-1H-1,5-methanobenzo[d]azepin-3-ium chloride was received from Pfitzer and used without further purification. (E)-N-(1-phenylethylidene)aniline,[1] tris(2,6-difluorophenyl)borane,[2] (bis(perfluorophenyl)borane,[3] were prepared according to literature methods.

NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer or a Varian Mercury Plus 400 MHz spectrometer at 25 ºC. Chemical shifts are given relative to $SiMe_4$ and referenced to the residual solvent signal (^1H, ^{13}C) or relative to an external standard (^{11}B: 15% $(Et_2O)BF_3$, ^{31}P: 85% H_3PO_4, ^{19}F: $CFCl_3$). Chemical shifts are reported in ppm and coupling constants as scalar values in Hz. Mass spectrometry was carried out using an AB/Sciex QStar mass spectrometer with an ESI source or on a Hewlett-Packard GC/MS 6890 N that works with the EI technique (70 eV). Elemental analyses (C, H, N) were performed in-house with a Perkin Elmer 2400 Series II CHNS Analyzer

Spectra

Figure S1. ^{1}H NMR spectrum of **1**

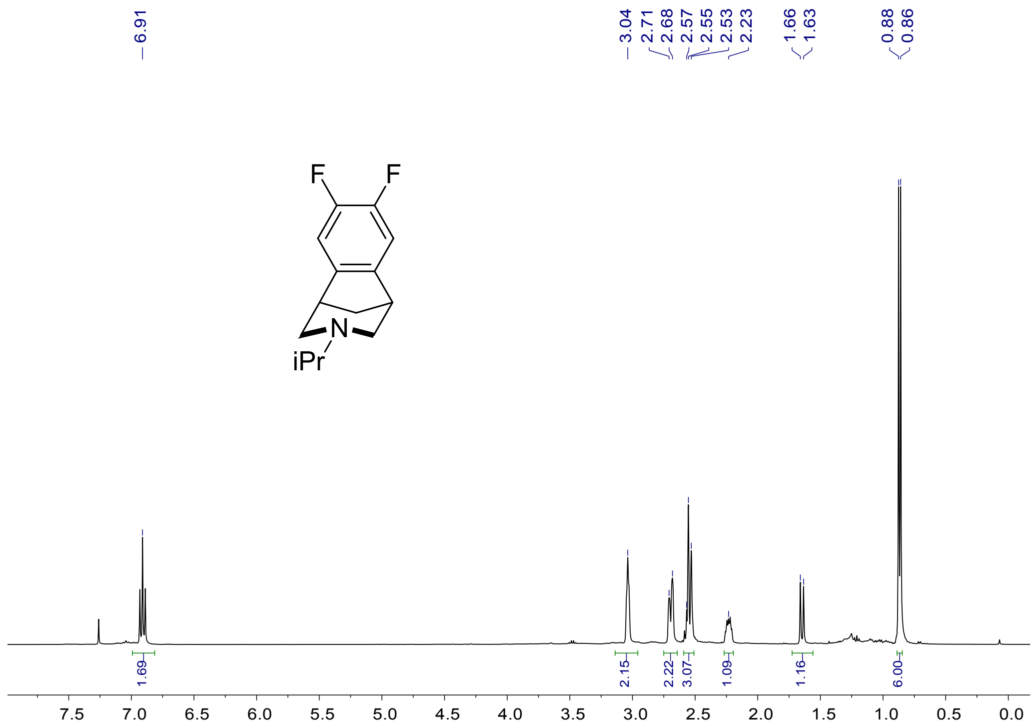


Figure S2. ^{13}C{H} NMR spectrum of **1**

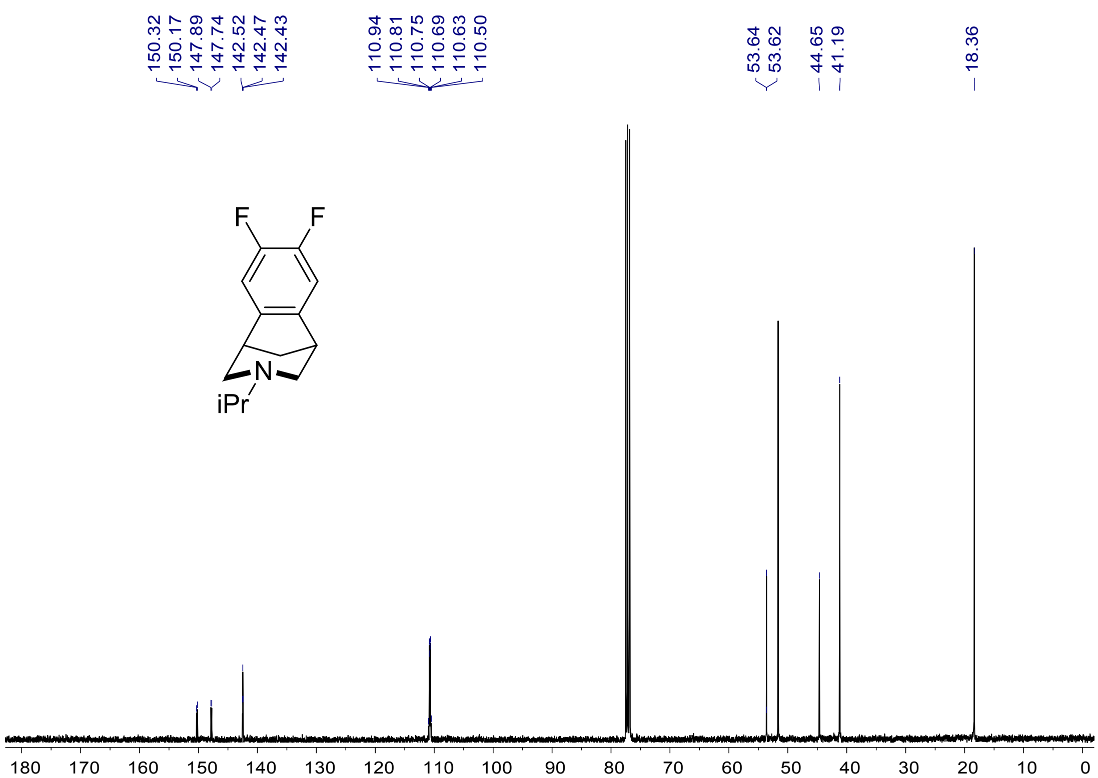


Figure S3. ^{19}F NMR spectrum of **1**

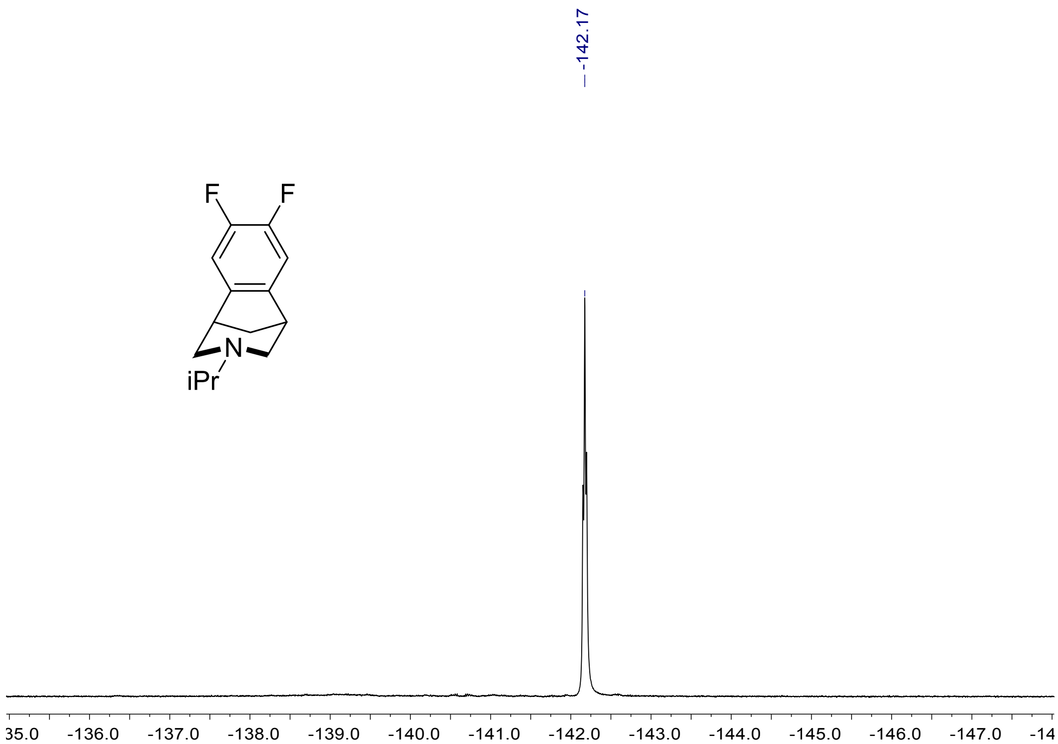


Figure S4. ^{1}H NMR spectrum of **2**

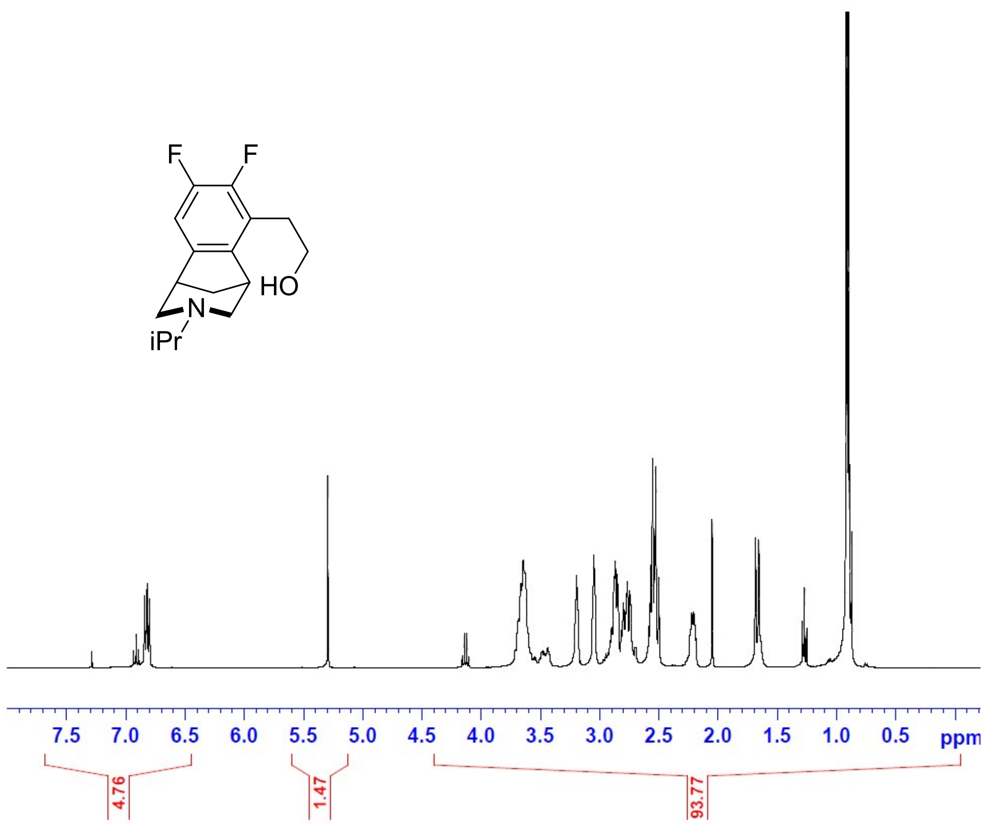


Figure S5. ^{13}C NMR spectrum of **2**

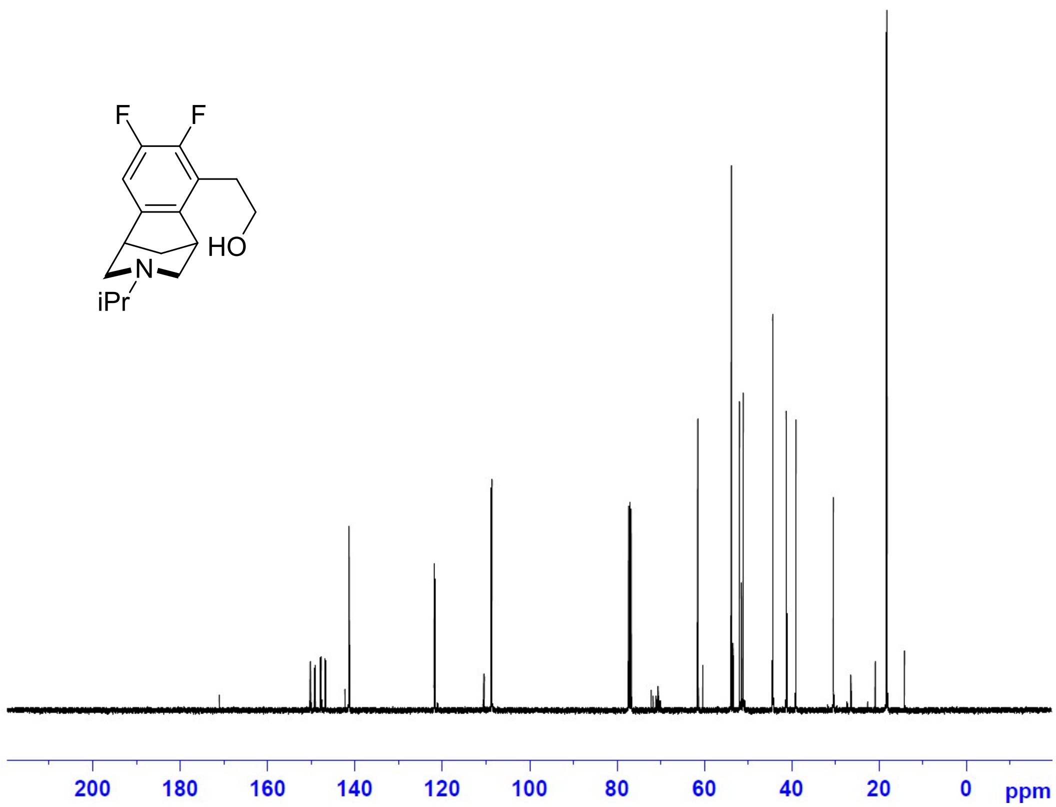


Figure S6. ^{19}F NMR spectrum of **2**

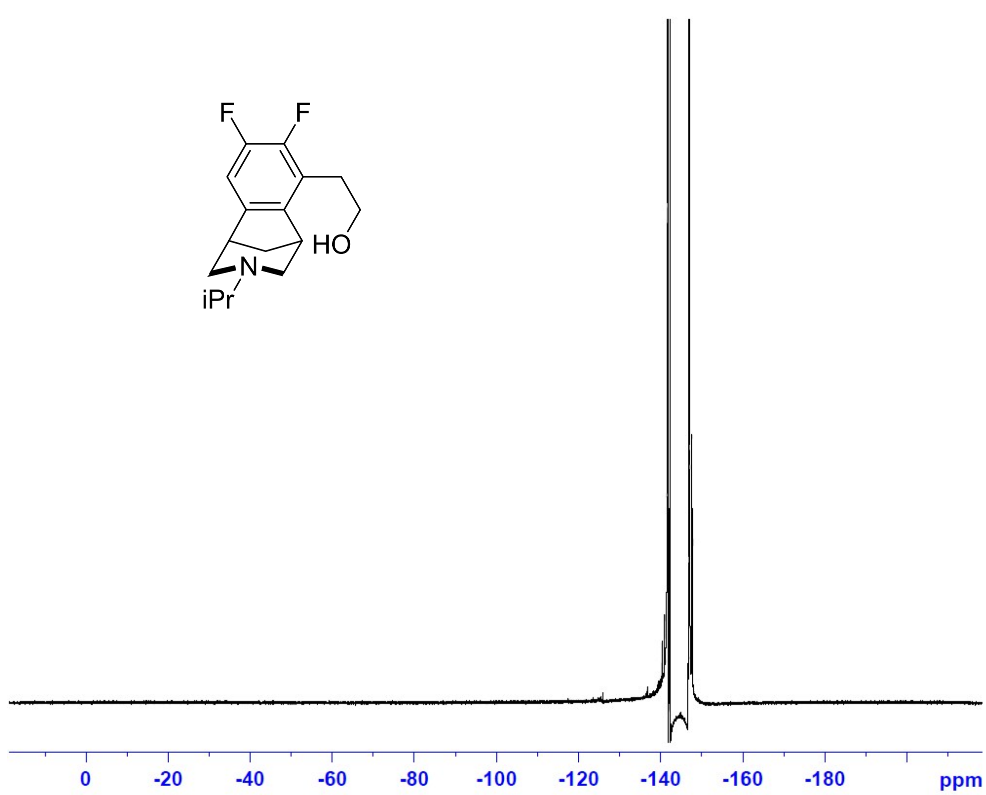


Figure S7. [1]H NMR spectrum of **3**

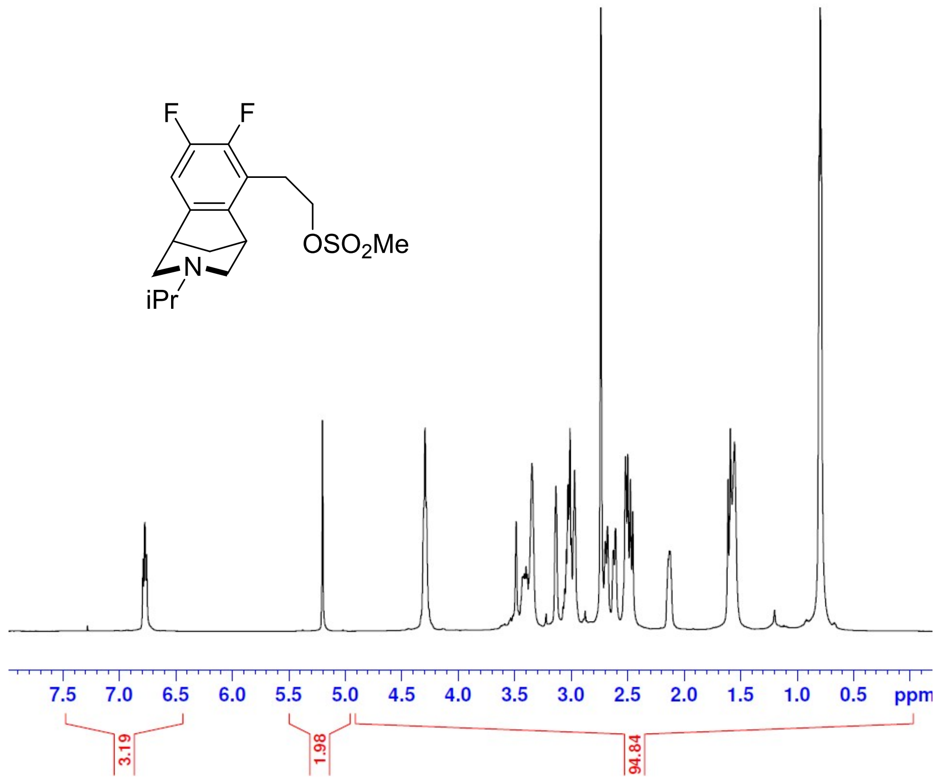


Figure S8. [13]C NMR spectrum of **3**

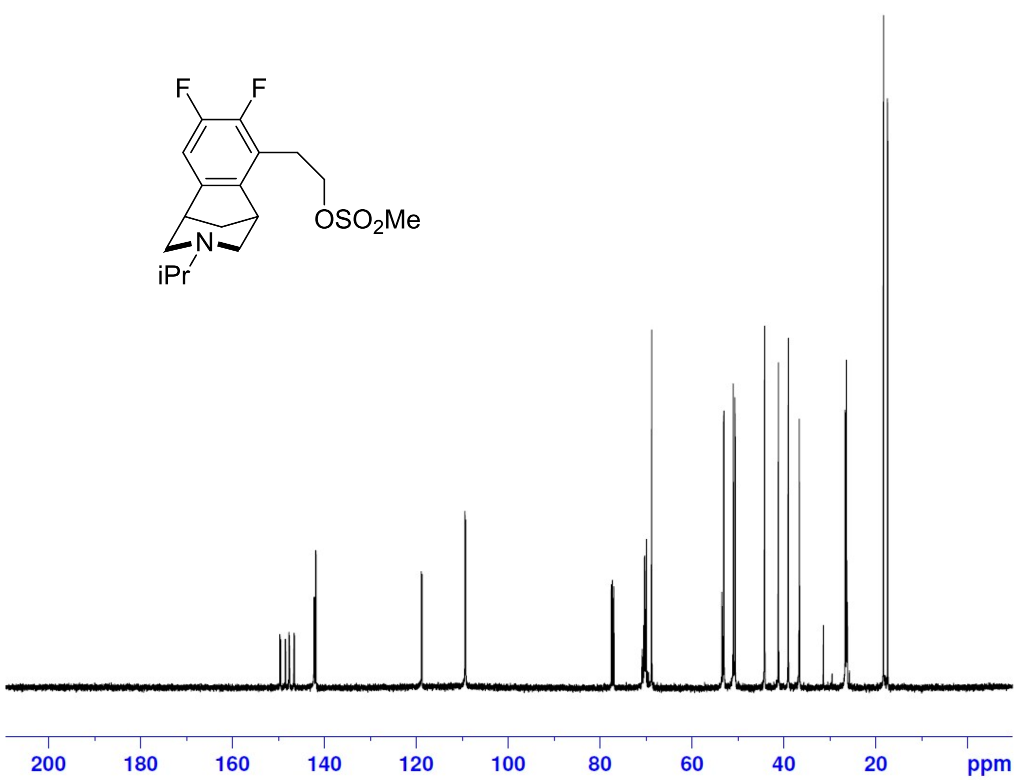


Figure S9. ^{1}H NMR spectrum of **4**

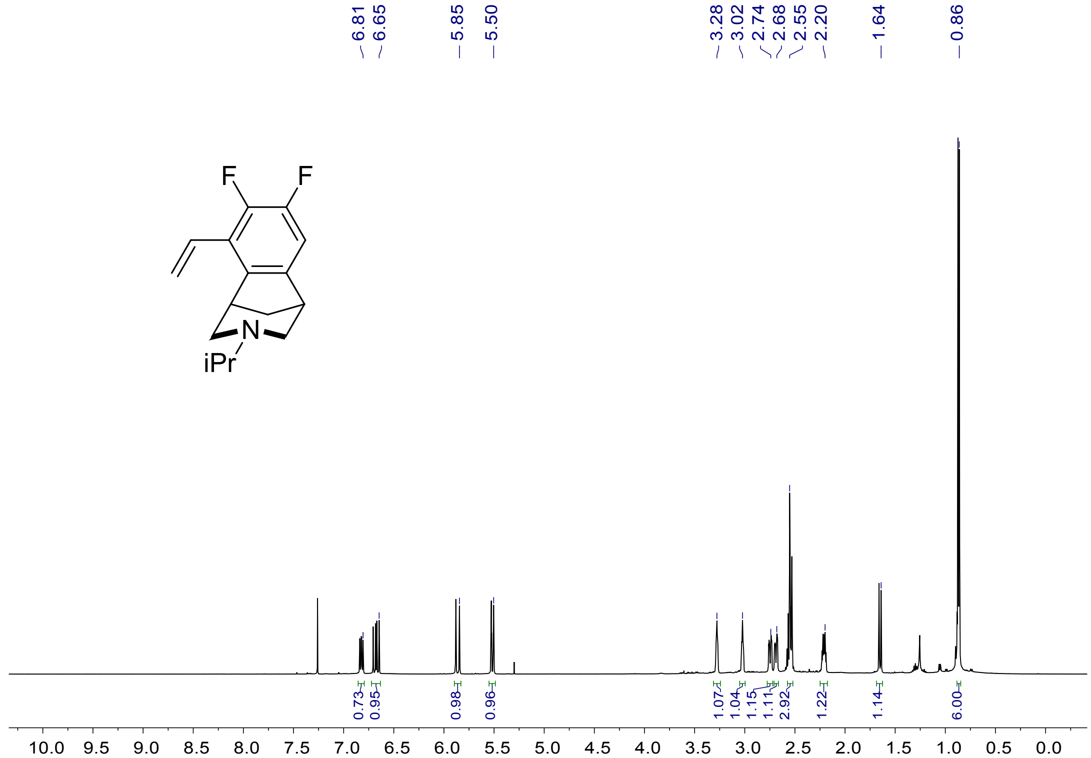


Figure S10. $^{13}C\{H\}$ NMR spectrum of **4**

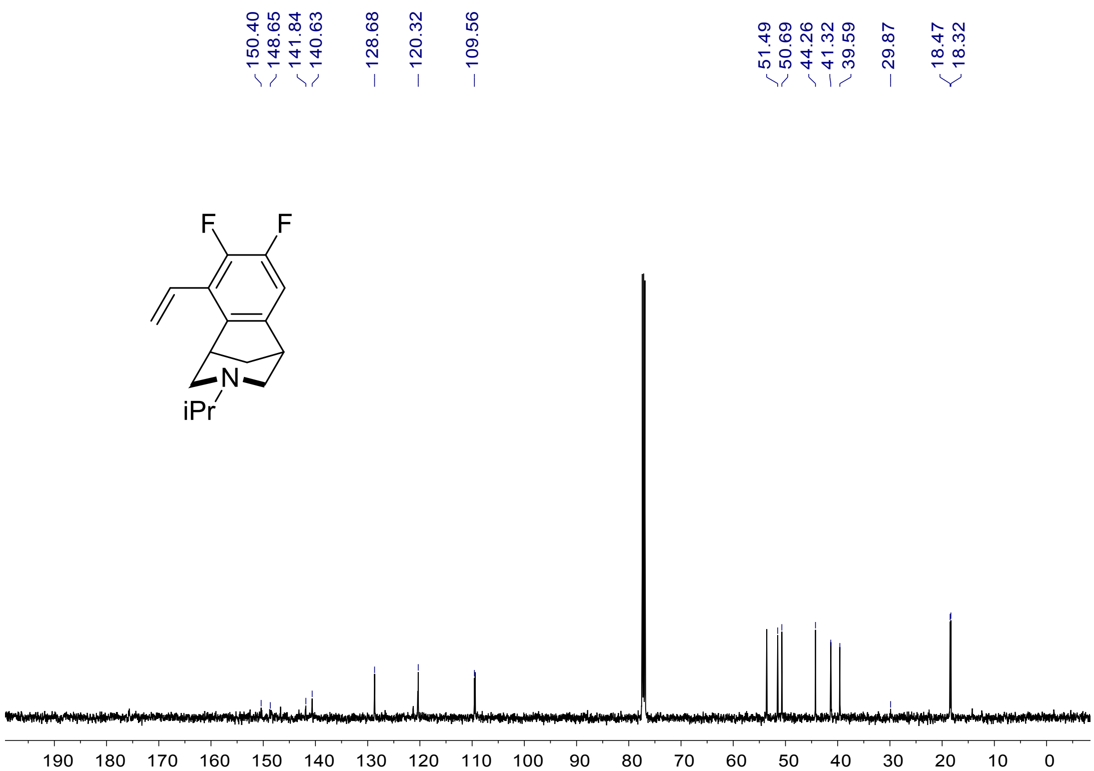


Figure S11. ^{19}F NMR spectrum of **4**

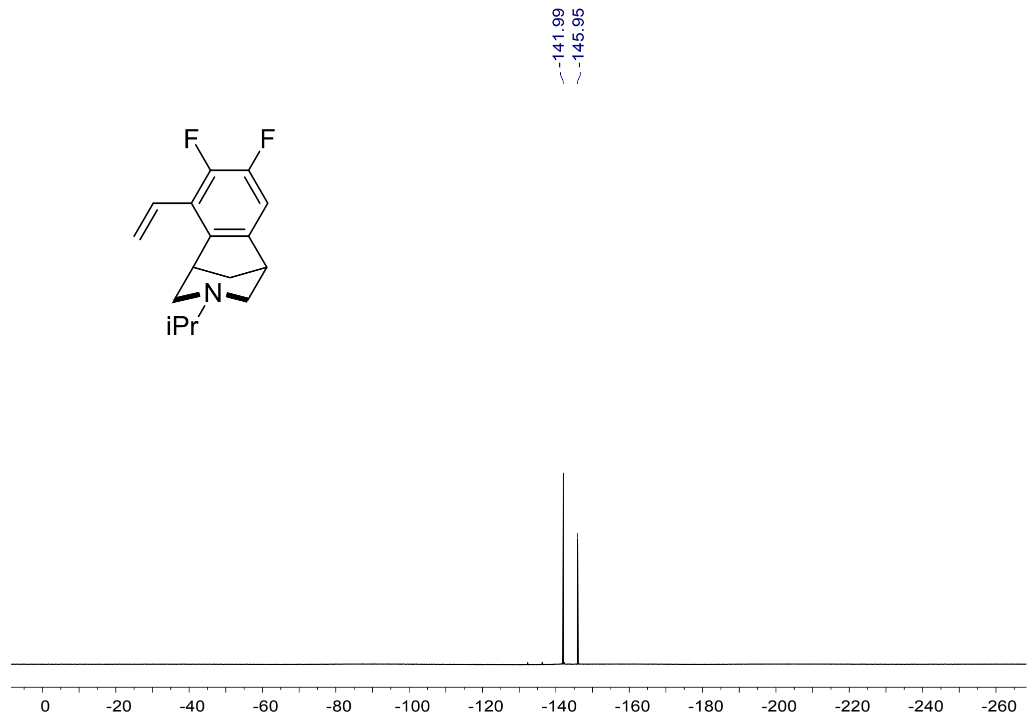


Figure S12. ^{1}H NMR spectrum of **6**

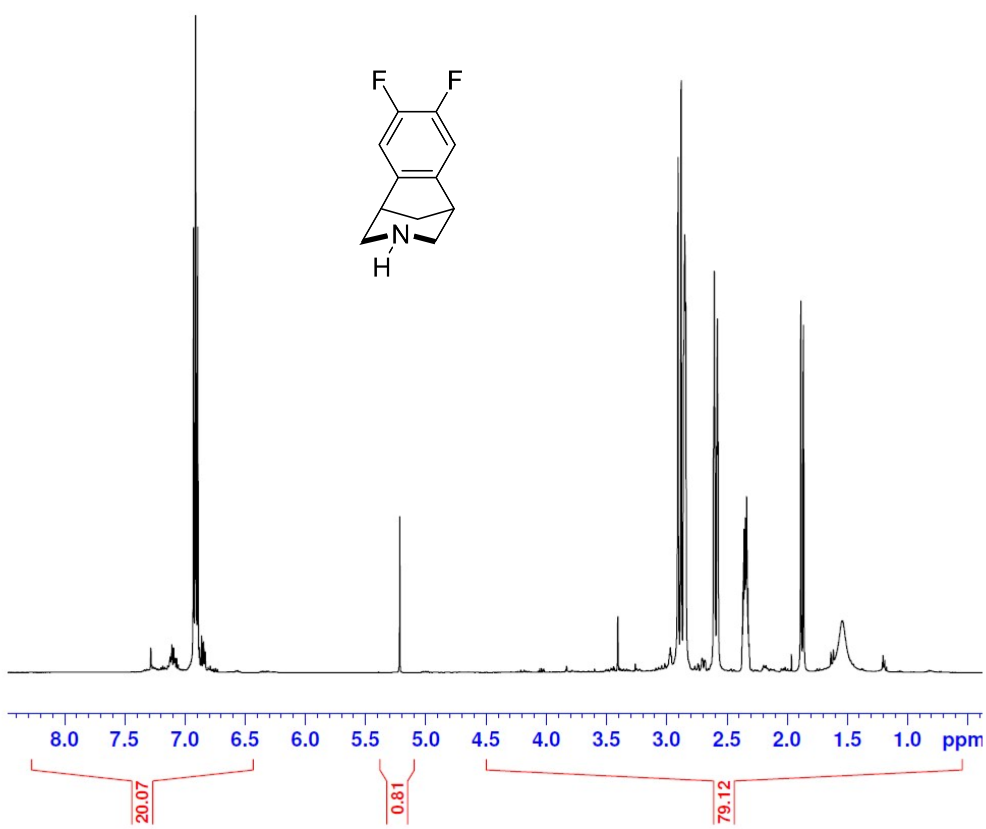


Figure S13. ^{1}H NMR spectrum of **7**

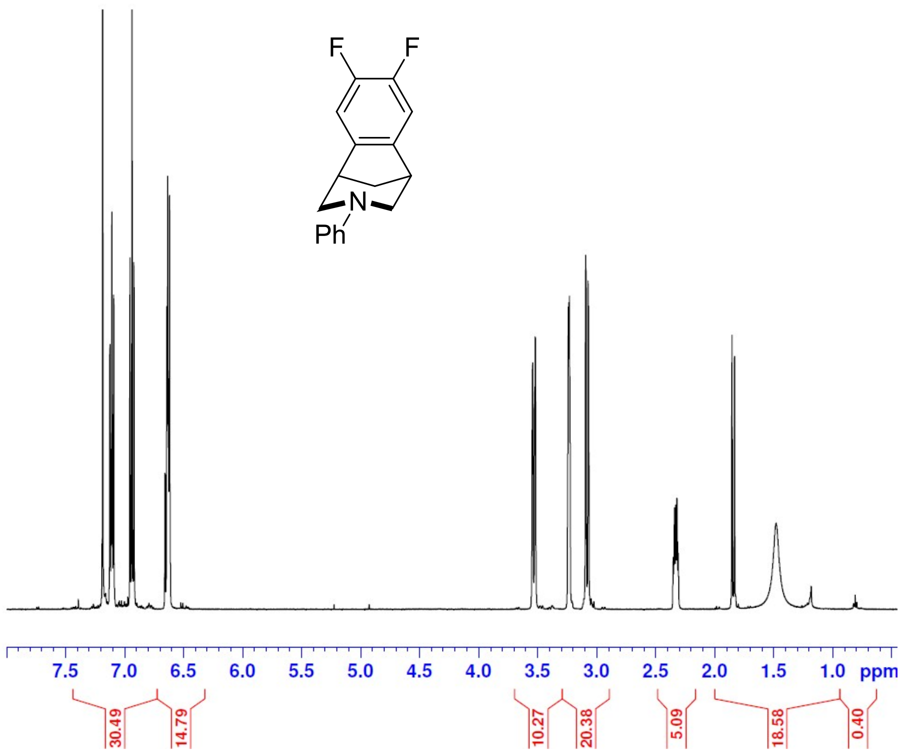


Figure S14. ^{13}C NMR spectrum of **7**

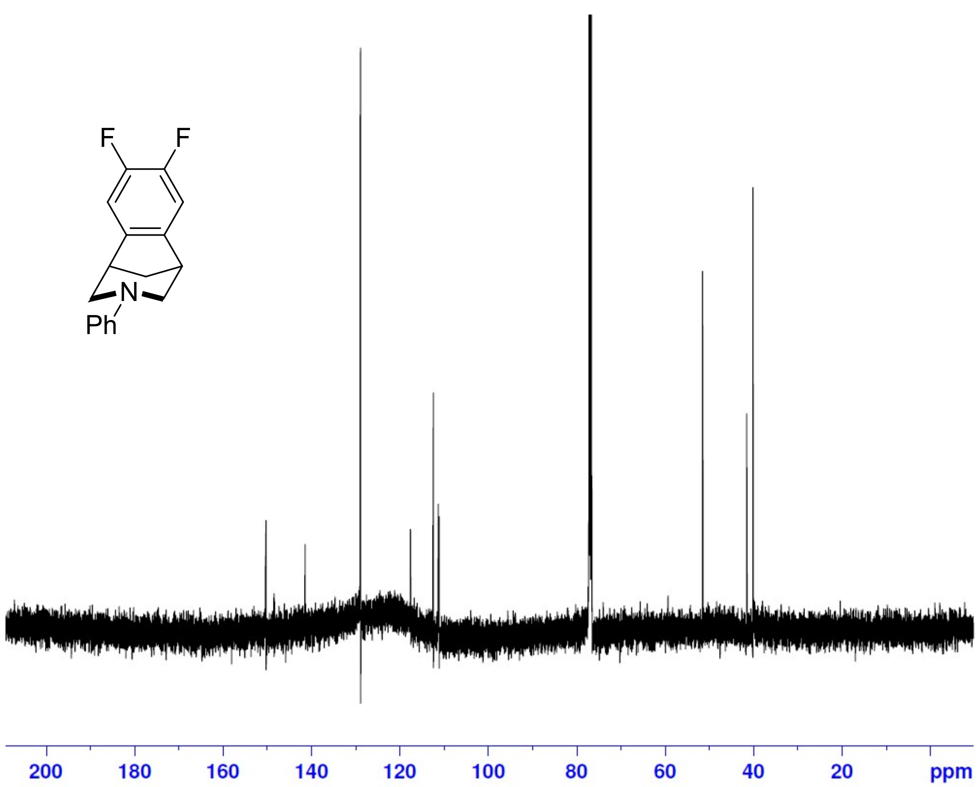


Figure S15. ^{1}H NMR spectrum of **8**

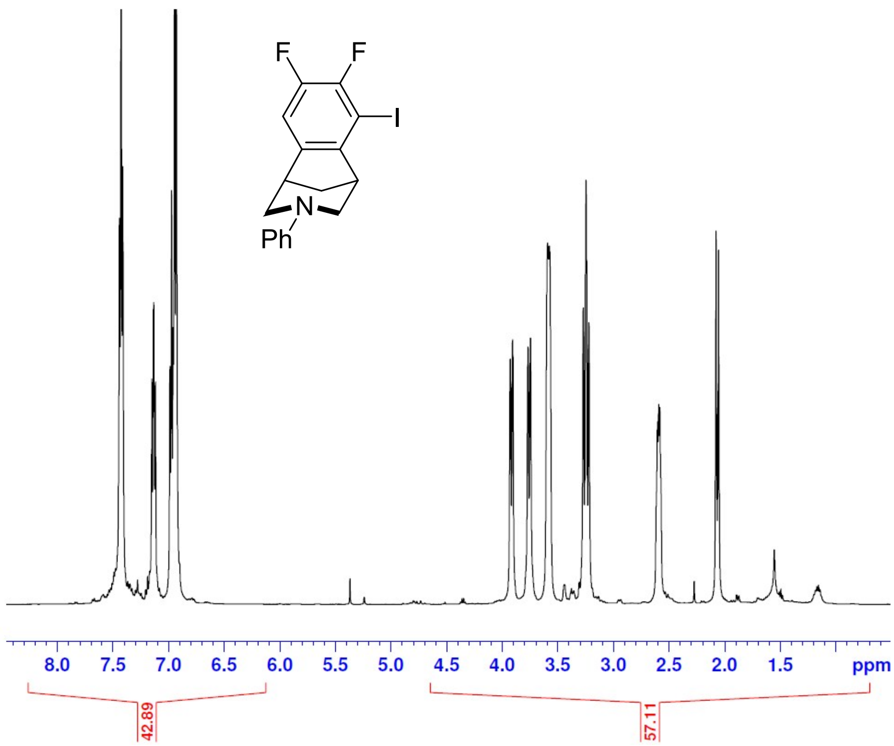


Figure S16. ^{13}C NMR spectrum of **8**

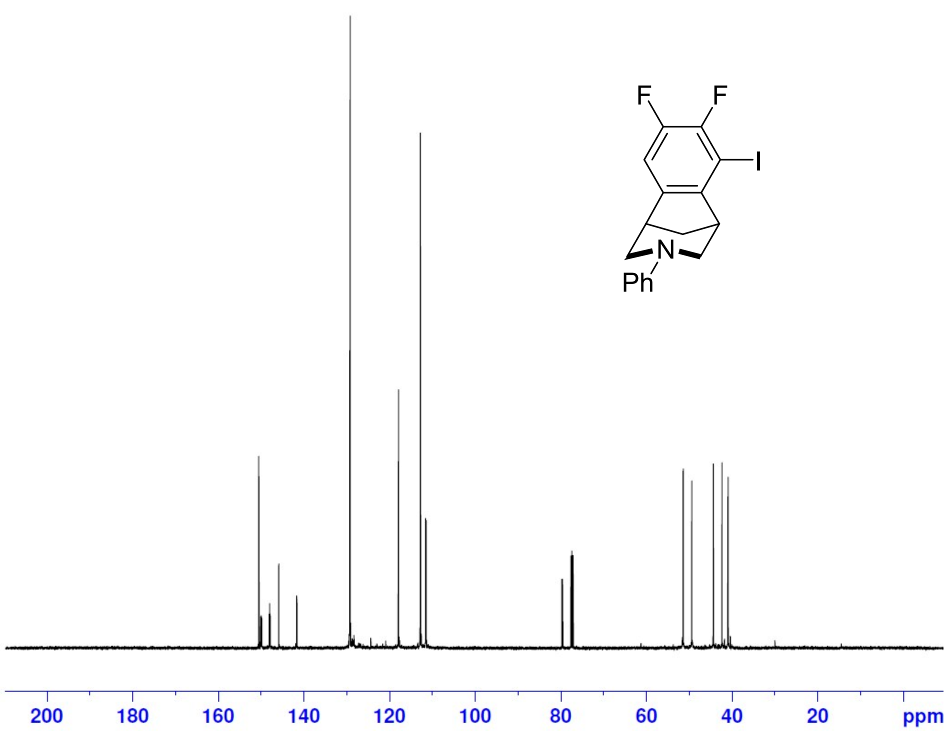


Figure S17. ^{1}H NMR spectrum of **9**

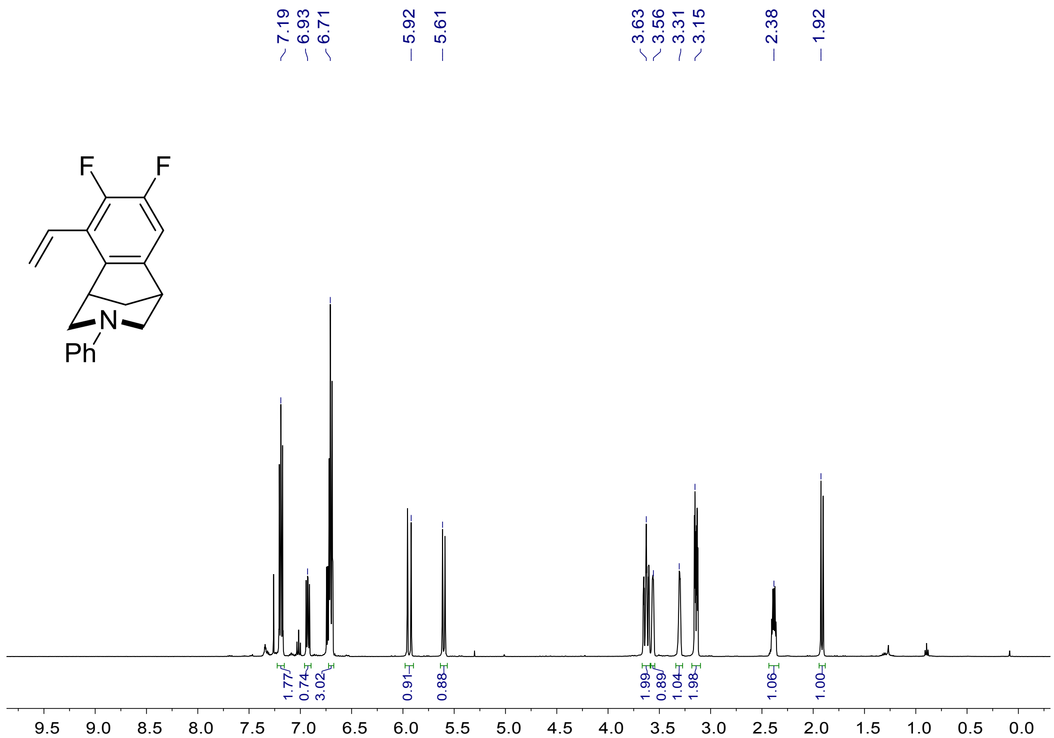


Figure S18. ^{13}C{H} NMR spectrum of **9**

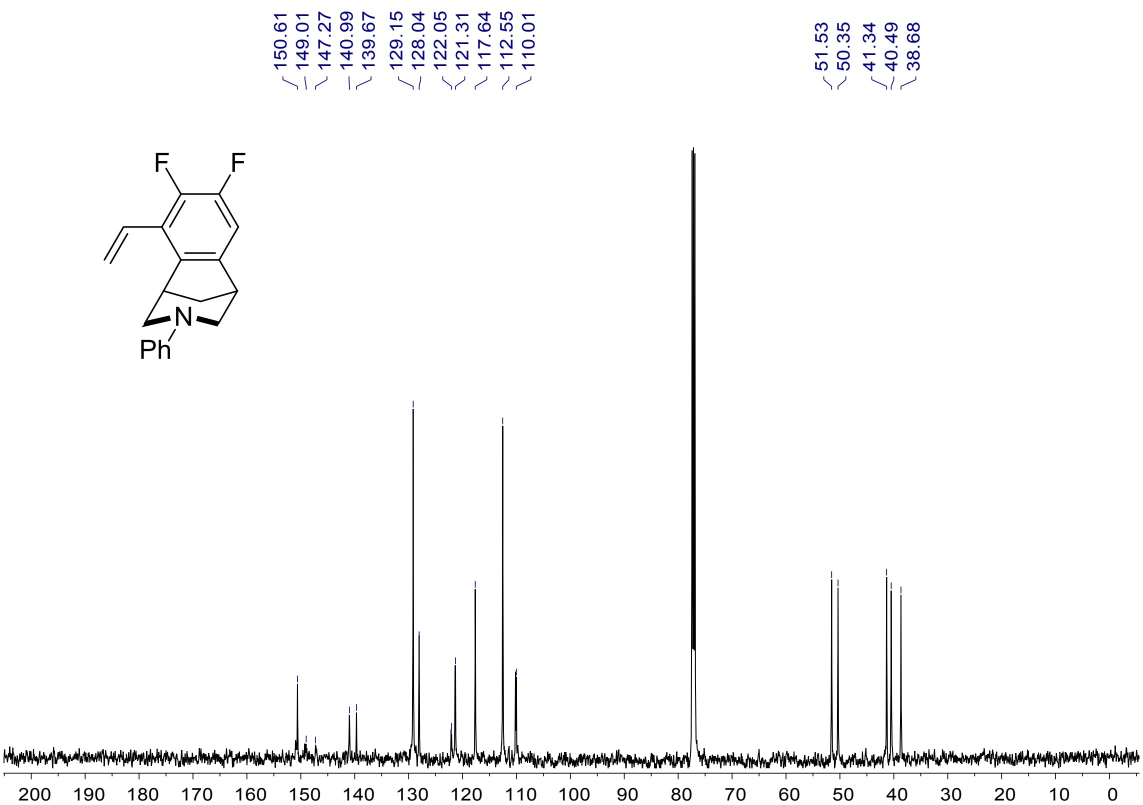


Figure S19. ^{19}F NMR spectrum of **9**

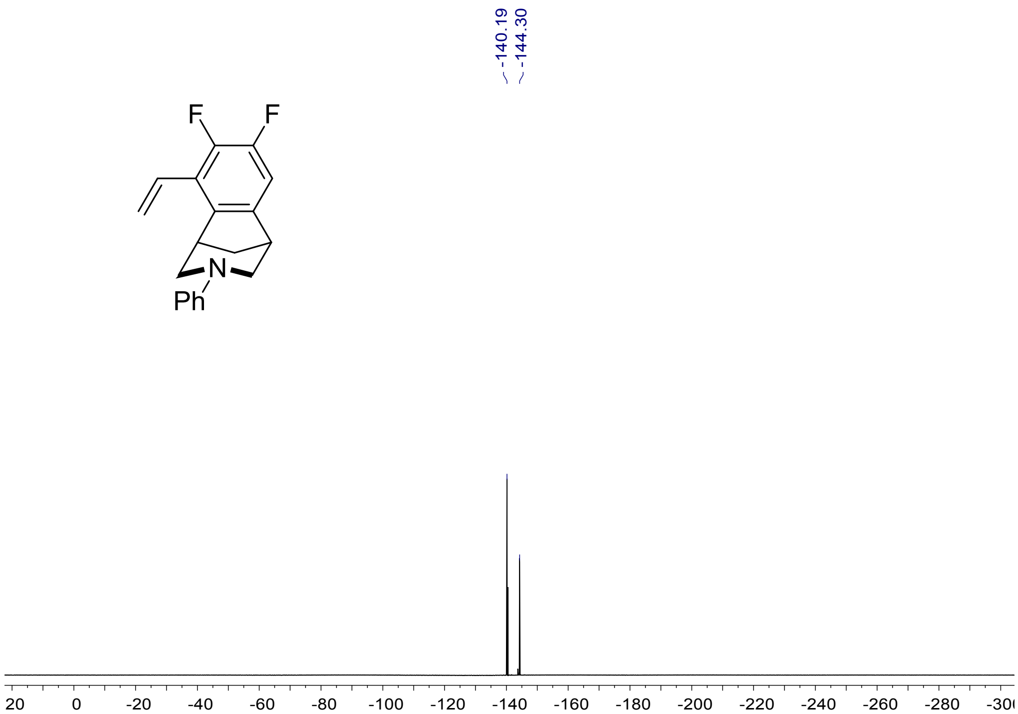


Figure S20. ^{1}H NMR spectrum of **10**

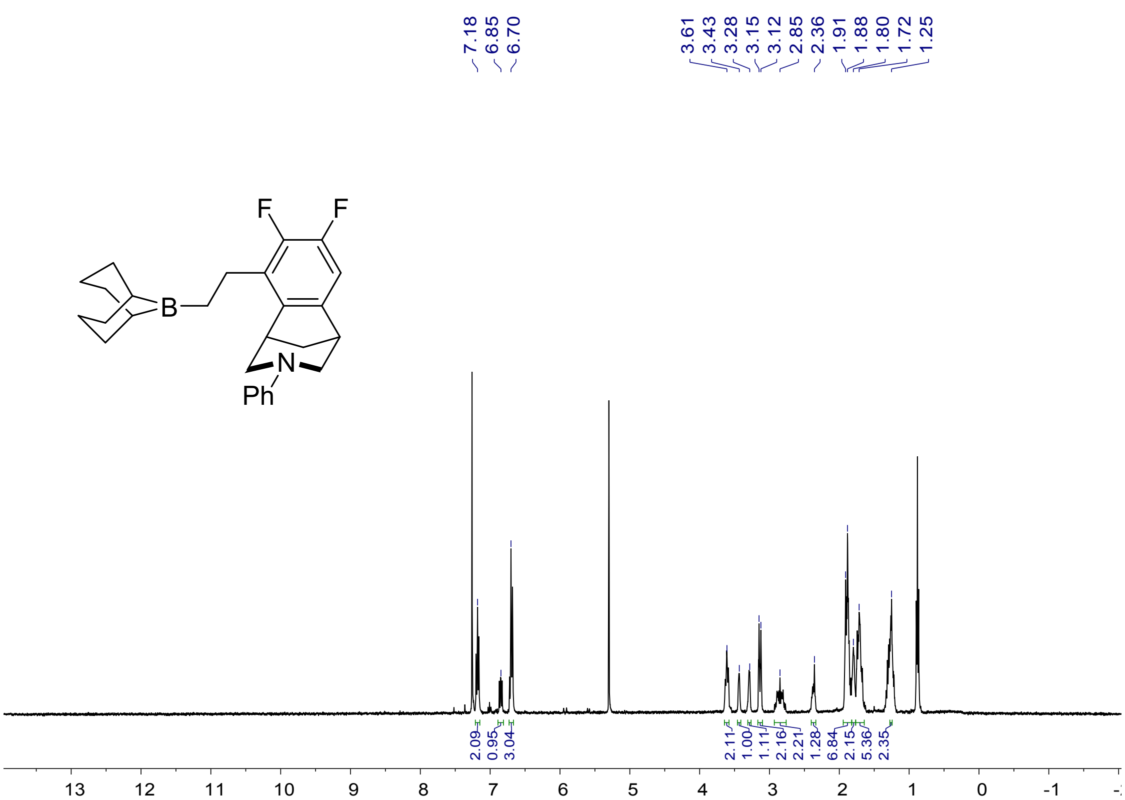


Figure S21. $^{13}C\{H\}$ NMR spectrum of **10**

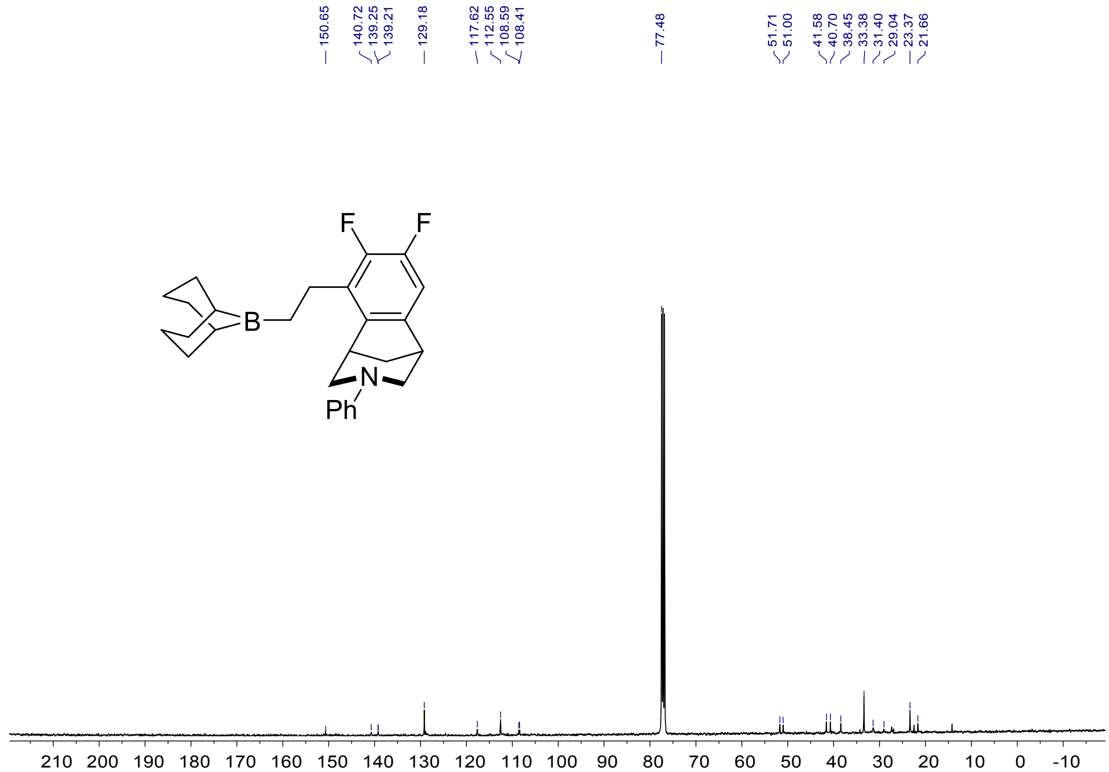


Figure S22. ^{11}B NMR spectrum of **10**

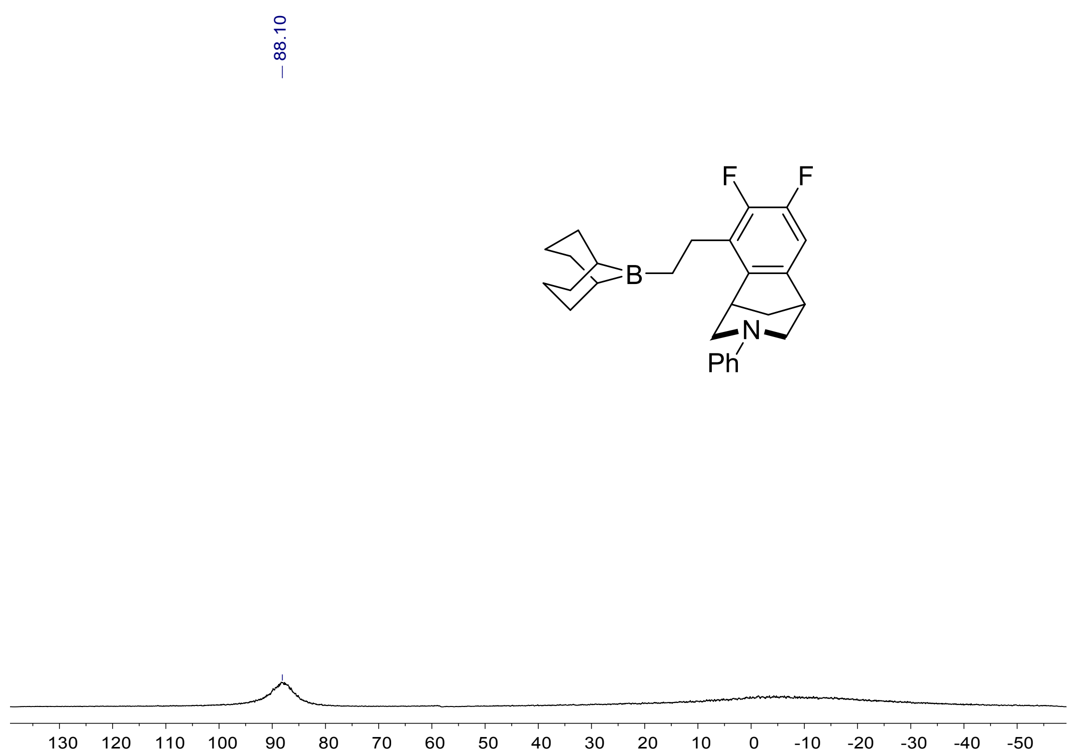


Figure S23. ^{19}F NMR spectrum of **10**

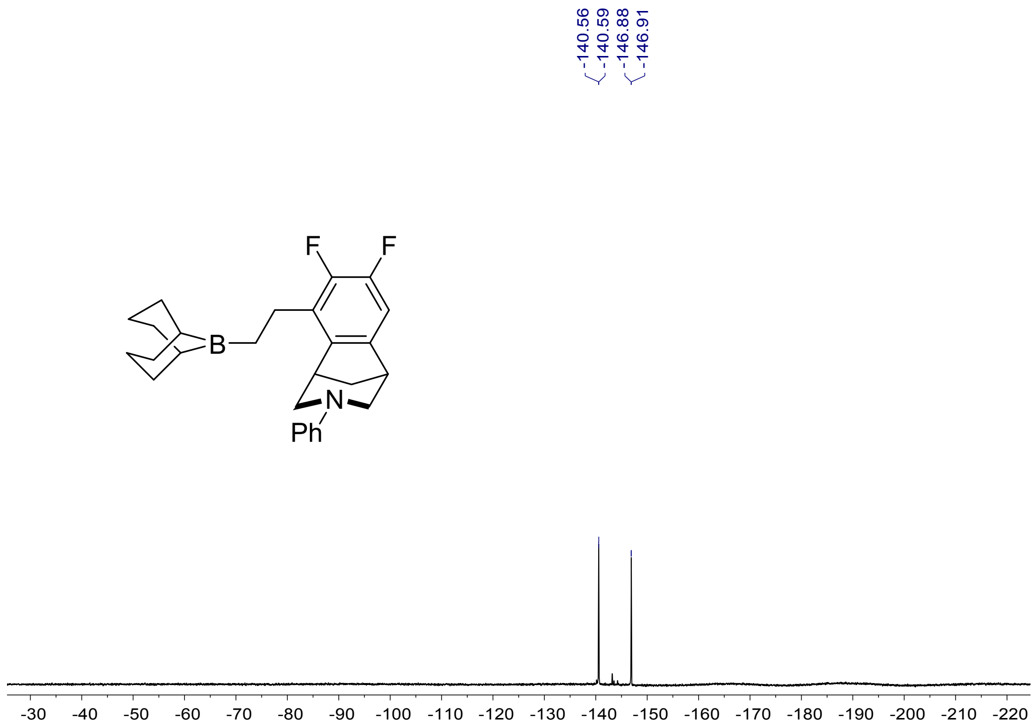


Figure S24. ^{1}H NMR spectrum of **11**

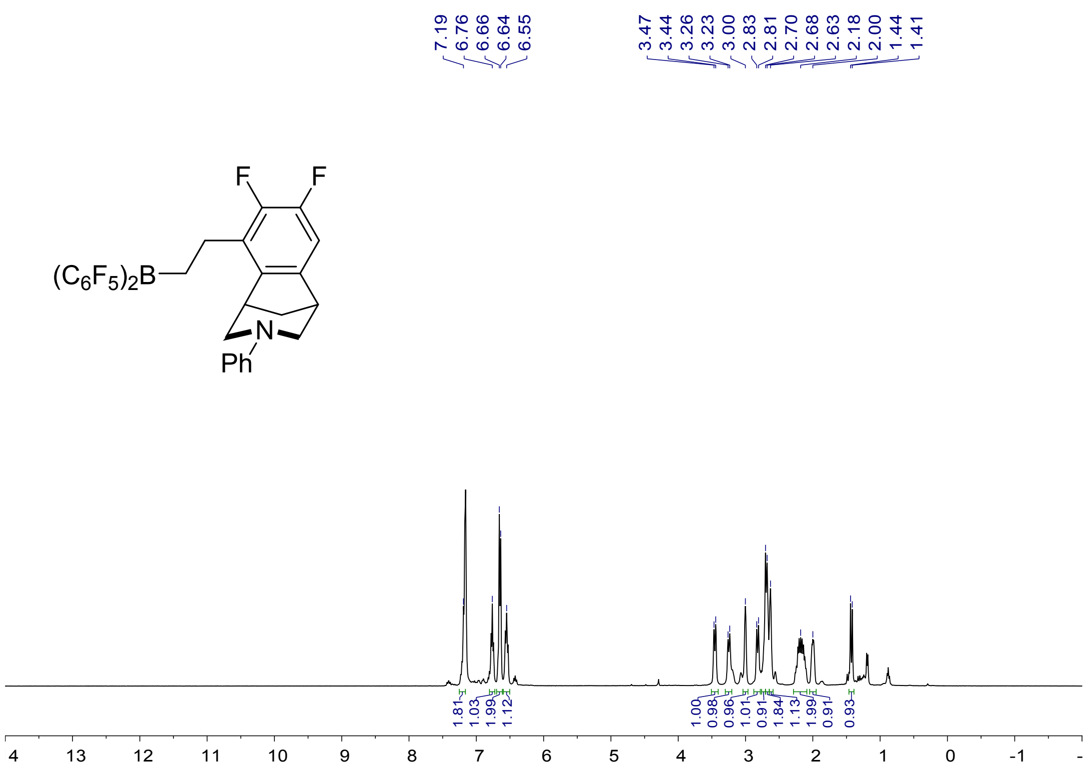


Figure S25. $^{13}C\{H\}$ NMR spectrum of **11**

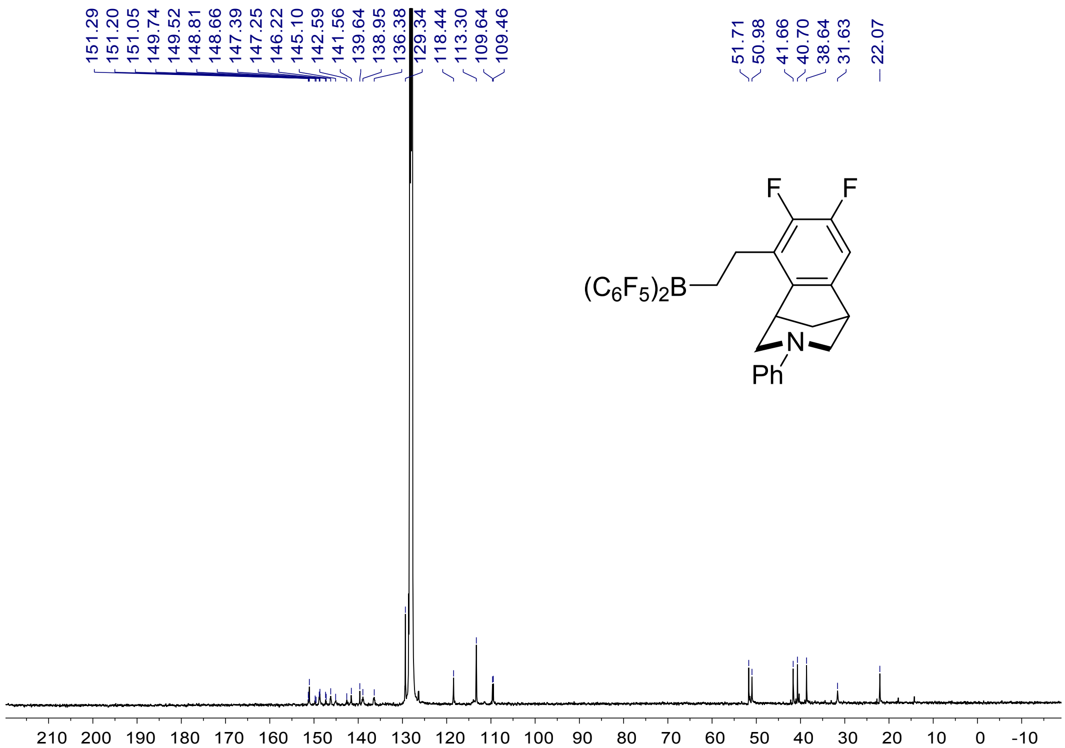


Figure S26. ^{11}B NMR spectrum of **11**

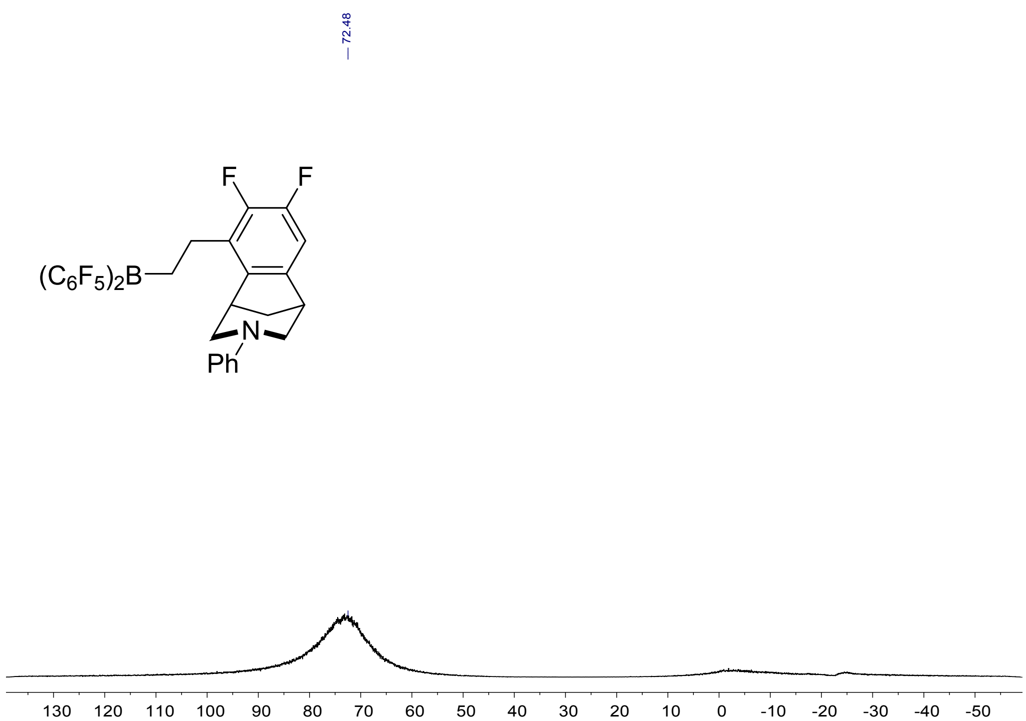


Figure S27. ^{19}F NMR spectrum of **11**

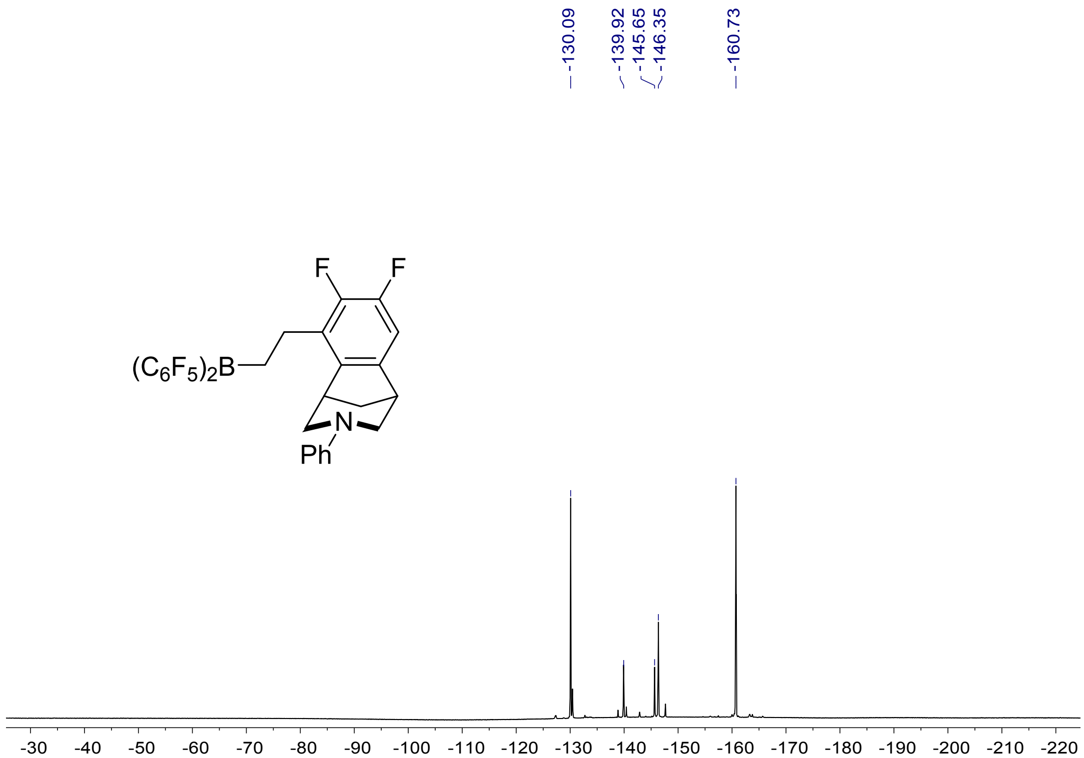


Figure S28. ^{1}H NMR spectrum of **12**

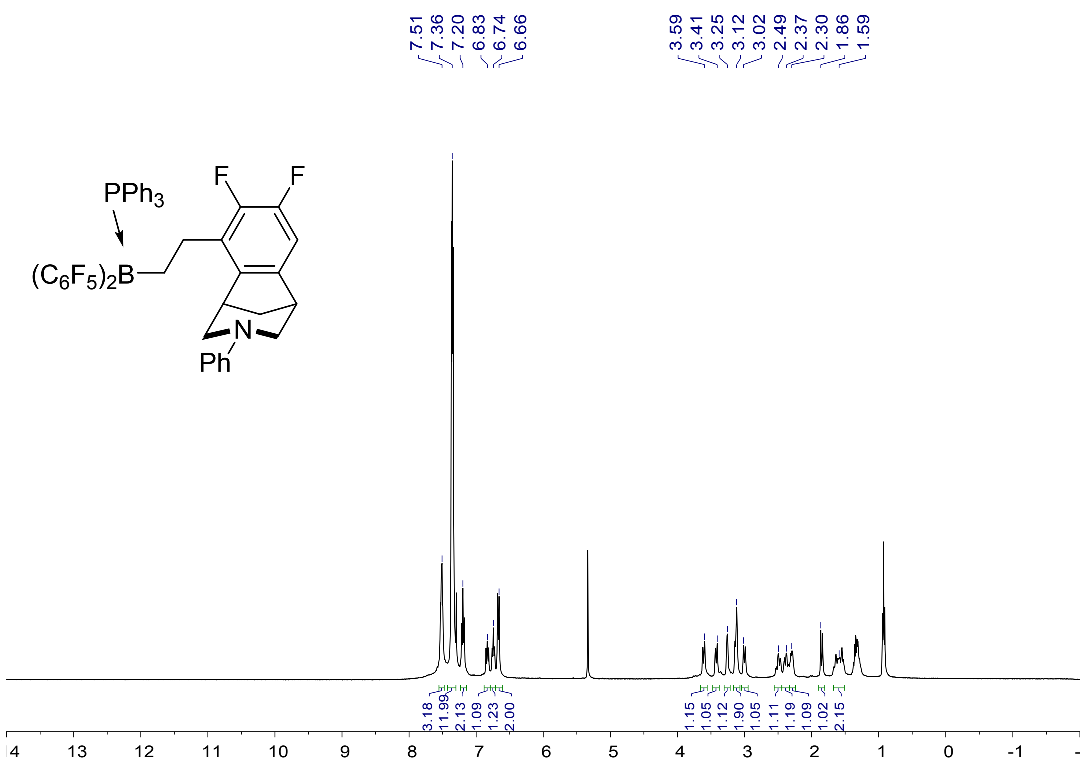


Figure S29. $^{13}C\{H\}$ NMR spectrum of **12**

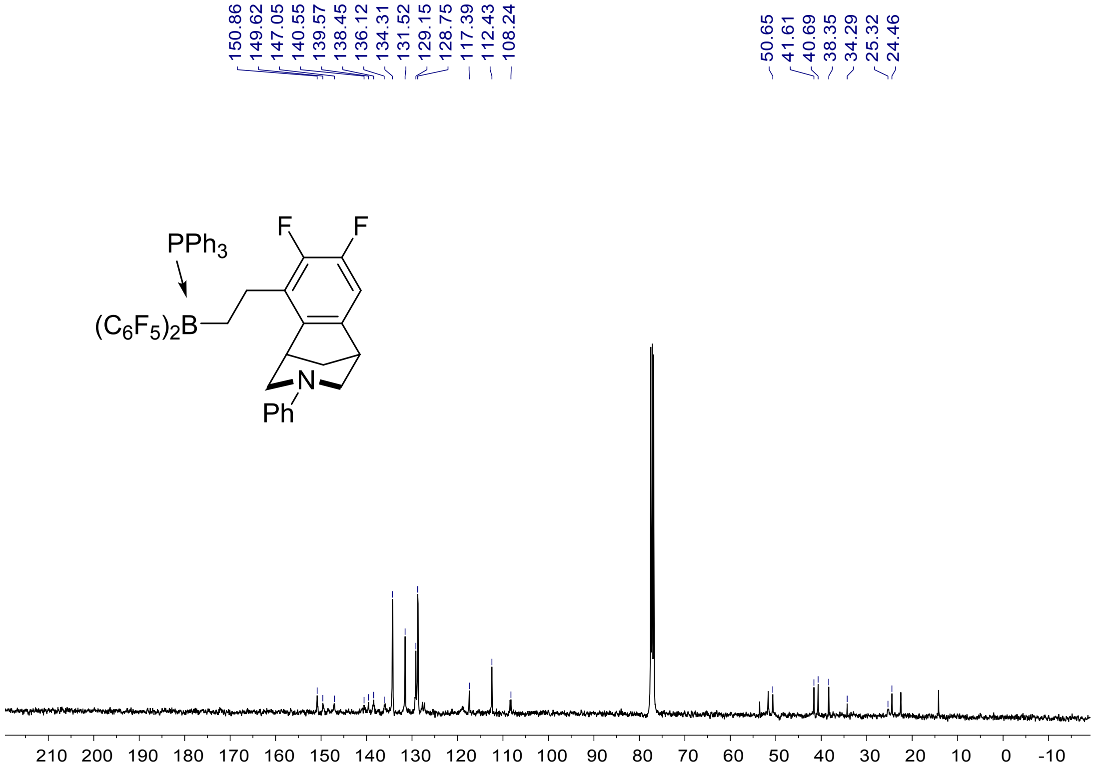


Figure S30. ^{31}P NMR spectrum of **12**

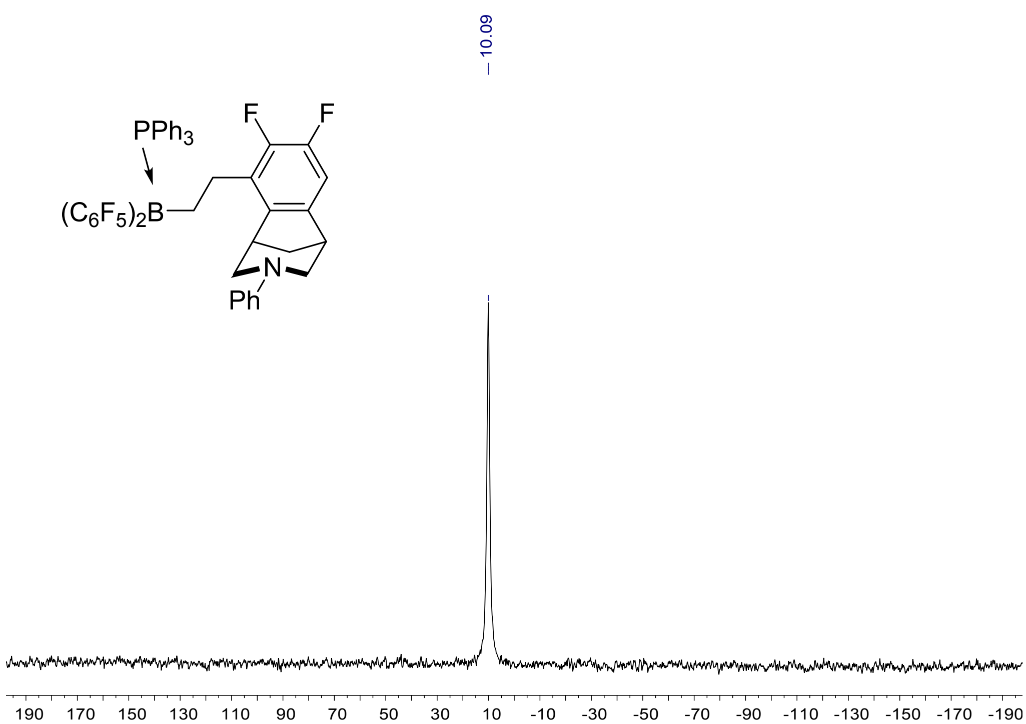


Figure S31. ^{11}B NMR spectrum of **12**

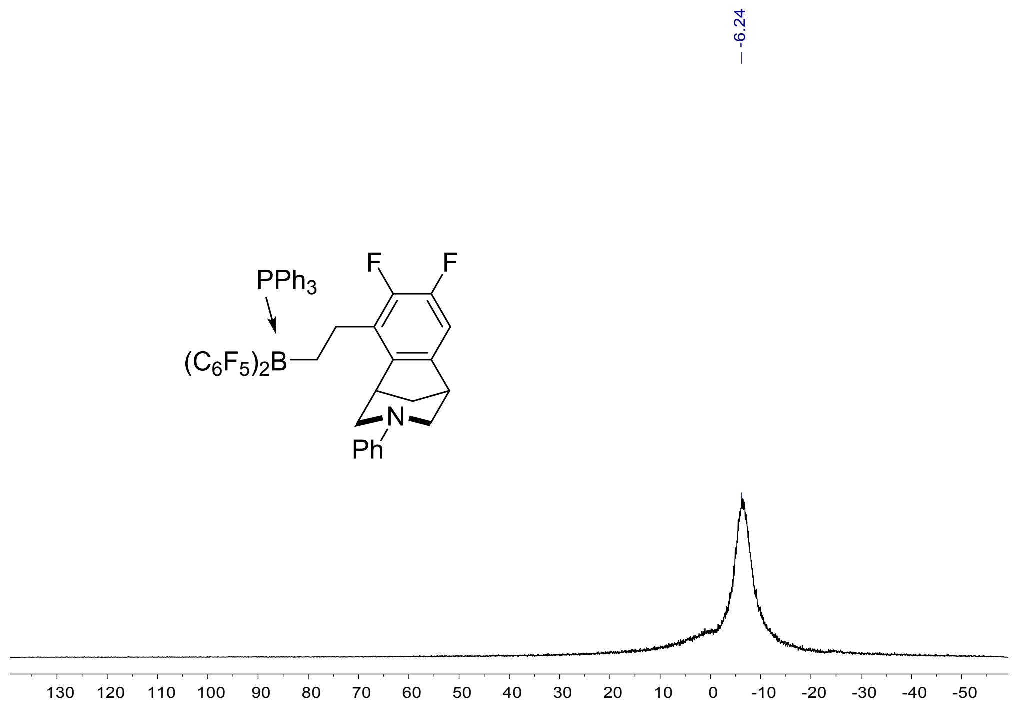


Figure S32. ^{19}F NMR spectrum of **12**

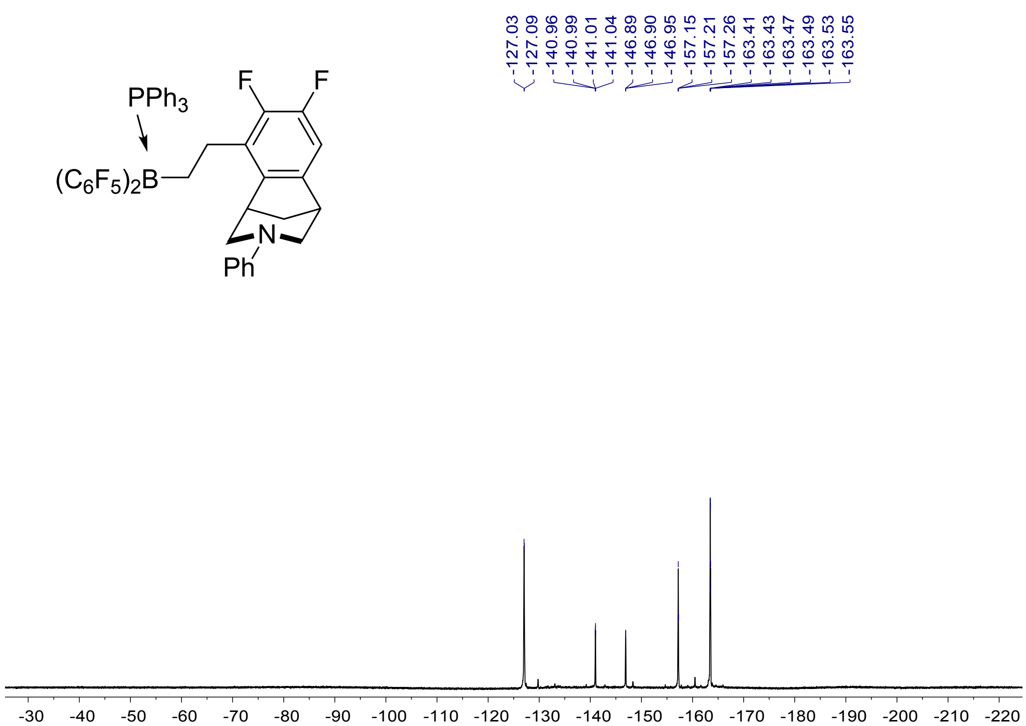
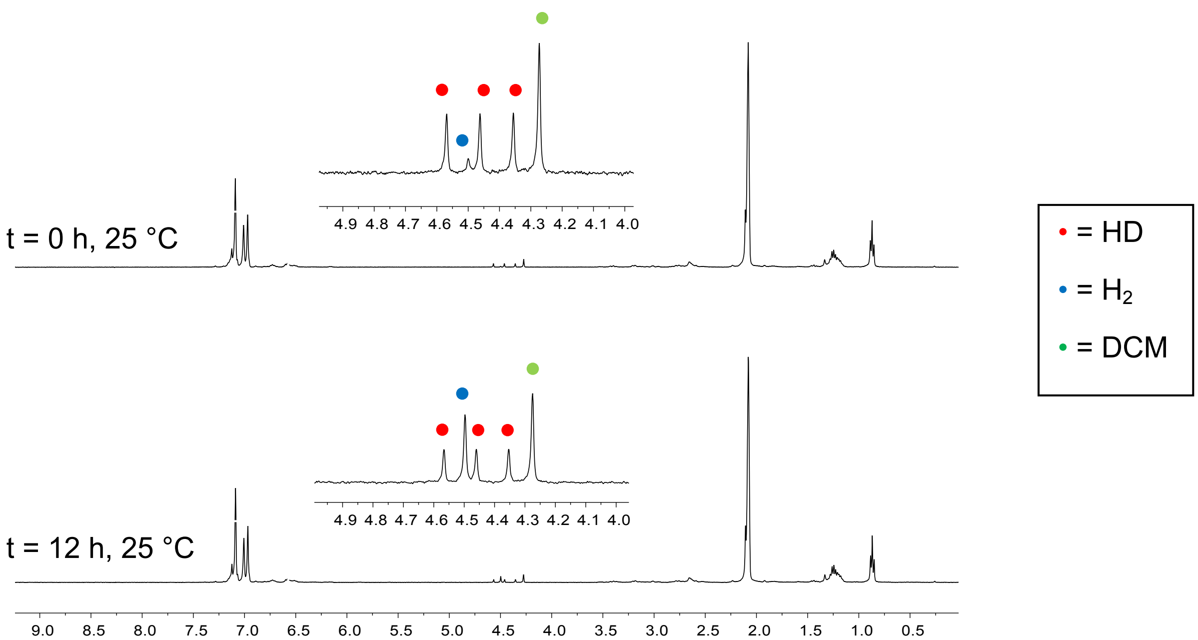


Figure S33. ^1H NMR spectrum for HD scrambling experiment with **11** in toluene-d_8



Gutmann-Beckett Test

In an inert atmosphere glovebox, 0.005 mmol of the Lewis acid (1 eqv., 2 mg for **12**, 5 mg for **13**) and 0.8 mg of Et_3PO (0.006 mmol, 1.2 eqv.) were added to 1 mL of solvent (DCM for **12**, C_6D_6 for **13**).[4] A clear colourless solution was formed and $^{31}P\{^1H\}$c NMR was collected.

Table S1. Gutmann-Beckett test results

	$^{31}P\{^1H\}$ (ppm)	Δ versus Et_3PO (ppm)
Et_3PO	52.2 (in DCM), 46.5 (in C_6D_6)	-
Et_3PO + **10**	52.4	0.2
Et_3PO + **11**	74.3	27.8

Computational details

The tables contain the optimized coordinates of the compounds and their fluoride adducts (denoted as **x**-F, additional possible geometries denoted alphabetically), calculated using the BP86 functional and the def2-TZVP basis set. All calculations were carried out in the gas phase.

Table S2. FIA data for boranes

Compound	Energy (kJ/mol)	Energy of F-adduct (kJ/mol)	FIA (kJ/mol)
10	-3478142.5	-3740334.9	350.1

BPh_3	-1885741.0	-2147911.5	328.1
$B(C_6H_3F_2)_3$	-3447380.9	-3709585.2	362.3
11	-6473827.8	-6736111.6	441.4
$B(C_6F_5)_3$	-5789595.6	-6051890.2	452.6

Table S3. GEI data for boranes

Compound	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)
10	-5.445	-0.713	1.00
BPh_3	-6.888	-2.256	2.04
$B(C_6H_3F_2)_3$	-6.993	-2.547	2.56
11	-5.538	-2.938	3.45
$B(C_6F_5)_3$	-7.651	-3.523	3.78

Table S4. Optimized Cartesian coordinates of **10**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-0.900631	2.717975	-1.934365
2	9	0	1.084712	4.499207	-1.578456
3	7	0	3.433290	-0.557609	0.615718
4	6	0	2.141240	-1.122122	1.022846
5	6	0	1.203826	-0.081218	1.669462
6	6	0	4.759286	-3.417969	-1.382940
7	6	0	0.045202	2.452190	-0.995158
8	6	0	4.308752	-1.379187	-0.100289
9	6	0	1.993330	2.017030	0.905385
10	6	0	1.073946	3.380495	-0.814543
11	6	0	3.889613	-2.624385	-0.634505
12	6	0	6.078259	-3.023436	-1.620612
13	6	0	-1.187658	0.308278	-0.464885
14	6	0	6.513225	-1.811140	-1.079186
15	6	0	-5.127180	0.166440	0.830215
16	6	0	-3.907926	-1.488621	-0.768759
17	6	0	2.072638	3.175101	0.137033
18	6	0	-2.488818	0.725044	0.258339
19	6	0	4.004726	0.574683	1.354659
20	6	0	0.959568	1.084660	0.719023
21	6	0	-0.041556	1.269405	-0.243589
22	6	0	5.657611	-1.004938	-0.328341
23	6	0	2.931735	1.488945	1.978259
24	6	0	-5.473167	-1.017696	1.782159
25	6	0	1.970443	0.617146	2.813475
26	6	0	-5.468458	-2.411987	1.123362
27	6	0	-4.264361	-2.663553	0.193092
28	5	0	-3.769352	-0.179963	0.101505
29	6	0	-6.329283	-0.664882	-1.341321
30	6	0	-6.192782	0.440256	-0.274332
31	6	0	-4.982223	-1.203889	-1.864236
32	1	0	2.864578	3.917126	0.253179
33	1	0	6.052185	-0.076773	0.080873
34	1	0	7.543010	-1.481007	-1.234617
35	1	0	6.753613	-3.650299	-2.204439
36	1	0	4.392561	-4.367448	-1.779974
37	1	0	2.876755	-2.986694	-0.468276
38	1	0	1.647453	-1.528375	0.126522
39	1	0	2.280668	-1.967890	1.729880
40	1	0	0.289627	-0.595166	1.998794
41	1	0	-0.883754	-0.694708	-0.128629
42	1	0	-1.385640	0.224575	-1.544709
43	1	0	-5.058428	1.077611	1.451429
44	1	0	-2.977711	-1.768678	-1.293207
45	1	0	-2.295116	0.854655	1.342277
46	1	0	-2.780042	1.746105	-0.060914
47	1	0	4.688780	0.223183	2.156441
48	1	0	4.606927	1.174234	0.654612
49	1	0	3.438044	2.278536	2.552540
50	1	0	-4.735965	-1.013008	2.606194
51	1	0	-6.453502	-0.838300	2.259869
52	1	0	1.296180	1.240271	3.419468
53	1	0	2.493401	-0.090364	3.475813
54	1	0	-5.474207	-3.181008	1.914478
55	1	0	-6.404023	-2.562180	0.566640
56	1	0	-4.437049	-3.583516	-0.394471
57	1	0	-3.374441	-2.871178	0.815454
58	1	0	-6.930447	-1.493821	-0.942038
59	1	0	-6.908411	-0.269089	-2.192790
60	1	0	-7.176303	0.625029	0.194661
61	1	0	-5.919997	1.386101	-0.777009
62	1	0	-4.556083	-0.467688	-2.569831
63	1	0	-5.155599	-2.119677	-2.458052

Table S5. Optimized Cartesian coordinates of **10-F**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-0.426637	3.411292	-1.983942
2	9	0	1.627442	4.894990	-1.096809
3	7	0	3.228228	-0.704888	0.573138
4	6	0	1.820146	-1.140027	0.659178
5	6	0	0.897388	-0.111786	1.339005
6	6	0	4.594141	-3.396912	-1.608537
7	6	0	0.346727	2.894827	-0.989426
8	6	0	4.125758	-1.510952	-0.111858
9	6	0	1.976847	1.981078	1.040922
10	6	0	1.415712	3.671828	-0.530511
11	6	0	3.687976	-2.611291	-0.898493
12	6	0	5.969517	-3.144903	-1.564794
13	6	0	-1.119347	0.796150	-0.899965
14	6	0	6.418654	-2.080683	-0.777777
15	6	0	-4.423434	-0.465065	1.245995
16	6	0	-3.797640	-1.115924	-1.196951
17	6	0	2.257512	3.231357	0.490234
18	6	0	-2.334599	0.891317	0.070824
19	6	0	3.770779	0.276712	1.519804
20	6	0	0.910194	1.203895	0.572287
21	6	0	0.056712	1.627357	-0.459863
22	6	0	5.528168	-1.282680	-0.059419
23	6	0	2.696014	1.197663	2.128467
24	6	0	-4.943142	-1.900440	1.495325
25	6	0	1.549518	0.316526	2.671575
26	6	0	-5.328372	-2.688538	0.221495
27	6	0	-4.325001	-2.549164	-0.947383
28	6	0	-5.986336	0.228482	-0.727784
29	6	0	-5.499179	0.509961	0.713078
30	6	0	-4.865087	-0.132206	-1.730189
31	1	0	3.079900	3.866919	0.824437
32	1	0	5.931654	-0.473845	0.547157
33	1	0	7.488109	-1.863385	-0.711146
34	1	0	6.672046	-3.766439	-2.122649
35	1	0	4.209603	-4.228251	-2.204927
36	1	0	2.629206	-2.855610	-0.958630
37	1	0	1.448793	-1.317967	-0.361167
38	1	0	1.749785	-2.103114	1.204702
39	1	0	-0.102773	-0.561025	1.431742
40	1	0	-0.796865	-0.257535	-0.941994
41	1	0	-1.422268	1.079321	-1.918440
42	1	0	-4.091048	-0.070640	2.229390
43	1	0	-3.020763	-1.202269	-1.985435
44	1	0	-1.958620	1.140022	1.082644
45	1	0	-2.957957	1.752976	-0.227361
46	1	0	4.313977	-0.236152	2.343583
47	1	0	4.507205	0.901734	0.987759
48	1	0	3.178962	1.833605	2.886905
49	1	0	-4.137532	-2.451090	2.011607
50	1	0	-5.813665	-1.900224	2.185849
51	1	0	0.847304	0.909055	3.276439
52	1	0	1.906626	-0.535406	3.273142
53	1	0	-5.433209	-3.759828	0.479156
54	1	0	-6.329999	-2.374905	-0.115001
55	1	0	-4.790357	-2.973147	-1.862816
56	1	0	-3.447371	-3.180908	-0.724983
57	1	0	-6.728778	-0.584891	-0.707588
58	1	0	-6.536354	1.112558	-1.102873
59	1	0	-6.385517	0.534379	1.382449
60	1	0	-5.074607	1.530111	0.743857
61	1	0	-4.347739	0.800274	-2.022951
62	1	0	-5.338192	-0.516578	-2.658731
63	9	0	-2.141823	-1.509069	0.717324
64	5	0	-3.155148	-0.533584	0.200664

Table S6. Optimized Cartesian coordinates of **11**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	2.242709	-2.423356	-1.978245
2	9	0	-0.958911	-1.417000	-3.675560
3	9	0	-3.420665	-2.243432	-4.380589
4	9	0	3.391175	-0.243722	2.107038
5	9	0	0.264411	2.056601	1.112721
6	9	0	3.892972	-4.457231	-1.340230
7	9	0	5.292456	-4.410337	1.008451
8	9	0	5.030405	-2.295424	2.723625
9	9	0	4.278856	0.998719	-1.231948
10	9	0	1.134696	4.589723	1.433909
11	9	0	3.562868	5.351115	0.424955
12	9	0	5.122621	3.541301	-0.909410
13	7	0	-4.355601	0.230476	1.016728
14	6	0	-3.306880	-1.273667	-3.443077
15	6	0	-2.031047	-0.843086	-3.071198
16	6	0	-2.982926	0.733534	-1.564522
17	6	0	-1.825652	0.165853	-2.115298
18	6	0	3.749481	-3.423776	-0.496538
19	6	0	2.730805	-1.247725	0.042670
20	6	0	-0.416303	0.577750	-1.750658
21	1	0	-0.437519	1.593506	-1.332344
22	1	0	0.188805	0.624421	-2.669326
23	6	0	2.890426	-2.365570	-0.795793
24	6	0	-3.147022	1.818019	-0.506172
25	1	0	-2.337609	2.561361	-0.490646
26	6	0	0.269225	-0.394785	-0.755466
27	1	0	0.194887	-1.424801	-1.132162
28	1	0	-0.312930	-0.404080	0.192147
29	6	0	-4.449876	-0.711166	-2.875821
30	1	0	-5.433952	-1.067439	-3.185588
31	6	0	3.493544	-1.262061	1.223815
32	6	0	-4.266999	0.303801	-1.941642
33	6	0	2.231045	1.416691	-0.079742
34	6	0	-4.460560	-0.498858	2.205587
35	6	0	-5.293907	1.091102	-1.144720
36	1	0	-6.251674	1.225666	-1.668138
37	6	0	4.473932	-3.398659	0.699463
38	6	0	-5.568302	0.404599	0.208161
39	1	0	-6.335573	0.988419	0.759962
40	1	0	-5.997434	-0.589559	0.010381
41	6	0	4.342670	-2.312893	1.570964
42	6	0	-5.600891	-1.291817	2.491416
43	1	0	-6.442027	-1.323097	1.801305
44	6	0	1.465324	2.389229	0.581344
45	6	0	-4.524865	2.403573	-0.884808
46	1	0	-4.967813	3.013047	-0.081833
47	1	0	-4.459918	3.012219	-1.798809
48	6	0	-3.259368	1.198436	0.901985
49	1	0	-2.317513	0.678315	1.133147
50	1	0	-3.366629	2.017182	1.644963
51	6	0	3.934514	3.164103	-0.412720
52	6	0	3.476994	1.853571	-0.560220
53	6	0	-5.677324	-2.051300	3.658884
54	1	0	-6.572162	-2.652502	3.835879
55	6	0	-3.429848	-0.482616	3.179548
56	1	0	-2.545714	0.137087	3.041721
57	6	0	3.138289	4.092640	0.264537
58	6	0	-4.641415	-2.046368	4.596544
59	1	0	-4.709537	-2.640176	5.509016
60	6	0	1.895158	3.702145	0.772681
61	6	0	-3.523378	-1.248555	4.342096
62	1	0	-2.704461	-1.208288	5.064136
63	5	0	1.737311	-0.070022	-0.290231

Table S7. Optimized Cartesian coordinates of **11-F**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-2.624225	2.721620	0.450934
2	9	0	0.284947	4.175665	-0.475275
3	9	0	2.632843	5.438615	-0.766334
4	9	0	-4.004220	-1.768325	1.361852
5	9	0	0.040811	-2.686969	1.197230
6	9	0	-5.160211	3.530873	0.693888
7	9	0	-7.158470	1.736275	1.268843
8	9	0	-6.543466	-0.920718	1.597256
9	9	0	-2.874101	-0.407448	-1.839518
10	9	0	0.267057	-4.695313	-0.557222
11	9	0	-1.047399	-4.608990	-2.965988
12	9	0	-2.614229	-2.435152	-3.579303
13	7	0	4.379176	-0.267524	0.193368
14	6	0	2.590139	4.091665	-0.957085
15	6	0	1.369155	3.428629	-0.801486
16	6	0	2.410191	1.372054	-1.363735
17	6	0	1.232665	2.042531	-0.992899
18	6	0	-4.860148	2.218869	0.856137
19	6	0	-3.164910	0.423981	0.894361
20	6	0	-0.100392	1.352980	-0.813402
21	1	0	-0.130173	0.492858	-1.502424
22	1	0	-0.904883	2.034447	-1.124186
23	6	0	-3.542843	1.759148	0.738328
24	6	0	2.647815	-0.109826	-1.628453
25	1	0	1.764315	-0.643630	-2.004638
26	6	0	-0.365402	0.863518	0.628834
27	1	0	-0.460403	1.736288	1.295846
28	1	0	0.529294	0.319465	0.984367
29	6	0	3.749425	3.409655	-1.323341
30	1	0	4.684620	3.959660	-1.444346
31	6	0	-4.228740	-0.440298	1.188920
32	6	0	3.633835	2.038442	-1.536117
33	6	0	-1.474606	-1.450230	-0.197108
34	6	0	4.847618	-0.767889	1.406726
35	6	0	4.690108	1.020441	-1.935328
36	1	0	5.486265	1.437118	-2.571317
37	6	0	-5.878473	1.314720	1.148330
38	6	0	5.344273	0.389261	-0.691726
39	1	0	6.131121	-0.324380	-1.022669
40	1	0	5.850462	1.185139	-0.121498
41	6	0	-5.558549	-0.032679	1.316303
42	6	0	6.161080	-0.489214	1.868540
43	1	0	6.845158	0.104872	1.264997
44	6	0	-0.671299	-2.572001	0.046688
45	6	0	3.823148	-0.052820	-2.628098
46	1	0	4.340394	-1.019131	-2.742305
47	1	0	3.484284	0.290126	-3.617255
48	6	0	3.133290	-0.830895	-0.353995
49	1	0	2.349032	-0.749895	0.411599
50	1	0	3.260609	-1.910183	-0.579414
51	6	0	-1.977221	-2.490610	-2.384293
52	6	0	-2.095024	-1.456292	-1.450801
53	6	0	6.609660	-0.965694	3.101258
54	1	0	7.626696	-0.721707	3.419450
55	6	0	4.033793	-1.581146	2.238241
56	1	0	3.023551	-1.849009	1.934944
57	6	0	-1.183716	-3.595618	-2.079990
58	6	0	5.788856	-1.746310	3.918730
59	1	0	6.145277	-2.116518	4.881508
60	6	0	-0.521839	-3.633236	-0.853305
61	6	0	4.499767	-2.046871	3.466388
62	1	0	3.833355	-2.660301	4.077269
63	9	0	-1.436874	-0.695754	2.240066
64	5	0	-1.605059	-0.187504	0.901782

Table S8. Optimized Cartesian coordinates of BPh_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000110	-0.000075	0.000132
2	6	0	0.182972	1.558776	0.000043
3	6	0	-0.733063	2.410996	0.660751
4	6	0	1.271644	2.175222	-0.660844
5	6	0	-0.564169	3.797040	0.676355
6	1	0	-1.584019	1.971213	1.186405
7	6	0	1.428709	3.562650	-0.676722
8	1	0	1.997393	1.549963	-1.186372
9	6	0	0.514243	4.377209	-0.000258
10	1	0	-1.277318	4.428591	1.210995
11	1	0	2.268838	4.011533	-1.211480
12	1	0	0.641761	5.462093	-0.000380
13	6	0	-1.441627	-0.621009	0.000152
14	6	0	-2.519643	0.012695	-0.661867
15	6	0	-1.721857	-1.839669	0.662180
16	6	0	-3.799693	-0.545080	-0.677594
17	1	0	-2.340948	0.953211	-1.188501
18	6	0	-3.006650	-2.386435	0.677966
19	1	0	-0.915731	-2.356062	1.188815
20	6	0	-4.048113	-1.743510	0.000185
21	1	0	-4.608302	-0.042597	-1.213265
22	1	0	-3.197129	-3.319196	1.213651
23	1	0	-5.051374	-2.175596	0.000225
24	6	0	1.258425	-0.937982	0.000140
25	6	0	2.453519	-0.571658	0.663104
26	6	0	1.249177	-2.187819	-0.662994
27	6	0	3.569609	-1.410715	0.678638
28	1	0	2.497176	0.384232	1.190567
29	6	0	2.372427	-3.017234	-0.678950
30	1	0	0.345607	-2.503015	-1.190308
31	6	0	3.534112	-2.633479	-0.000289
32	1	0	4.472348	-1.109613	1.214998
33	1	0	2.342024	-3.968277	-1.215488
34	1	0	4.410092	-3.286084	-0.000495

Table S9. Optimized Cartesian coordinates of BPh_3-F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000253	-0.000274	0.735952
2	9	0	0.000427	0.000167	2.201826
3	6	0	-1.526800	-0.346361	0.230514
4	6	0	-2.401121	-1.056993	1.079811
5	6	0	-2.041340	0.007297	-1.033359
6	6	0	-3.700494	-1.403764	0.693183
7	1	0	-2.041747	-1.333076	2.075019
8	6	0	-3.337658	-0.337398	-1.437662
9	1	0	-1.416252	0.591425	-1.716710
10	6	0	-4.177506	-1.049111	-0.574542
11	1	0	-4.347809	-1.954365	1.383910
12	1	0	-3.698089	-0.040113	-2.427854
13	1	0	-5.192476	-1.317001	-0.882172
14	6	0	0.463152	1.494624	0.229598
15	6	0	1.027424	1.763321	-1.033967
16	6	0	0.283872	2.607259	1.078505
17	6	0	1.376981	3.058366	-1.438206
18	1	0	1.221323	0.929967	-1.717220
19	6	0	0.633123	3.905972	0.691939
20	1	0	-0.135745	2.434012	2.073339
21	6	0	1.179658	4.141664	-0.575430
22	1	0	1.815293	3.221823	-2.428122
23	1	0	0.479103	4.741943	1.382383
24	1	0	1.455099	5.154611	-0.883052
25	6	0	1.062893	-1.149079	0.230189
26	6	0	2.117899	-1.547134	1.078272
27	6	0	1.012357	-1.774507	-1.032097
28	6	0	3.068687	-2.498376	0.692044
29	1	0	2.178414	-1.095251	2.072214
30	6	0	1.959862	-2.724163	-1.436064
31	1	0	0.192347	-1.527979	-1.714524
32	6	0	2.998478	-3.091908	-0.574163
33	1	0	3.871090	-2.780629	1.381803
34	1	0	1.881466	-3.187327	-2.425056
35	1	0	3.738599	-3.836420	-0.881547

Figure S34. Depictions of HOMO (left) and LUMO (right) of **10**

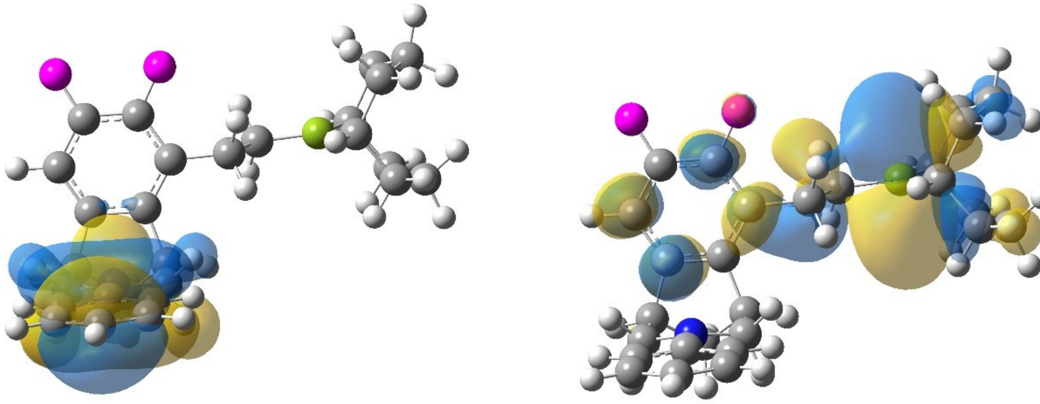
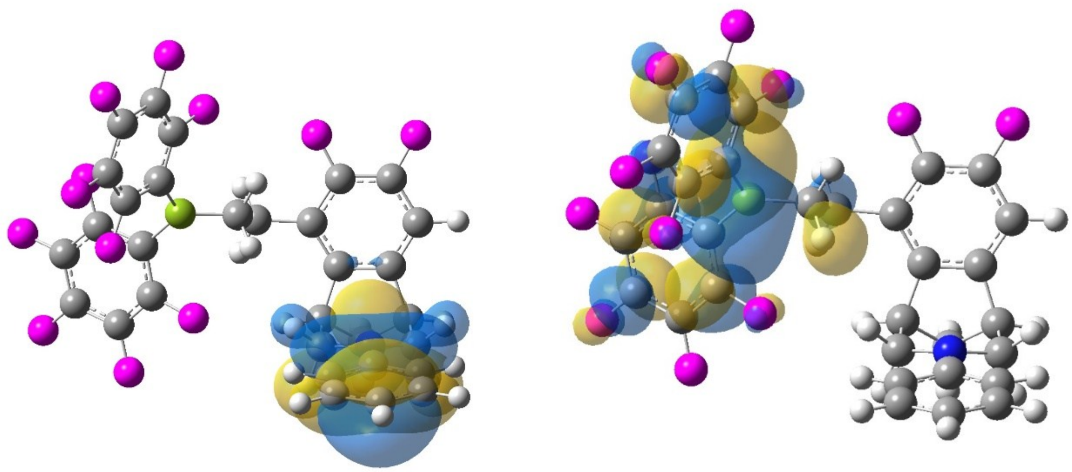


Figure S35. Depictions of HOMO (left) and LUMO (right) of **11**



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