Electronic Supplementary Material (ESI) for Dalton Transactions.

Reactions of Carbene-Stabilized Borenium Cations

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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 or an Innovative Technology 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. Spectrograde chloroform was obtained from ACP Chemicals, dried over CaH_2, and vacuum-transferred into Young bombs. Tetrahydrofuran was obtained from Sigma-Aldrich, dried over Na/benzophenone, and vacuum-transferred into Young bombs. Dichloromethane-d_2 and chloroform-d were obtained from Cambridge Isotope Laboratories, dried over CaH_2, and vacuum-transferred into Young bombs. All solvents were degassed after purification 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. 1,3-dibenzylimidazolium bromide[1] 1,3-dibenzylimidazolyl-2-ylidene-borane[2], di-t-butyl(ethynyl)phosphane,[3] di-tert-butyl(phenylethynyl)phosphane[3] and dimesityl(1-phenylvinyl)phosphane[4] were prepared using literature methods.

NMR spectra were recorded on a Bruker Avance 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. GC-MS spectra were obtained on an Agilent Technologies 5975C VL MSD with Triple Axis Detector and 7890A GC System. Column Agilent 19091S-433 (30m x 250 µm x 0.25 µm). Helium was used as the carrier gas. Elemental analyses (C, H, N) were performed in-house with a Perkin Elmer 2400 Series II CHNS Analyzer.

NMR Spectra of 4

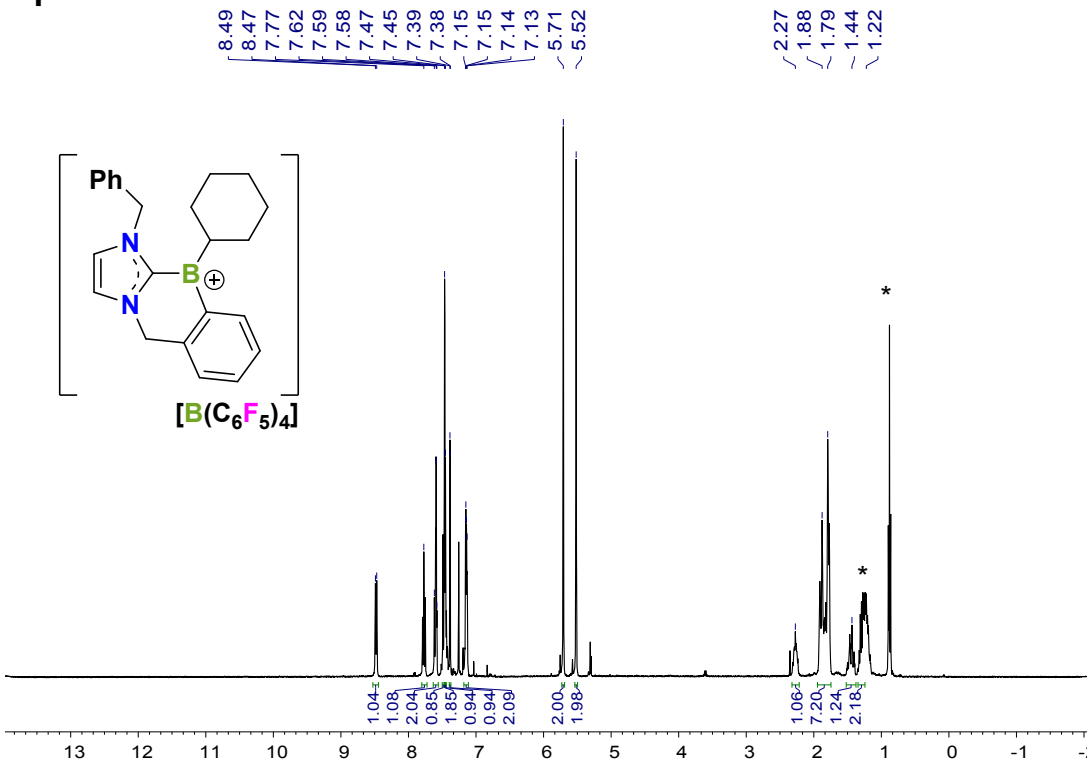

Figure S1. ^{1}H NMR spectrum of **4**. (* residual pentane)

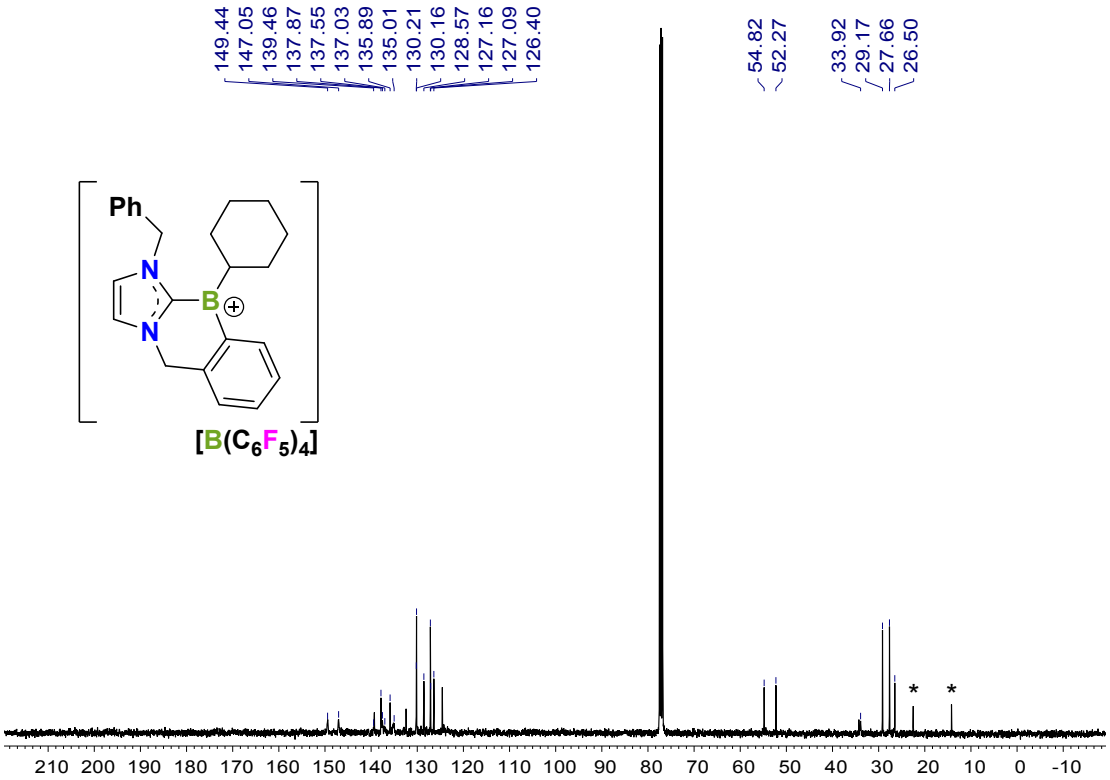

Figure S2. ^{13}C{H} NMR spectrum of **4**. (* residual pentane)

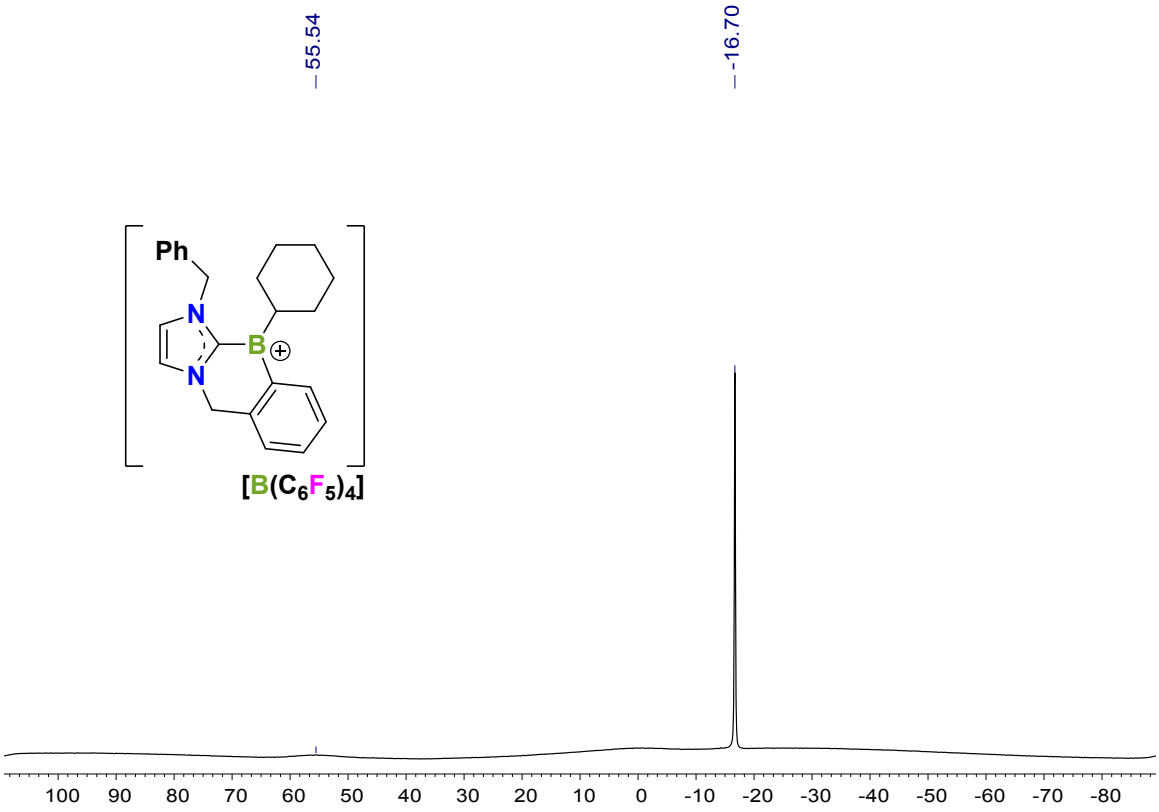

Figure S3. ^{11}B NMR spectrum of **4**.

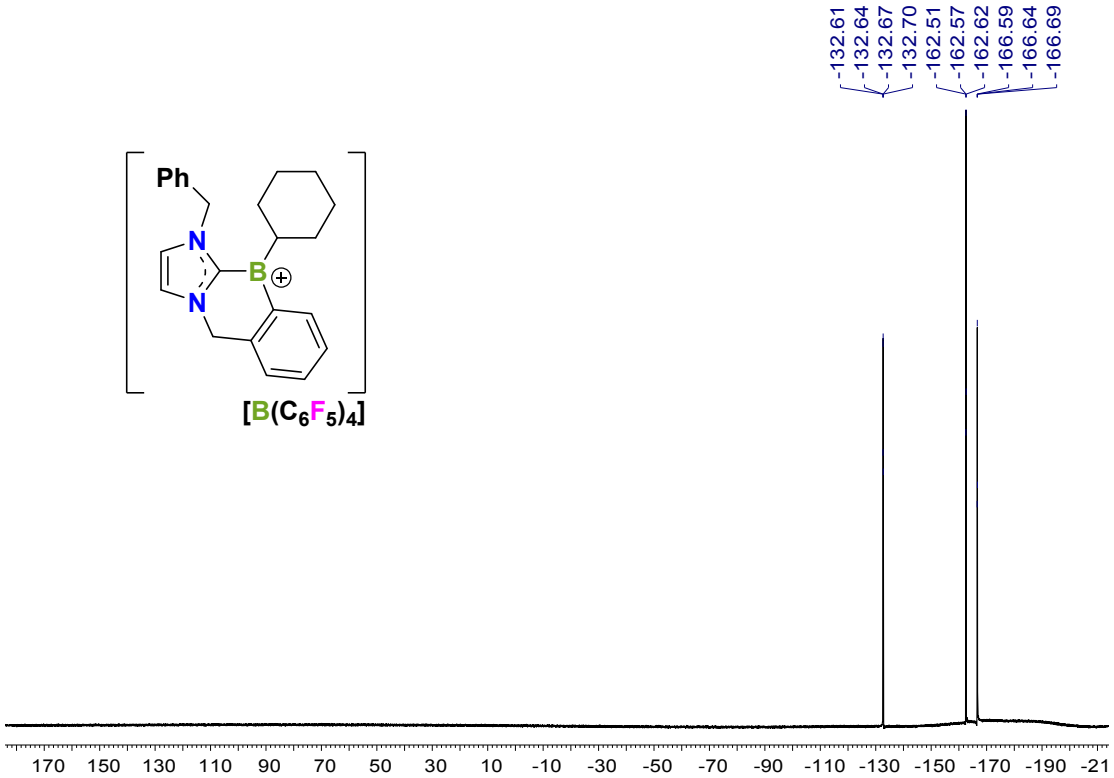

Figure S4. ^{19}F NMR spectrum of **4**.

NMR Spectra of 5

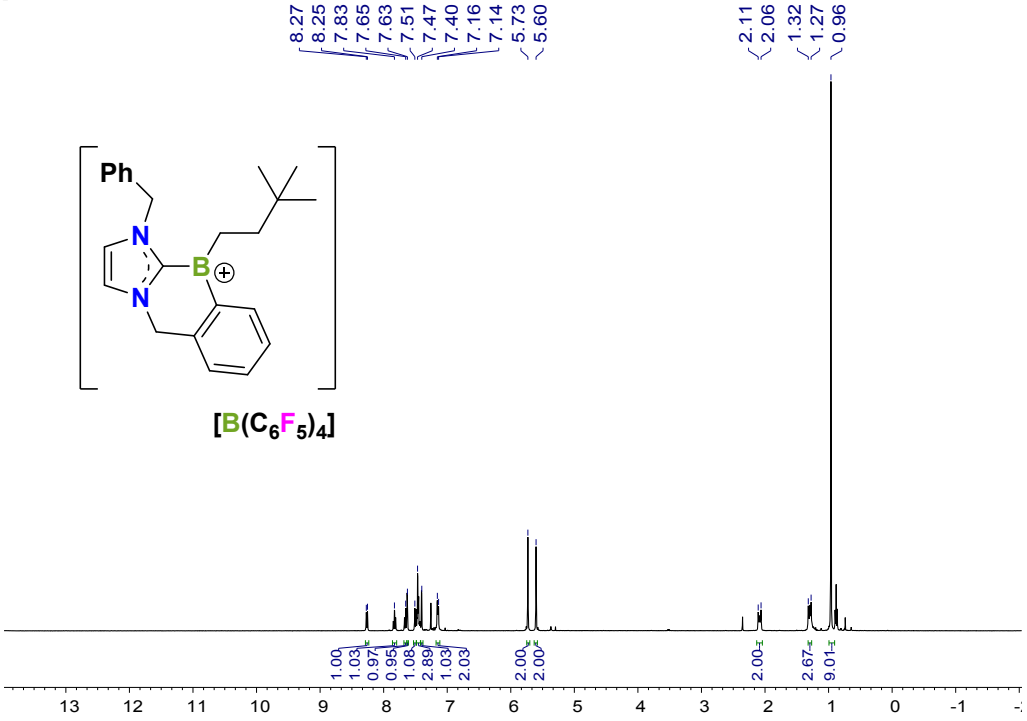

Figure S5.^{1}H NMR spectrum of **5**.

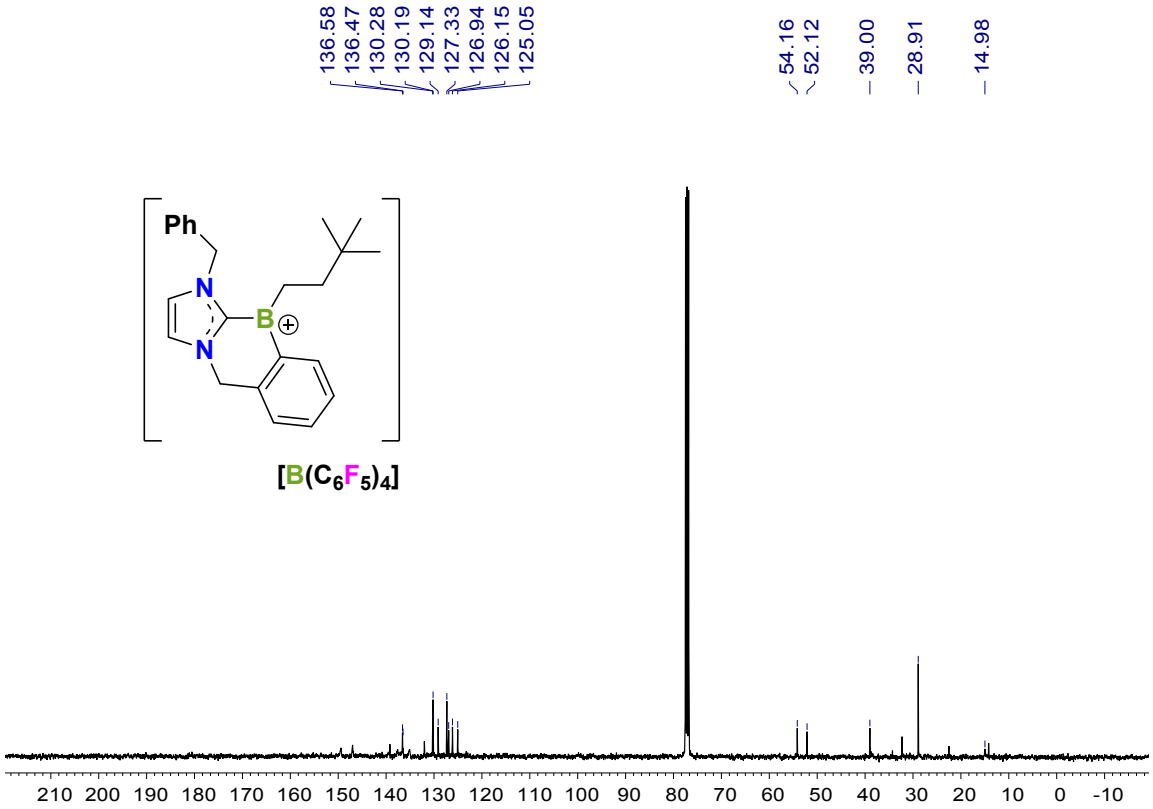

Figure S6. ^{13}C{H} NMR spectrum of **5** (in $CDCl_3$)

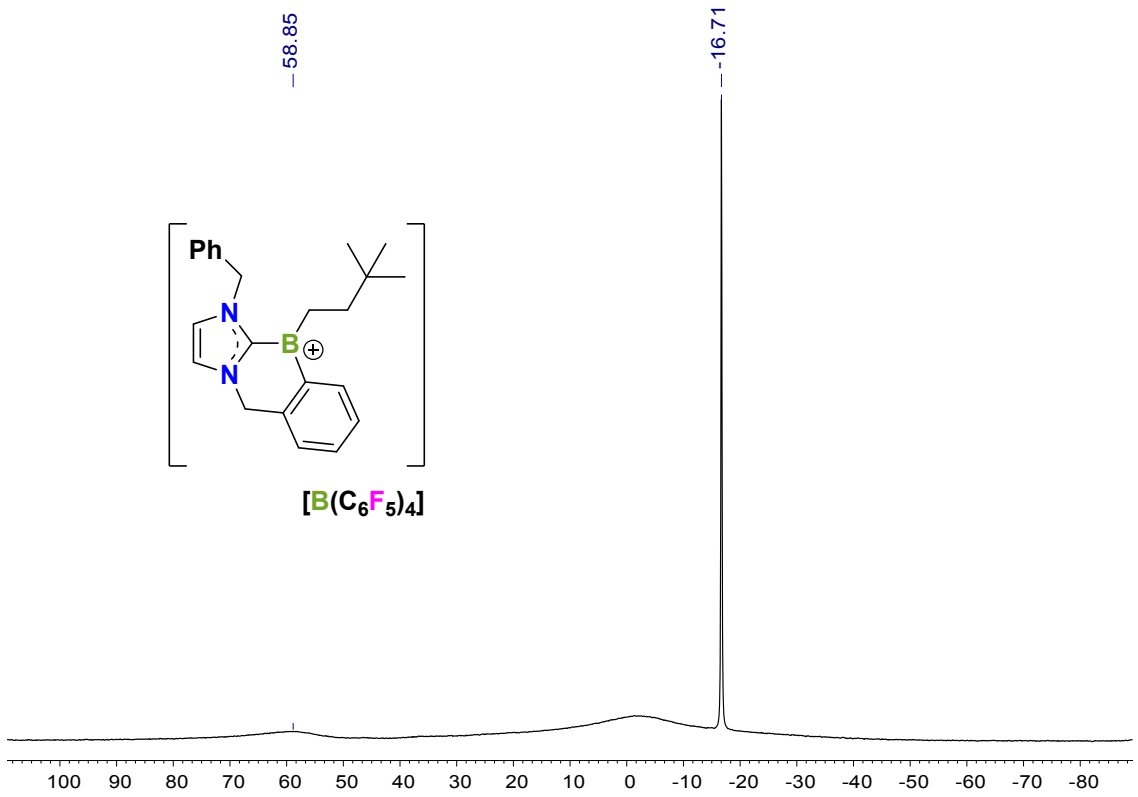

Figure S7. ^{11}B NMR spectrum of **5**.

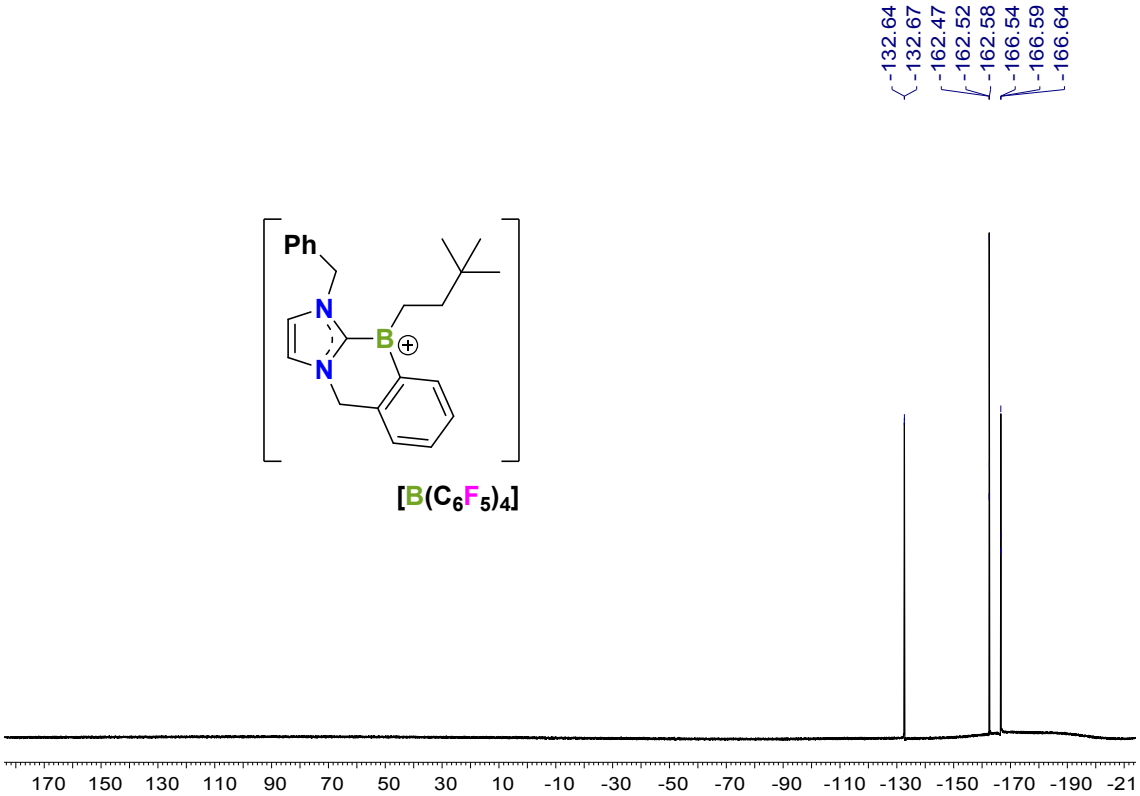

Figure S8. ^{19}F NMR spectrum of **5**.

In-situ NMR Spectra of Oxidation of 4

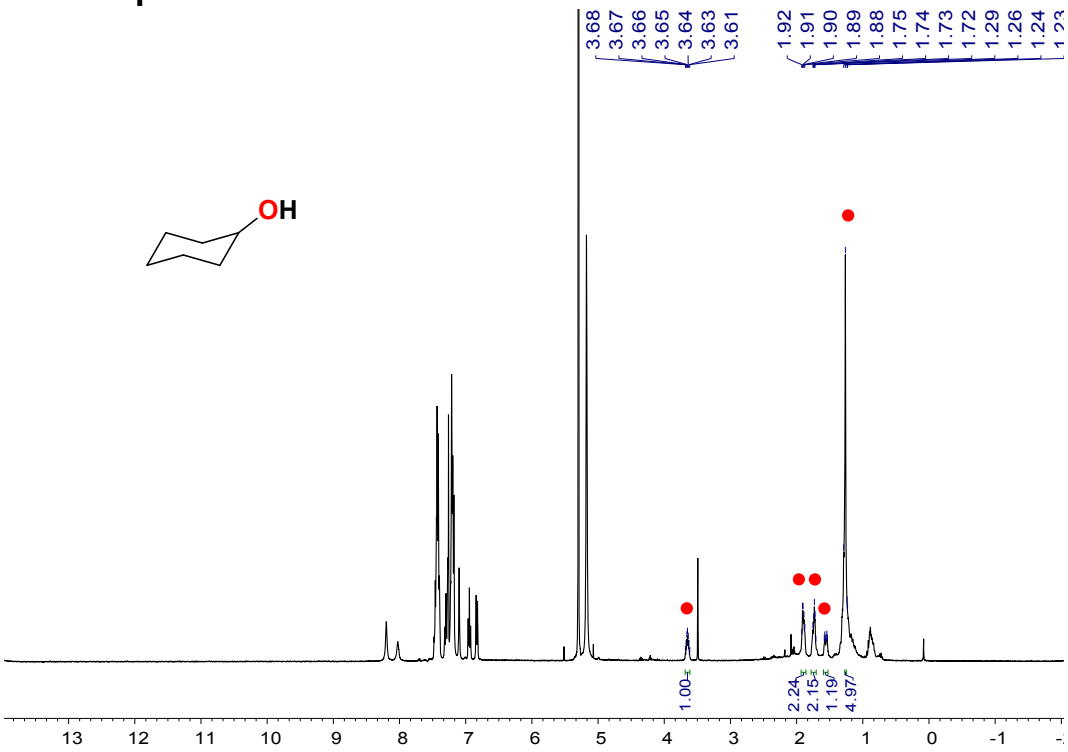

Figure S9. In-situ ^{1}H NMR spectrum of cyclohexanol in the reaction mixture.

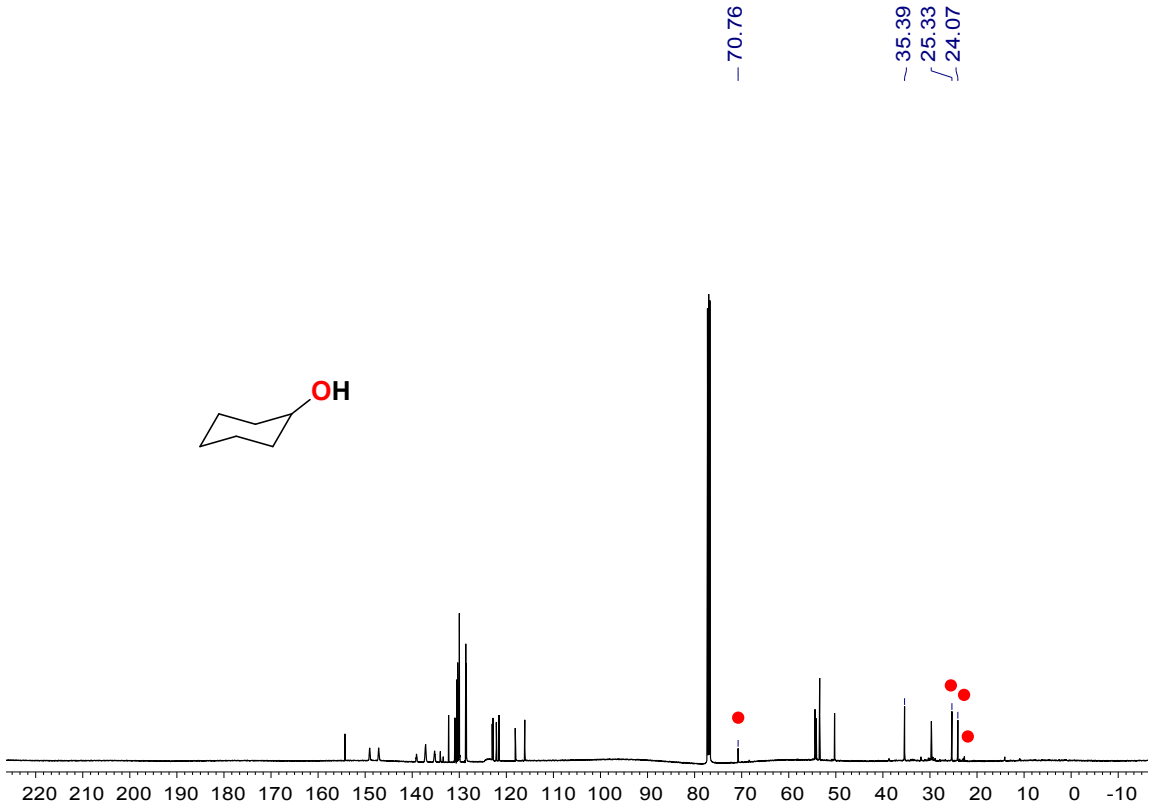

Figure S10. In-situ $^{13}C\{H\}$ NMR spectrum of cyclohexanol in the reaction mixture. (in $CDCl_3$).

In-situ NMR Spectra of Oxidation of 5

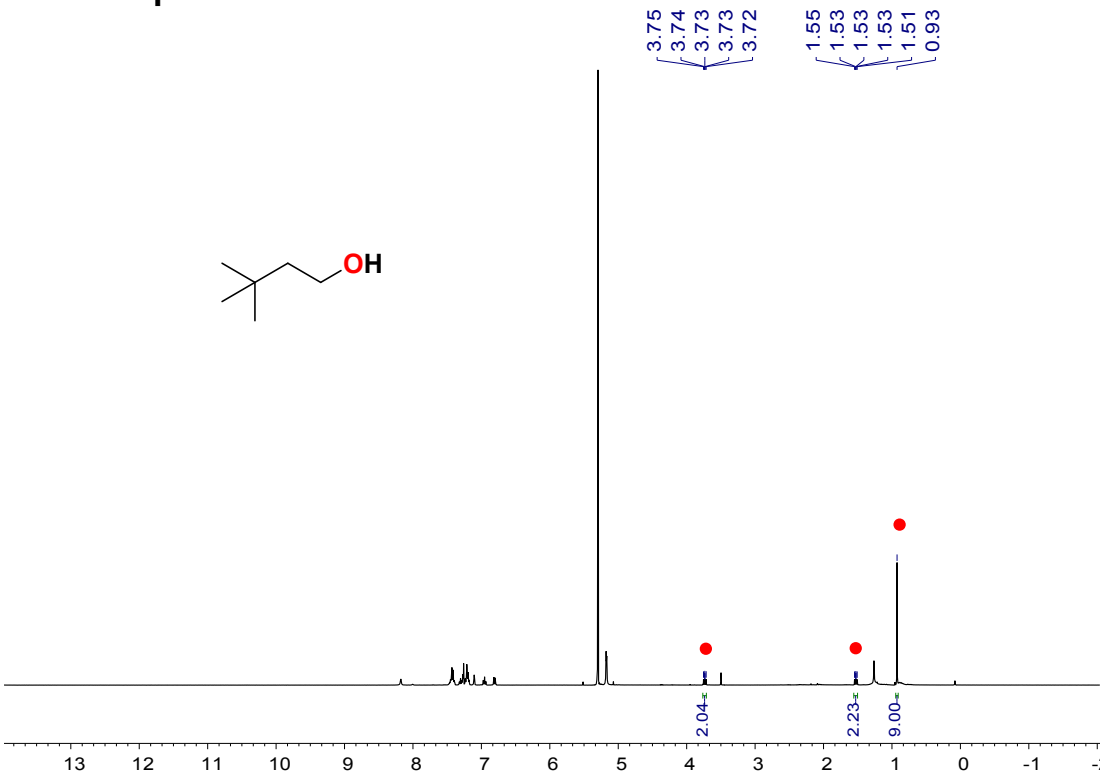

Figure S11. ^{1}H NMR spectrum of 3,3-dimethylbutan-1-ol in the reaction mixture..

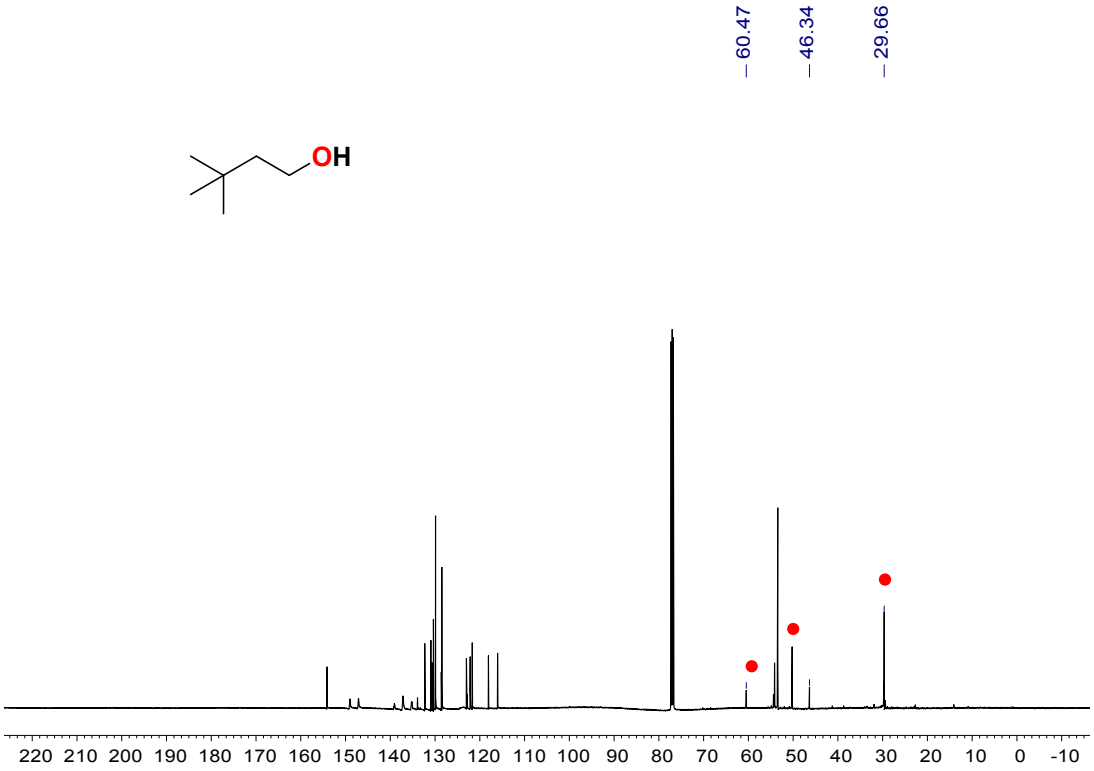

Figure S12. $^{13}C\{H\}$ NMR spectrum 3,3-dimethylbutan-1-ol in the reaction mixture.

NMR Spectra of 6

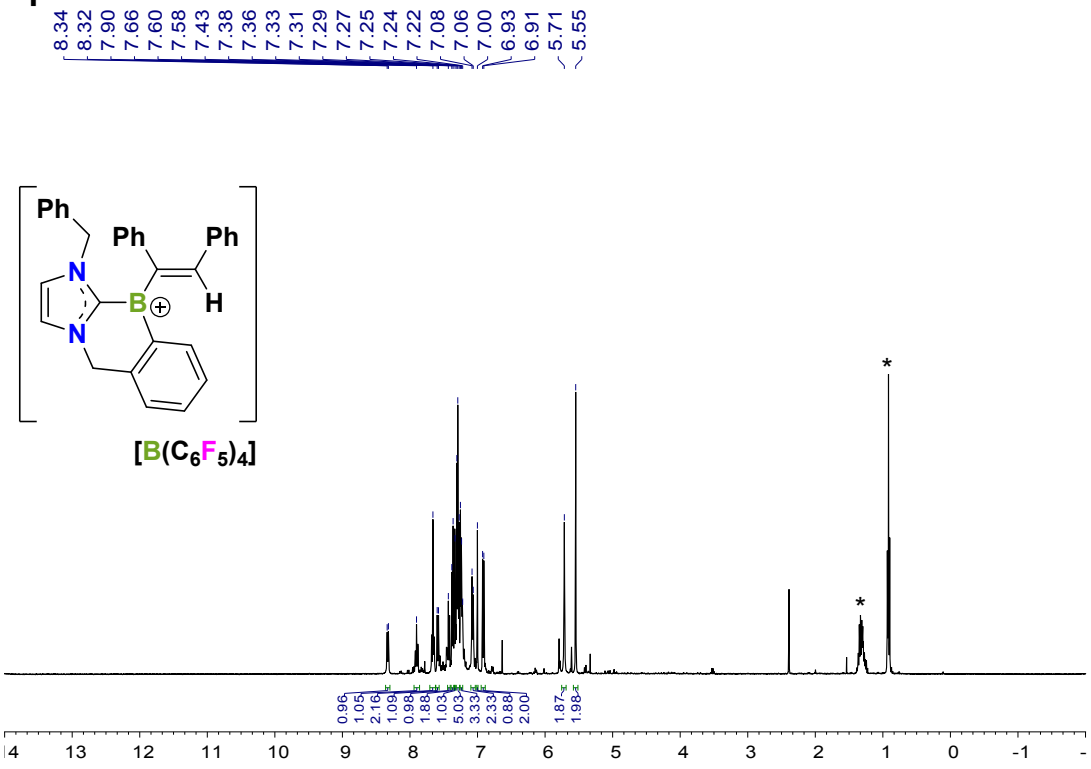

Figure S13. ^{1}H NMR spectrum of **6** with minor unknown impurities. (* residual pentane)

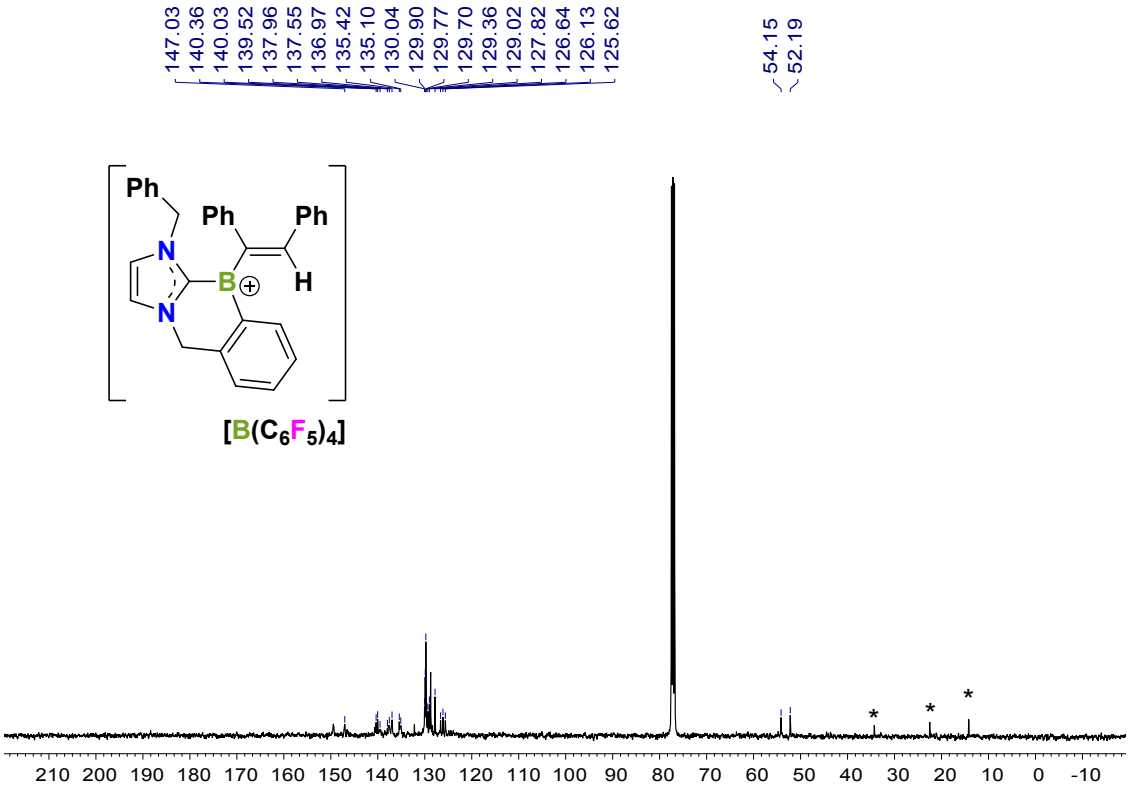

Figure S14. ^{13}C{H} NMR spectrum of **6**. (* residual pentane) (in $CDCl_3$)

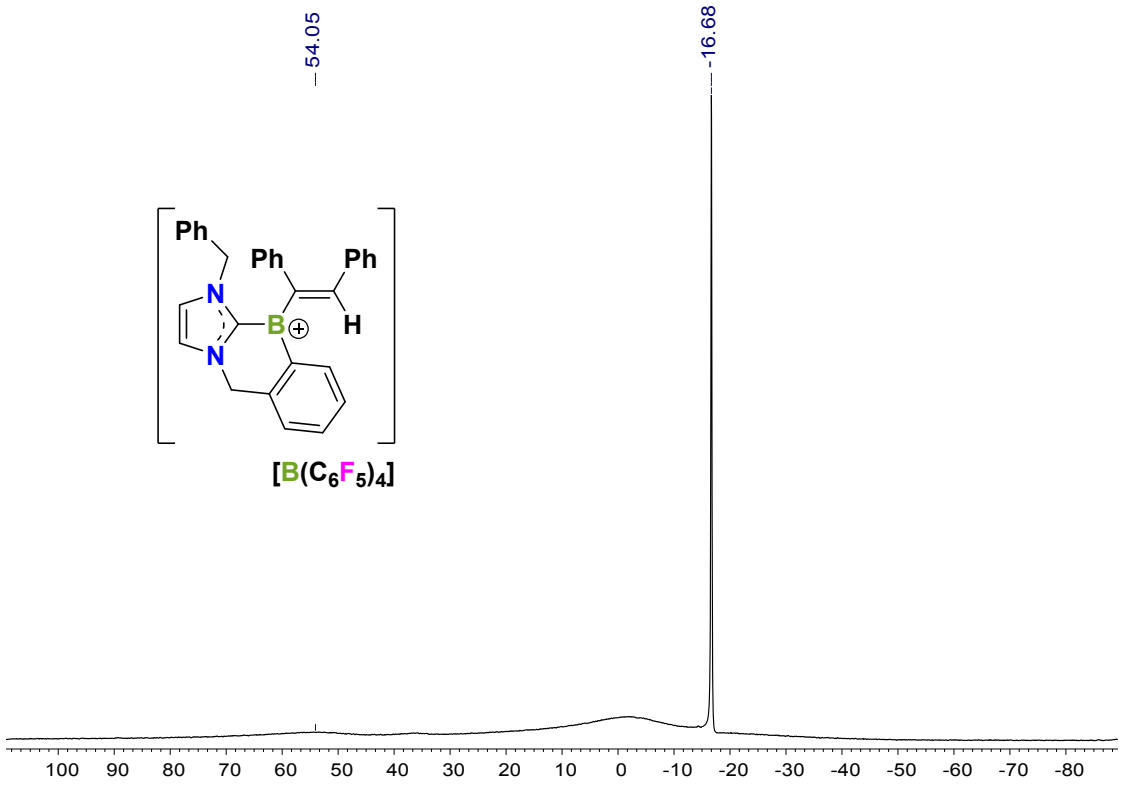

Figure S15. ^{11}B NMR spectrum of **6**.

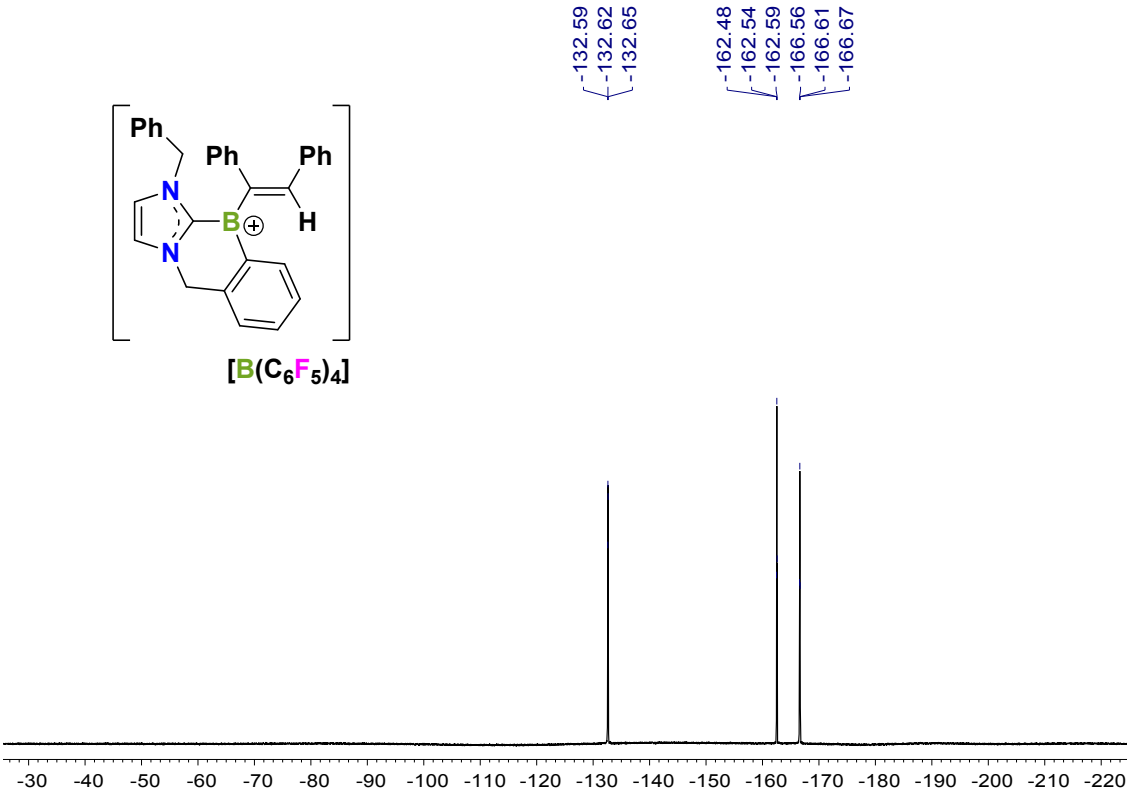

Figure S16. ^{19}F NMR spectrum of **6**.

NMR Spectra of 7

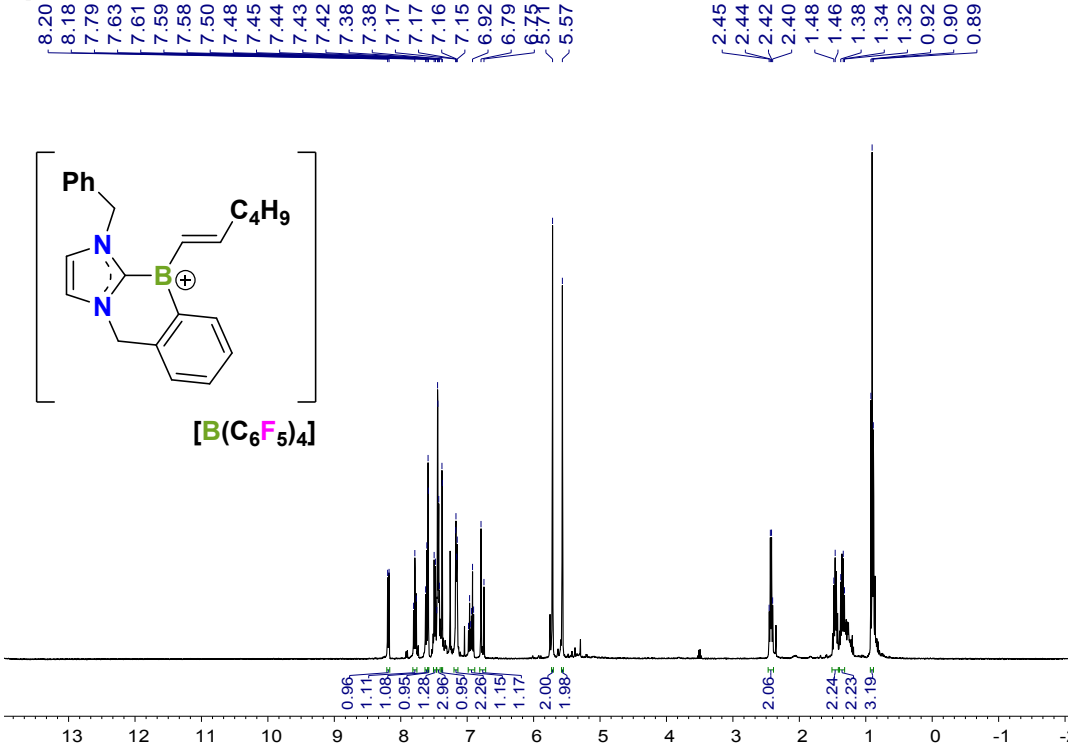

Figure S17. ^{1}H NMR spectrum of **7**.

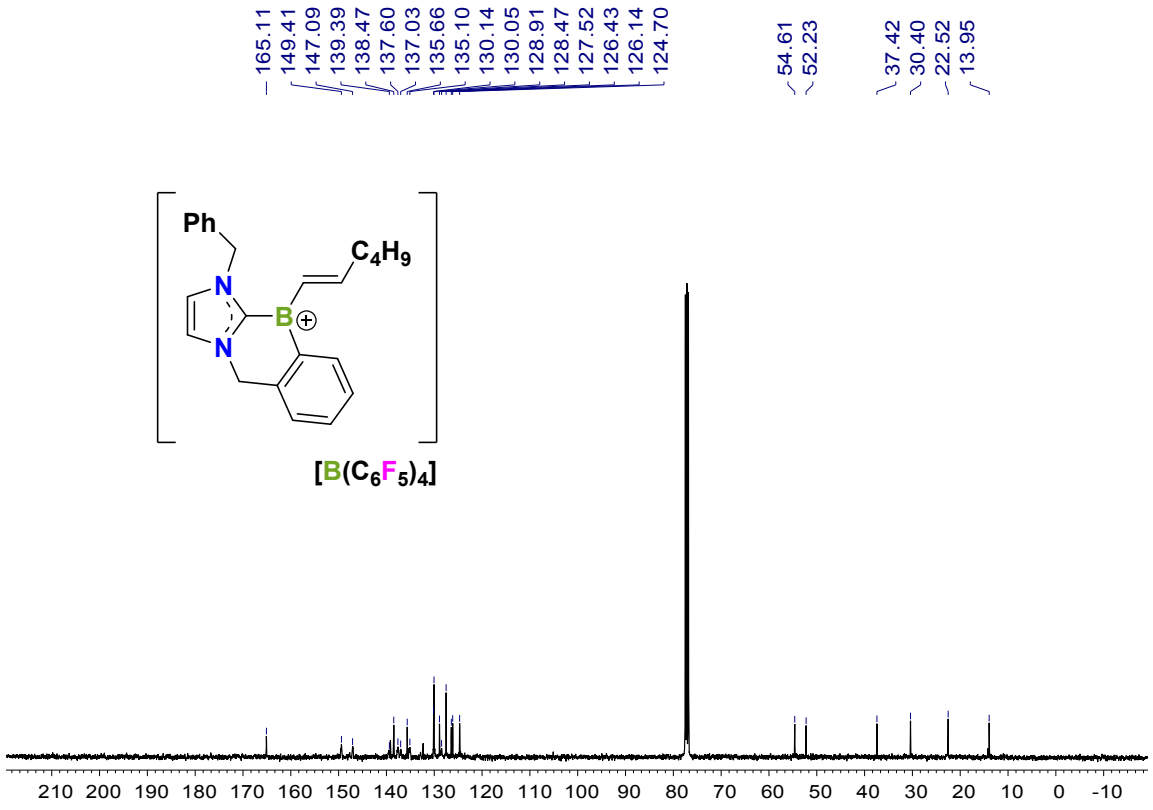

Figure S18. ^{13}C{H} NMR spectrum of **7**. (in $CDCl_3$)

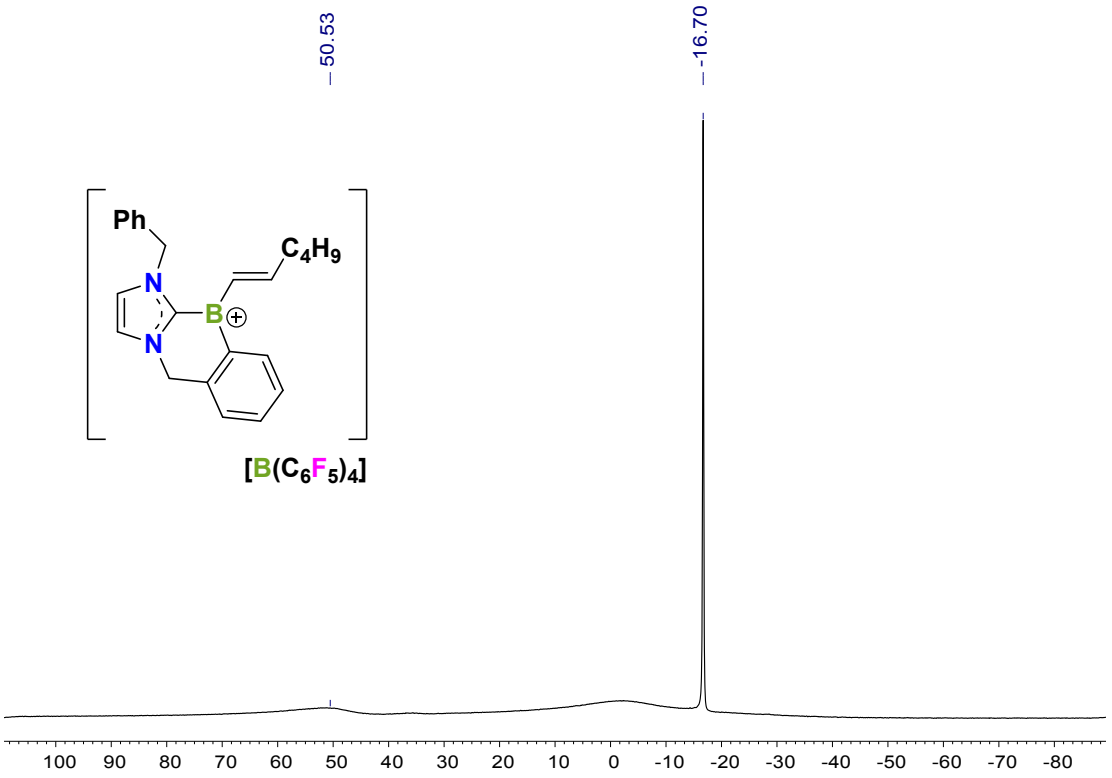

Figure S19. ^{11}B NMR spectrum of **7**.

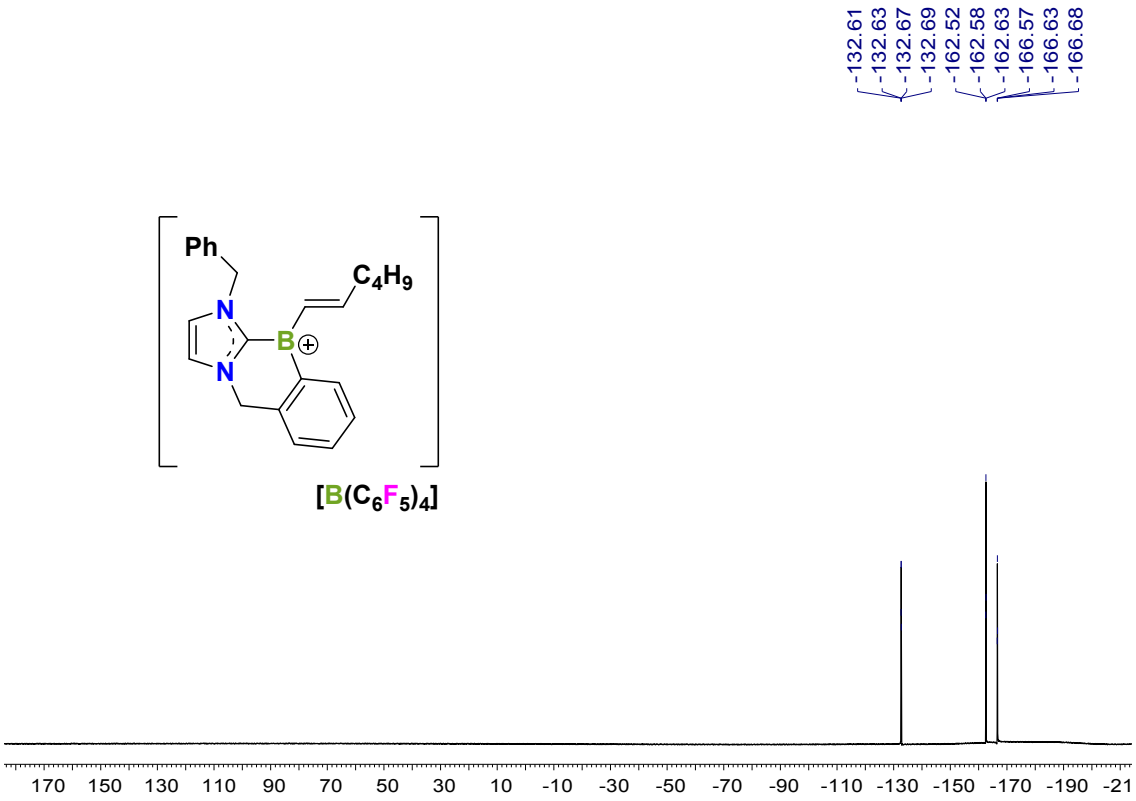

Figure S20. ^{19}F NMR spectrum of **7**.

NMR Spectra of 8a/8b

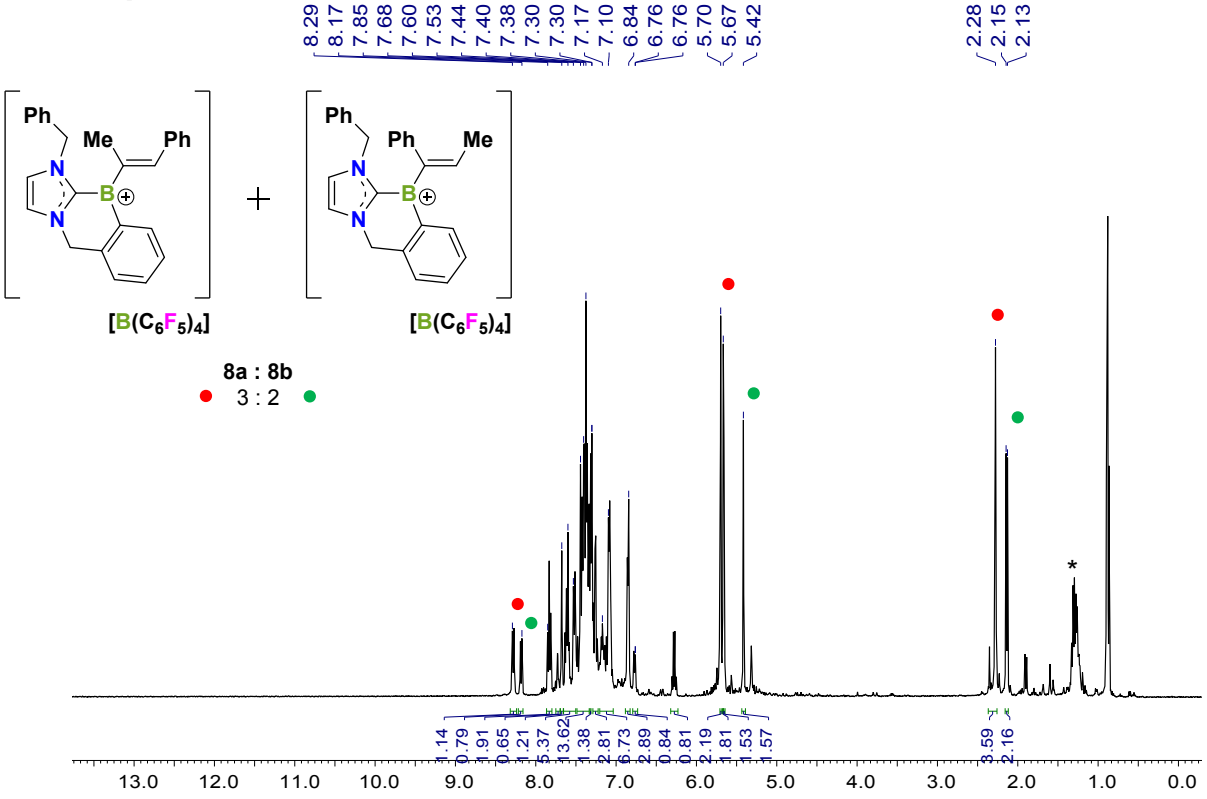

Figure S21. ^{1}H NMR spectrum of **8a/8b** with minor unknown impurities. (* residual pentane)

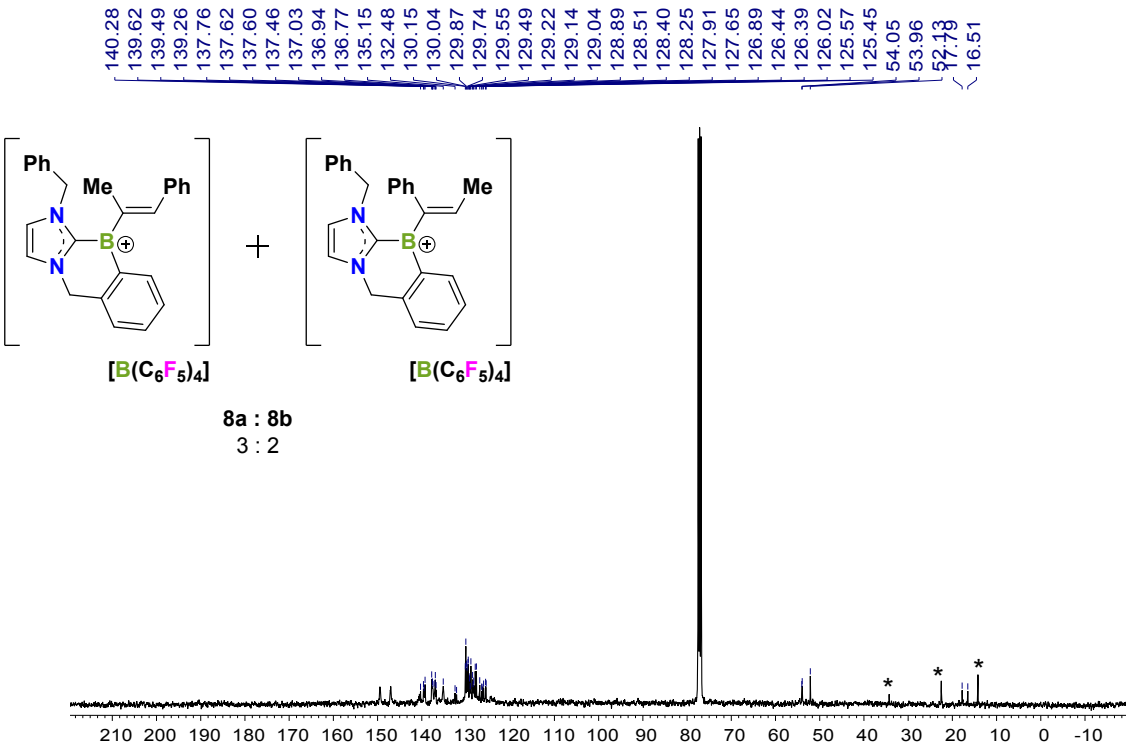

Figure S22. $^{13}C\{H\}$ NMR spectrum of **8a/8b**. (* residual pentane) (in $CDCl_3$)

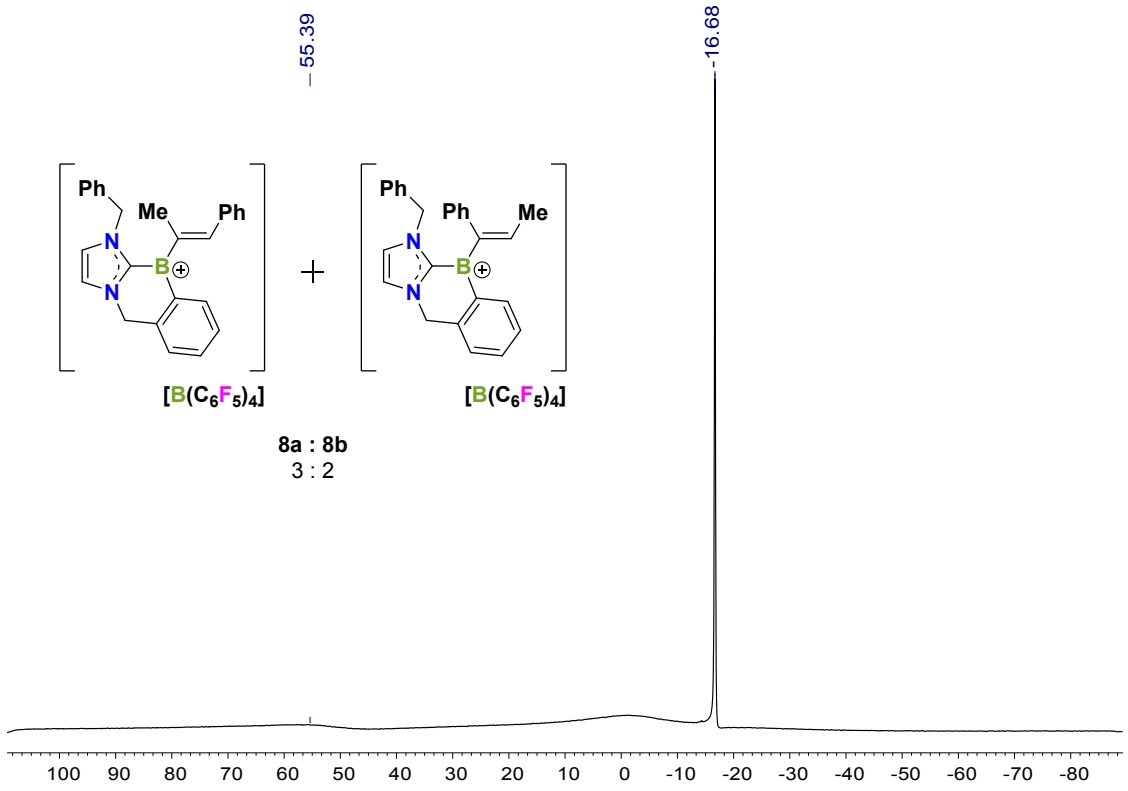

Figure S23. ^{11}B NMR spectrum of **8a/8b**.

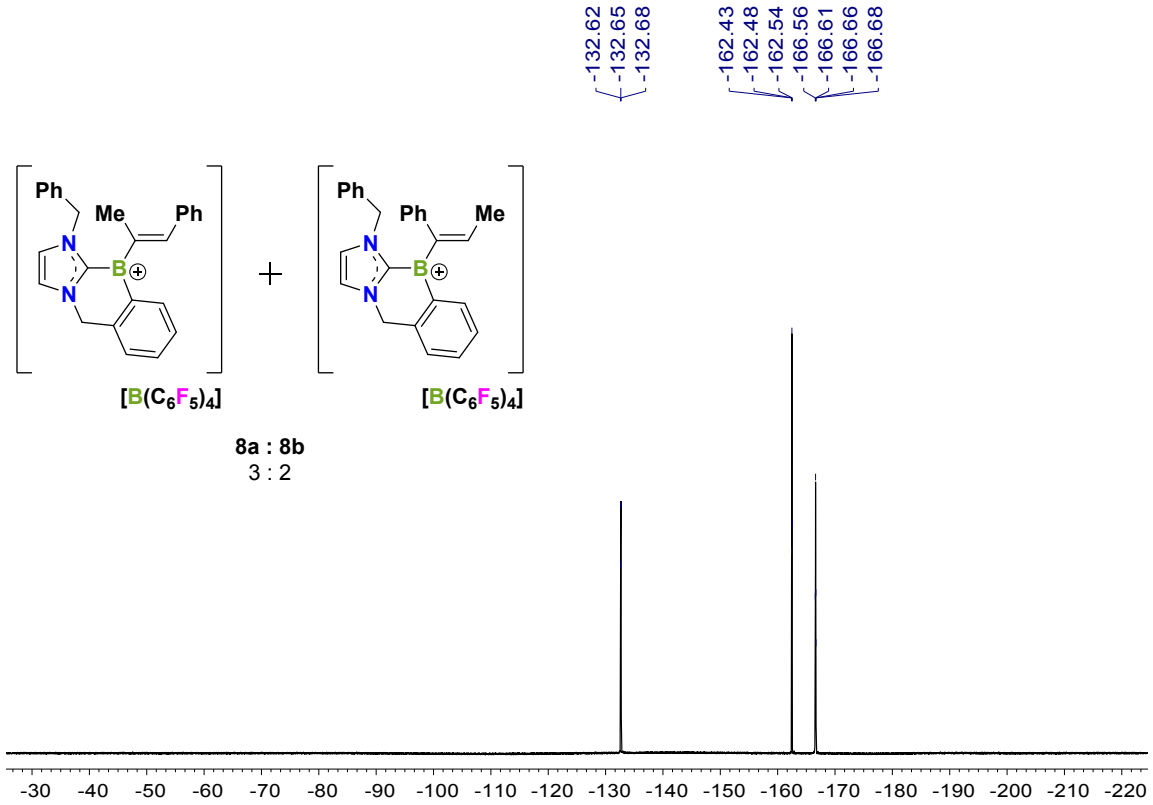

Figure S24. ^{19}F NMR spectrum of **8a/8b**.

NMR Spectra of 9

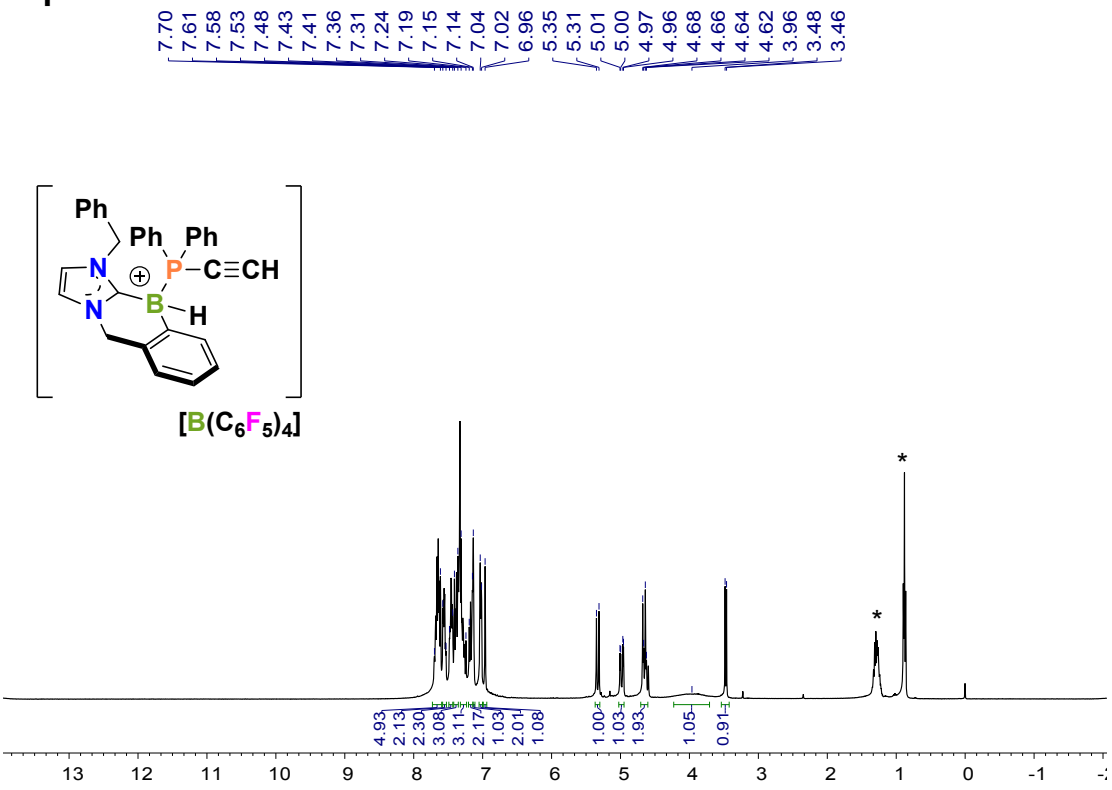

Figure S25. ^{1}H NMR spectrum of **9**. (* residual pentane)

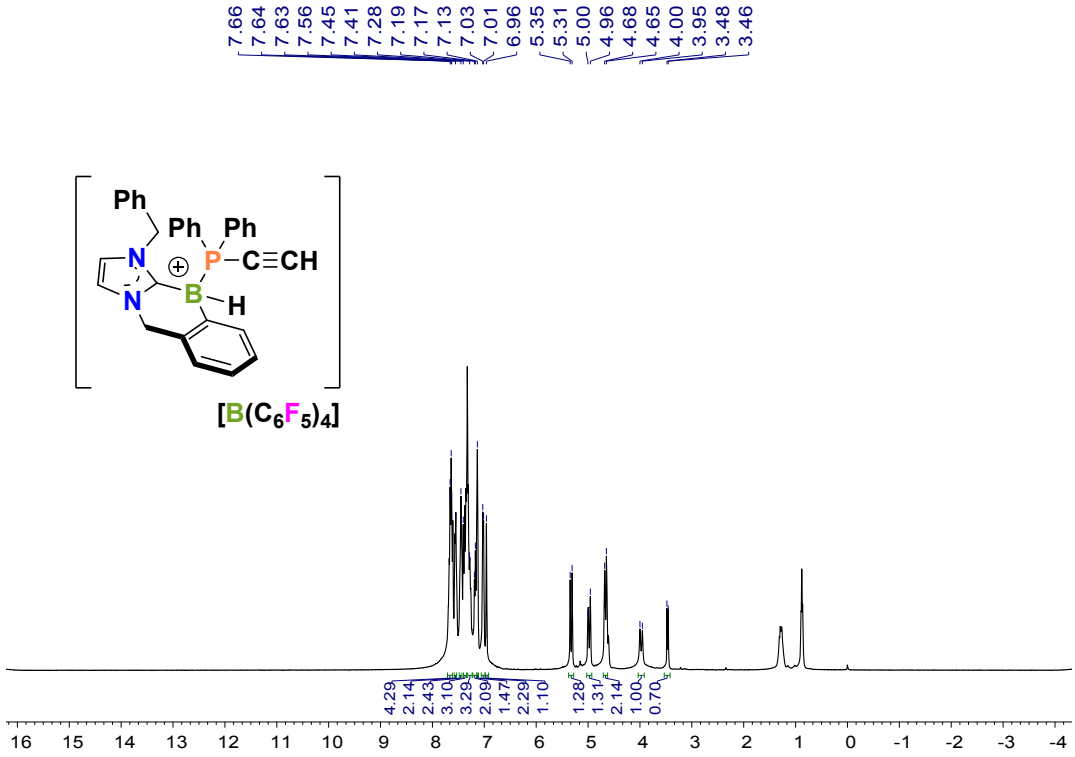

Figure S26. $^{1}H\{^{11}B\}$ NMR spectrum of **9**.

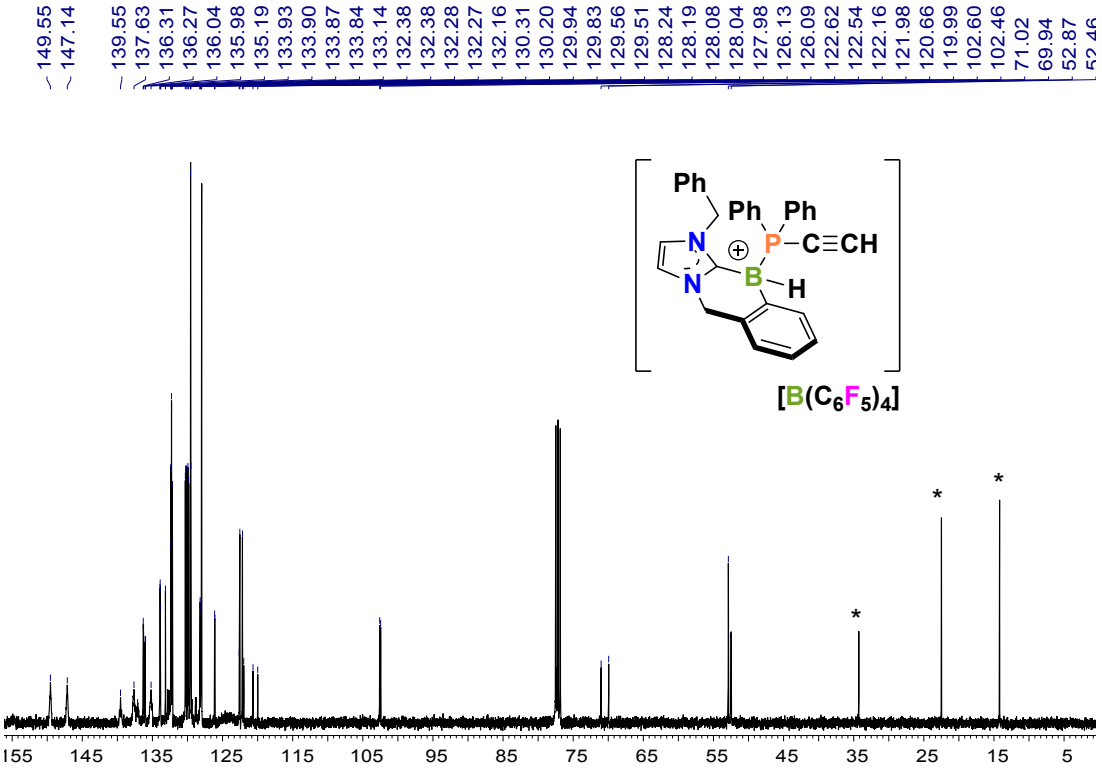

Figure S27. $^{13}C\{H\}$ NMR spectrum of **9**. (* residual pentane) (in $CDCl_3$)

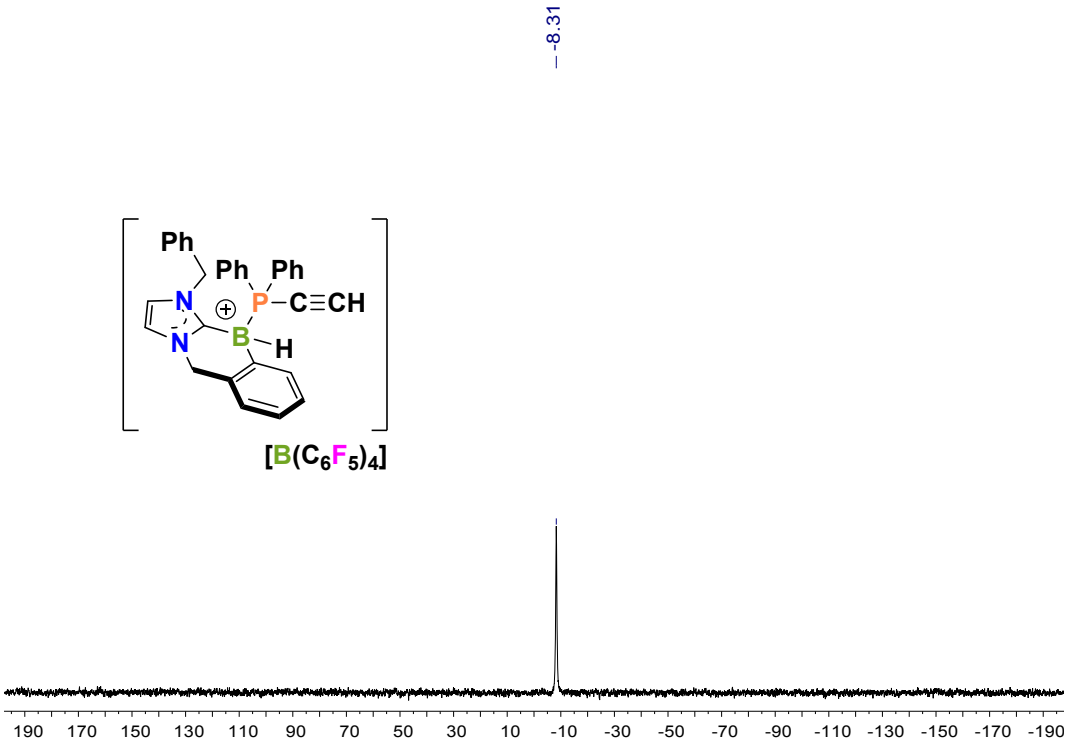

Figure S28. $^{31}P\{H\}$ NMR spectrum of **9**.

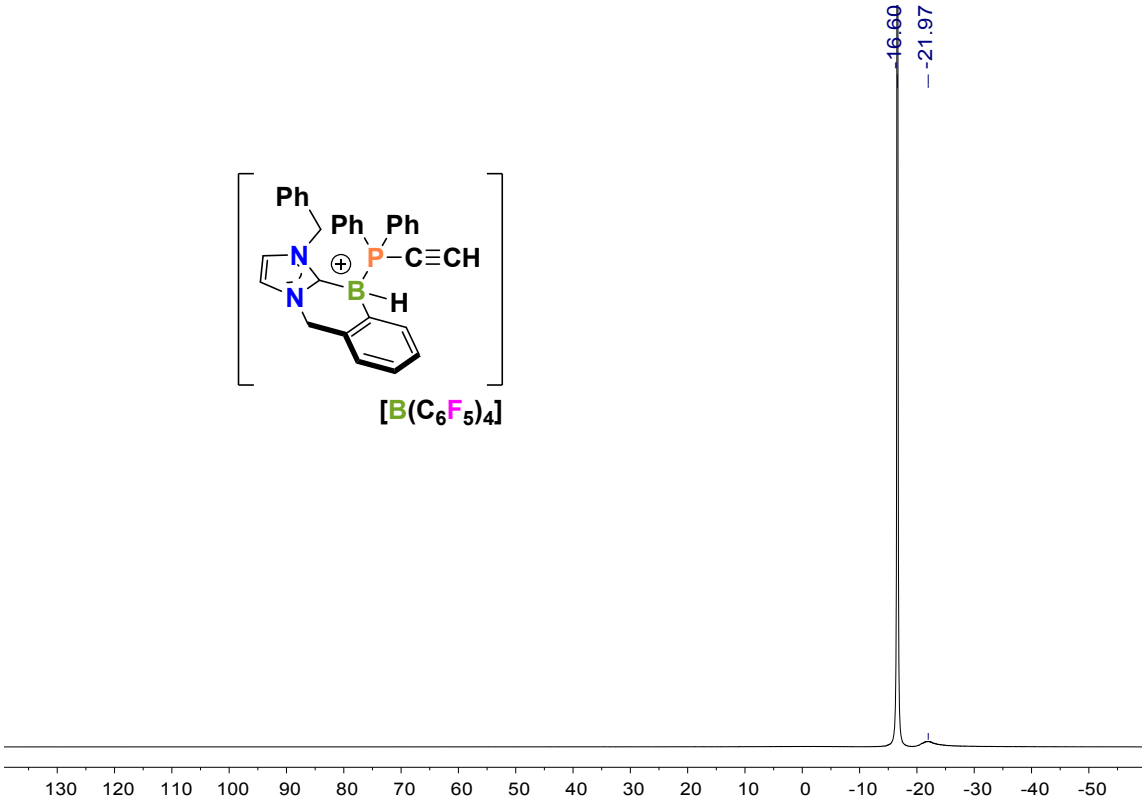

Figure S29. ^{11}B NMR spectrum of **9**.

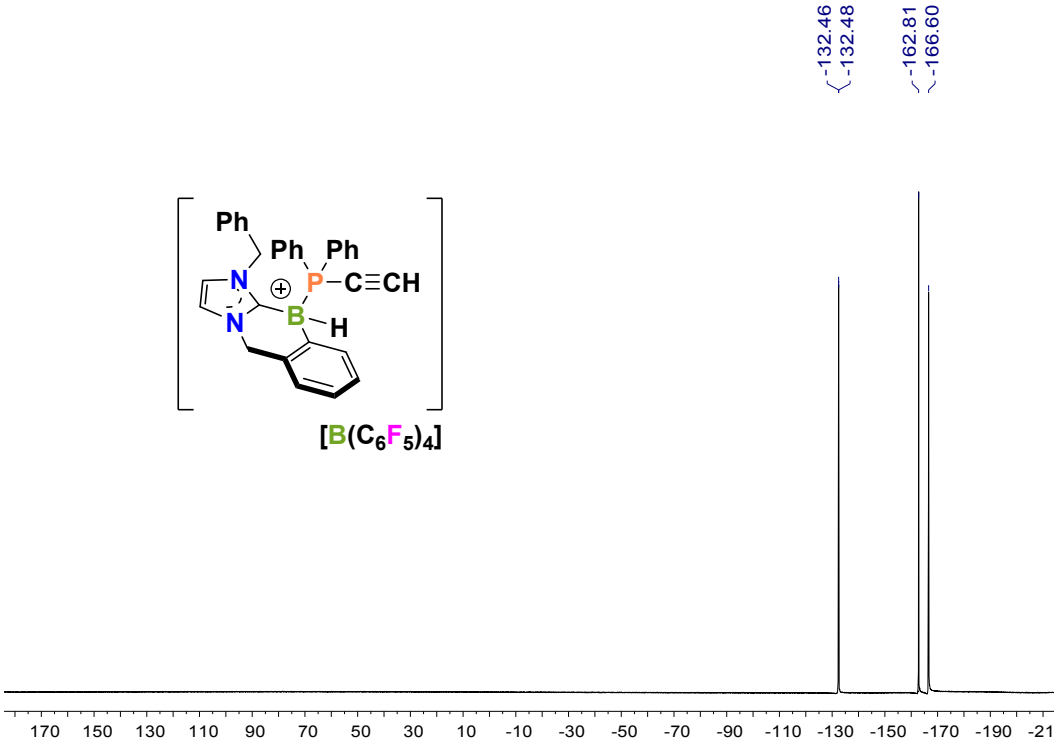

Figure S30. ^{19}F NMR spectrum of **9**.

NMR Spectra of 10

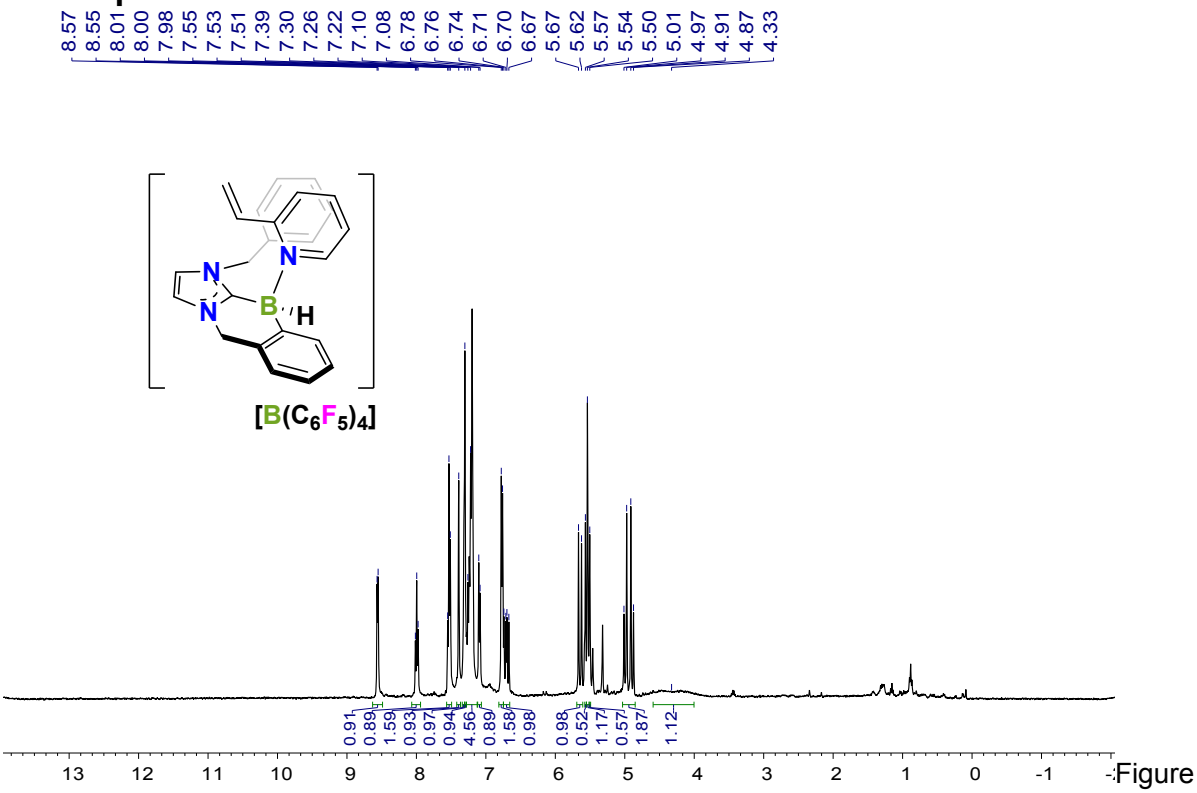

Figure S31. ^{1}H NMR spectrum of **10** with minor impurities.

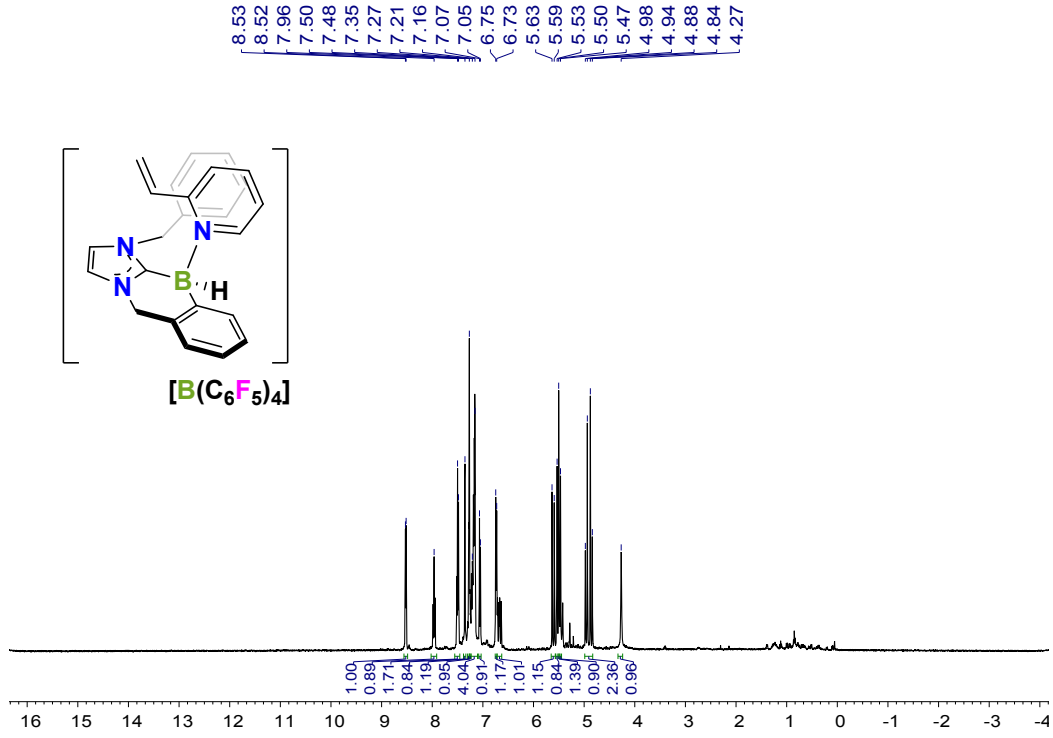

Figure S32. $^{1}H\{^{11}B\}$ NMR spectrum of **10** with minor impurities.

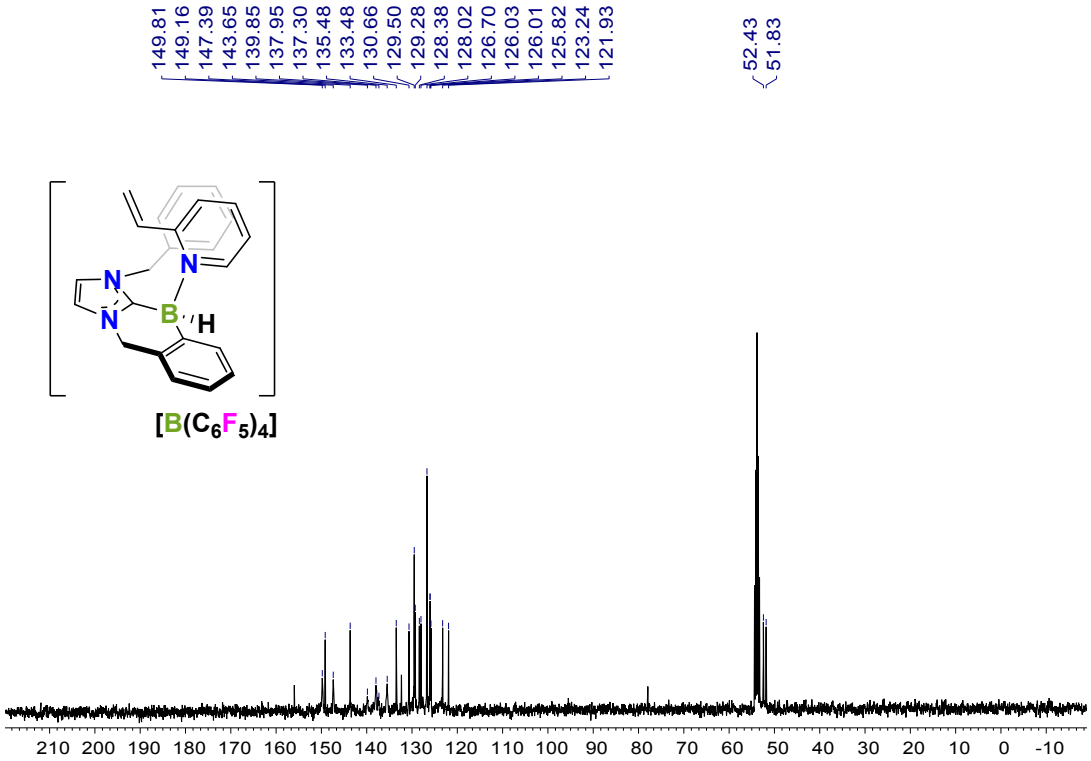

Figure S33. $^{13}C\{H\}$ NMR spectrum of **10**.

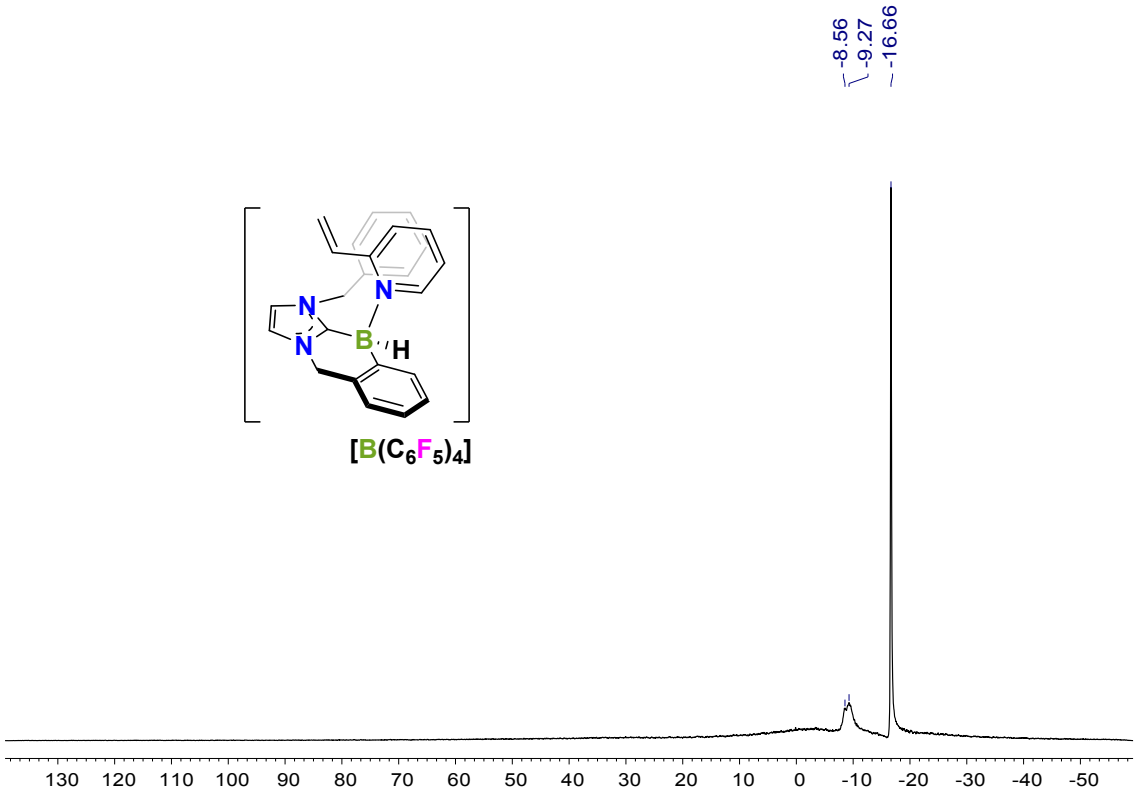

Figure S34. ^{11}B NMR spectrum of **10**.

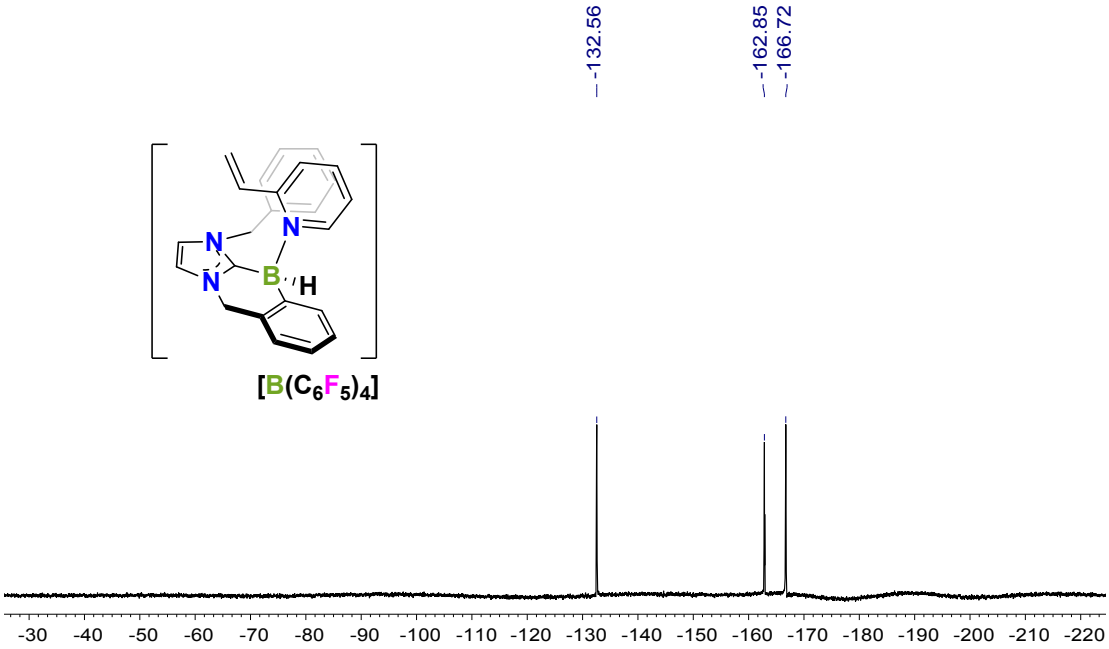

Figure S35. ^{19}F NMR spectrum of **10**.

NMR Spectra of 11

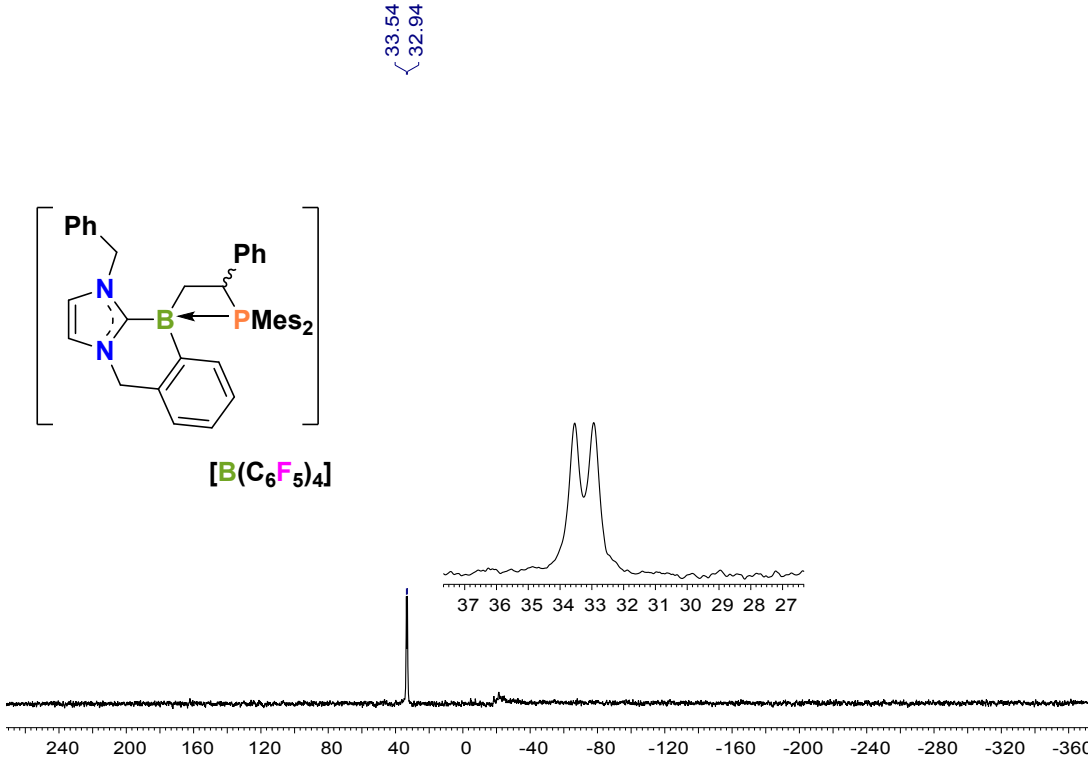

Figure S36. ^{31}P NMR spectrum of **11**.

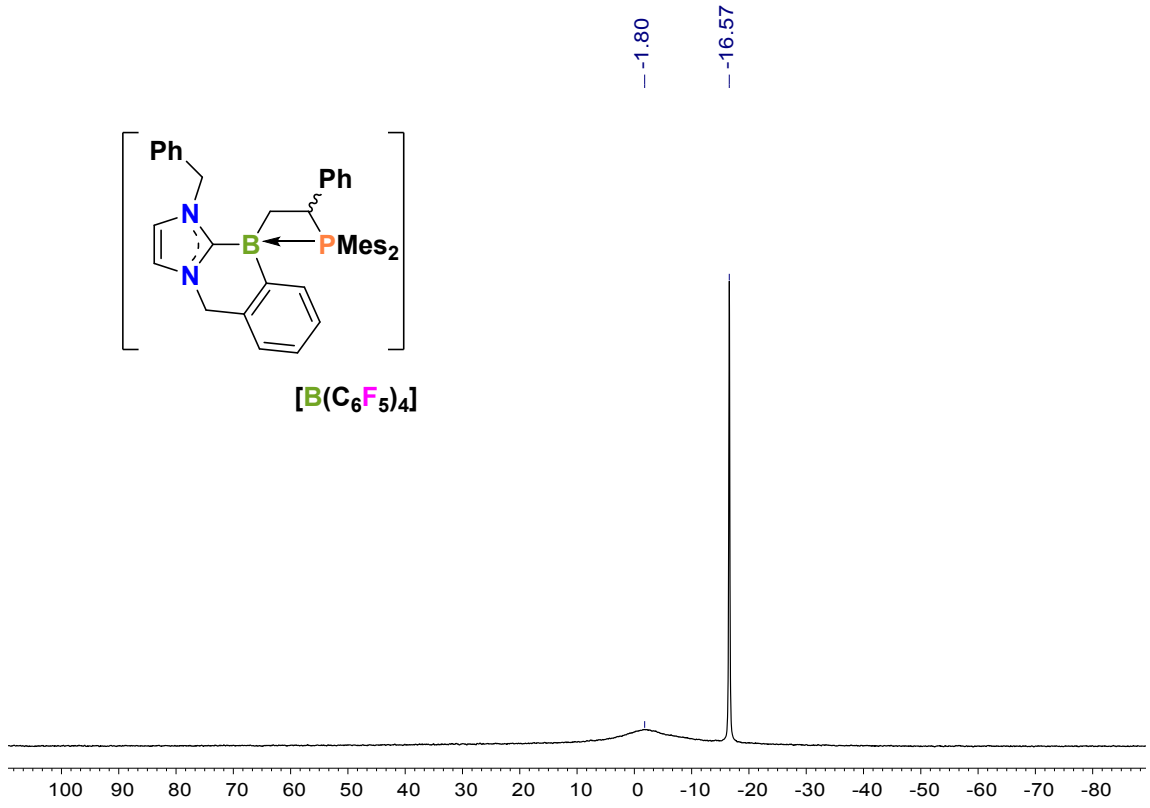

Figure S37. ^{11}B NMR spectrum of **11**.

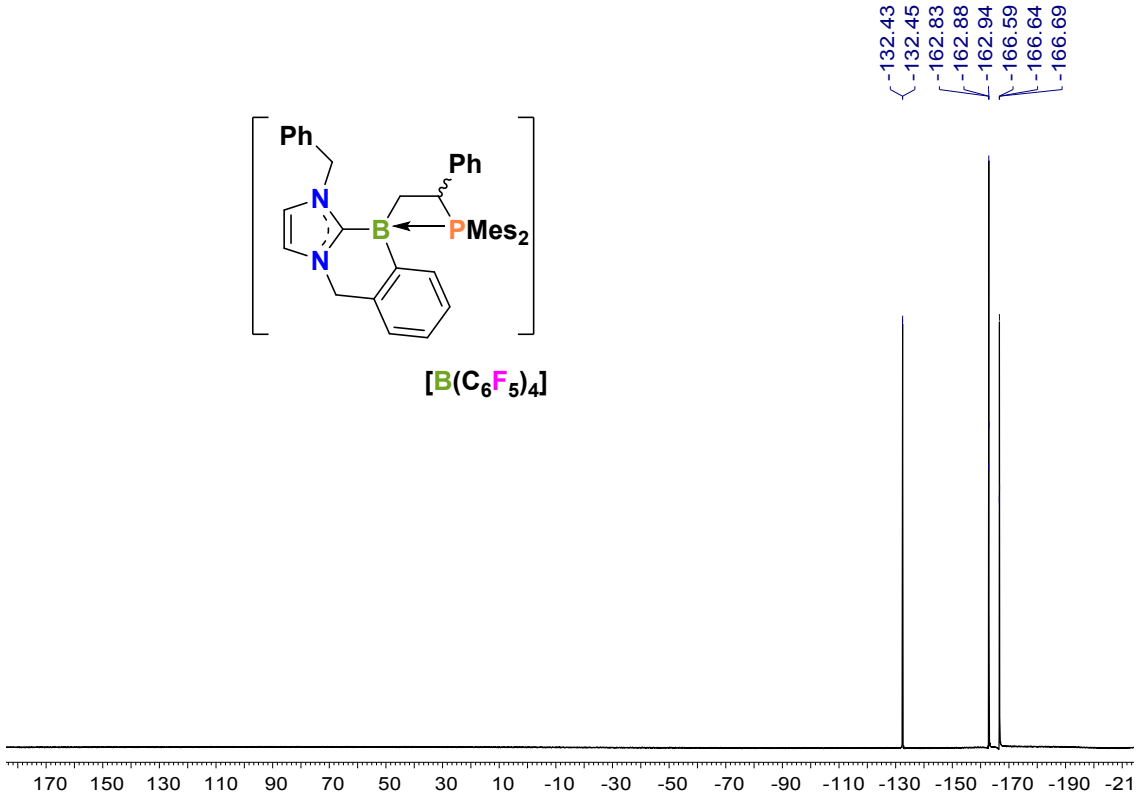

Figure S38. ^{19}F spectrum of **11**.

NMR Spectra of 12

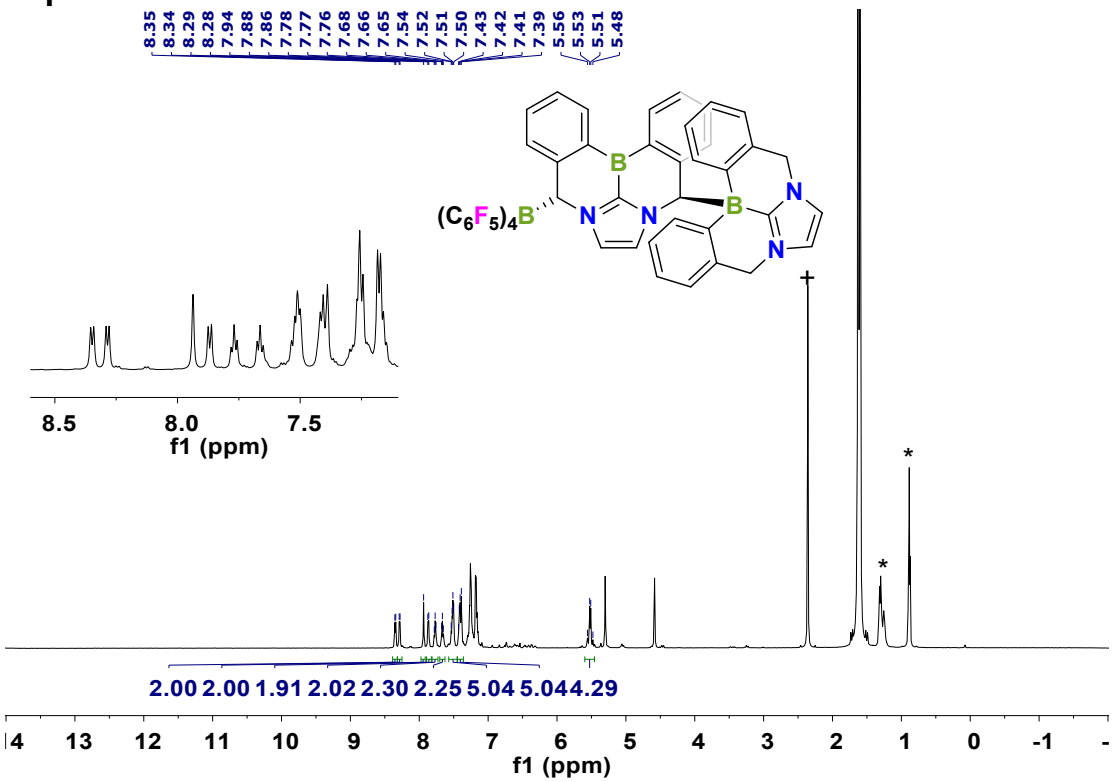

Figure S39. ^{1}H NMR spectrum of **12**. (* residual pentane, $^{+}$ residual toluene)

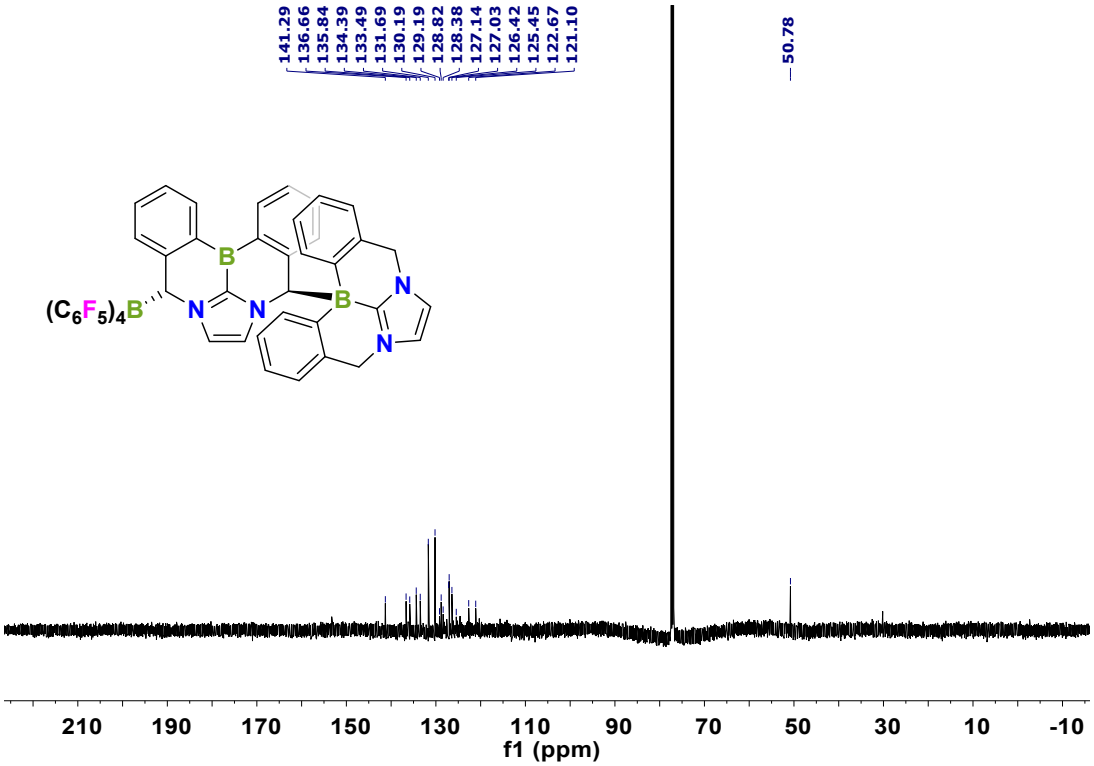

Figure S40. ^{13}C{H} NMR spectrum of **12**. (in $CDCl_3$)

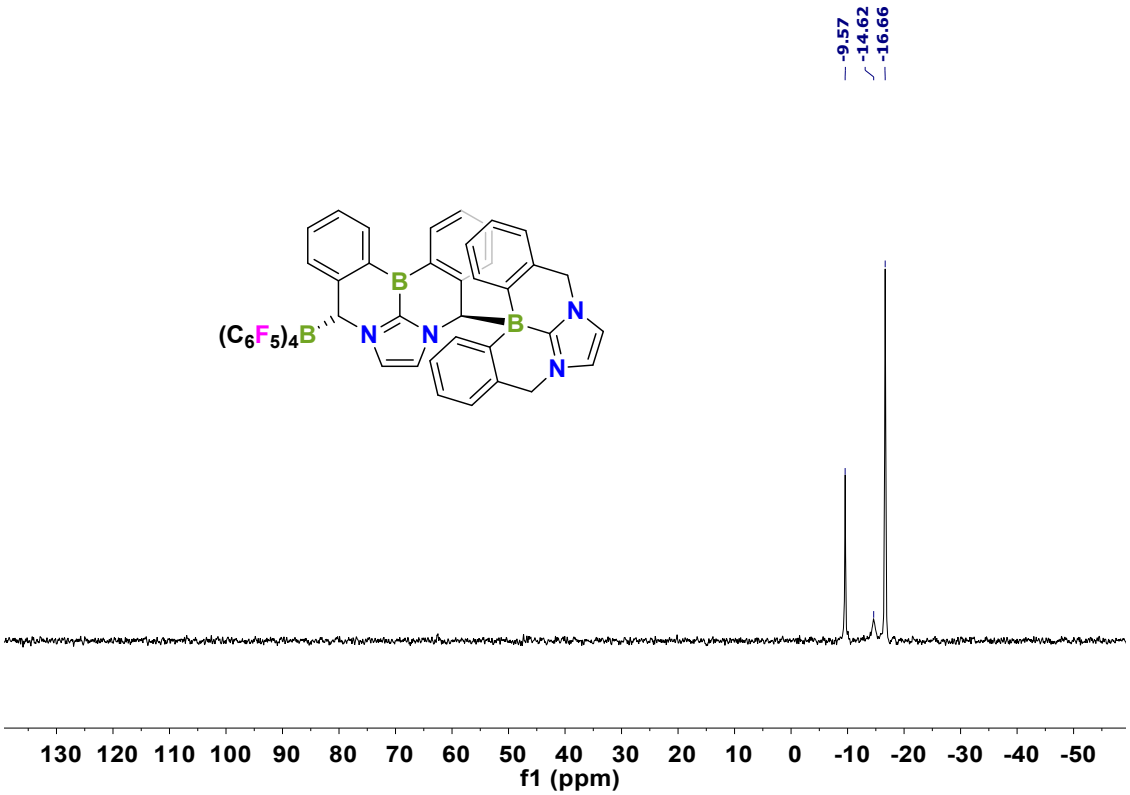

Figure S41. ^{11}B NMR spectrum of **12**.

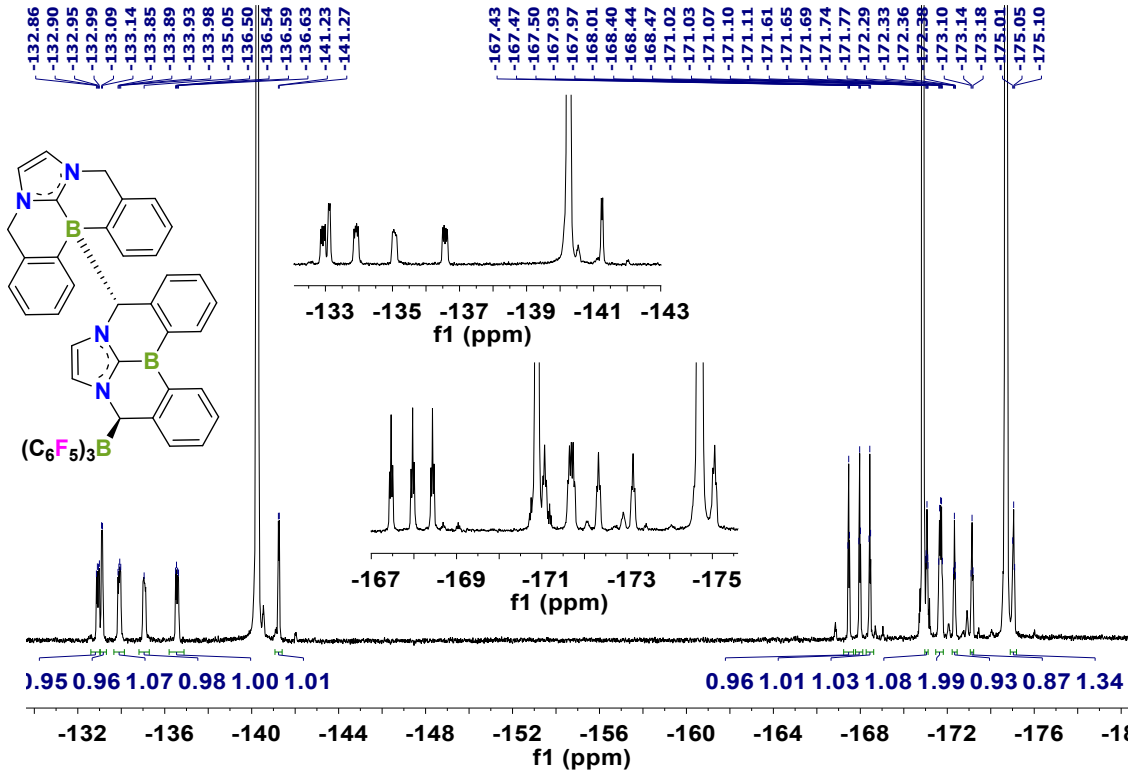

Figure S42. ^{19}F NMR spectrum of **12**.

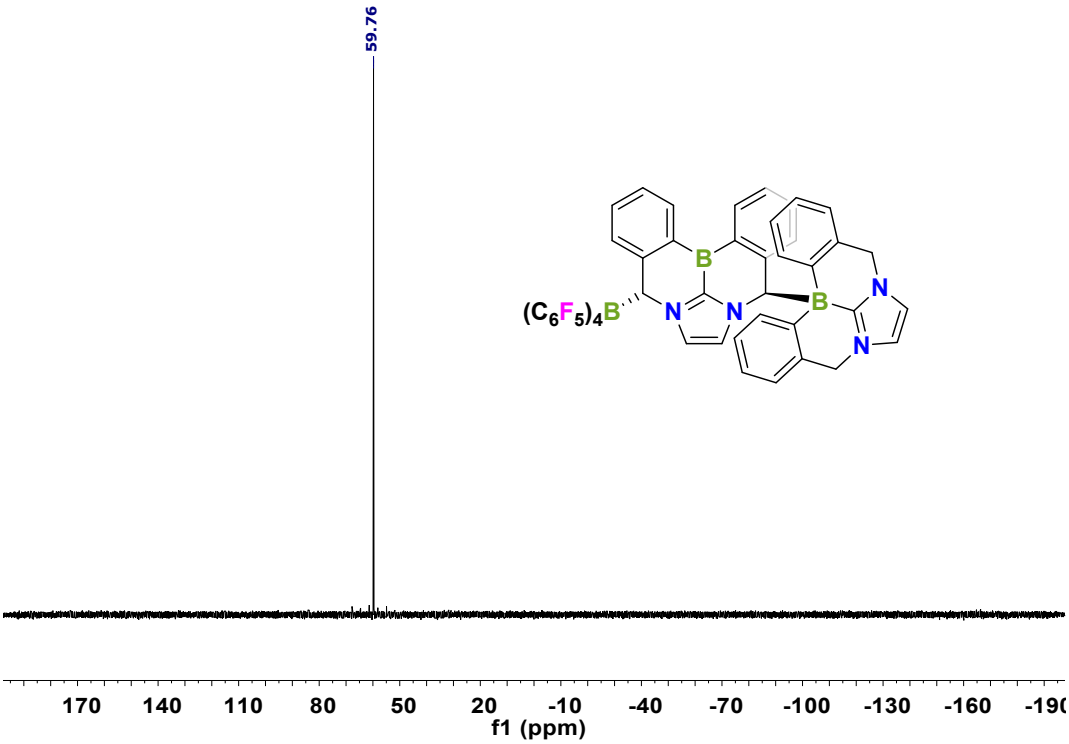

Figure S43. $^{31}P\{H\}$ NMR spectrum of **12**.

NMR Spectra of 13

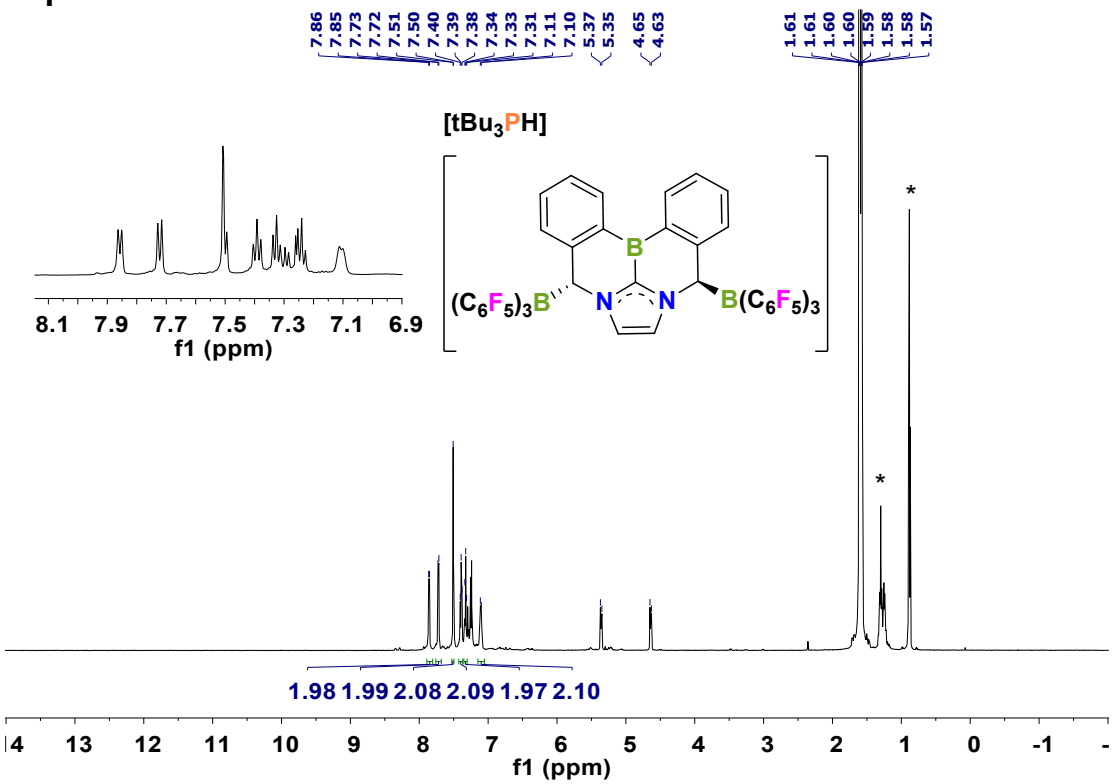

Figure S44. 1H NMR spectrum of **13**. (* residual pentane)

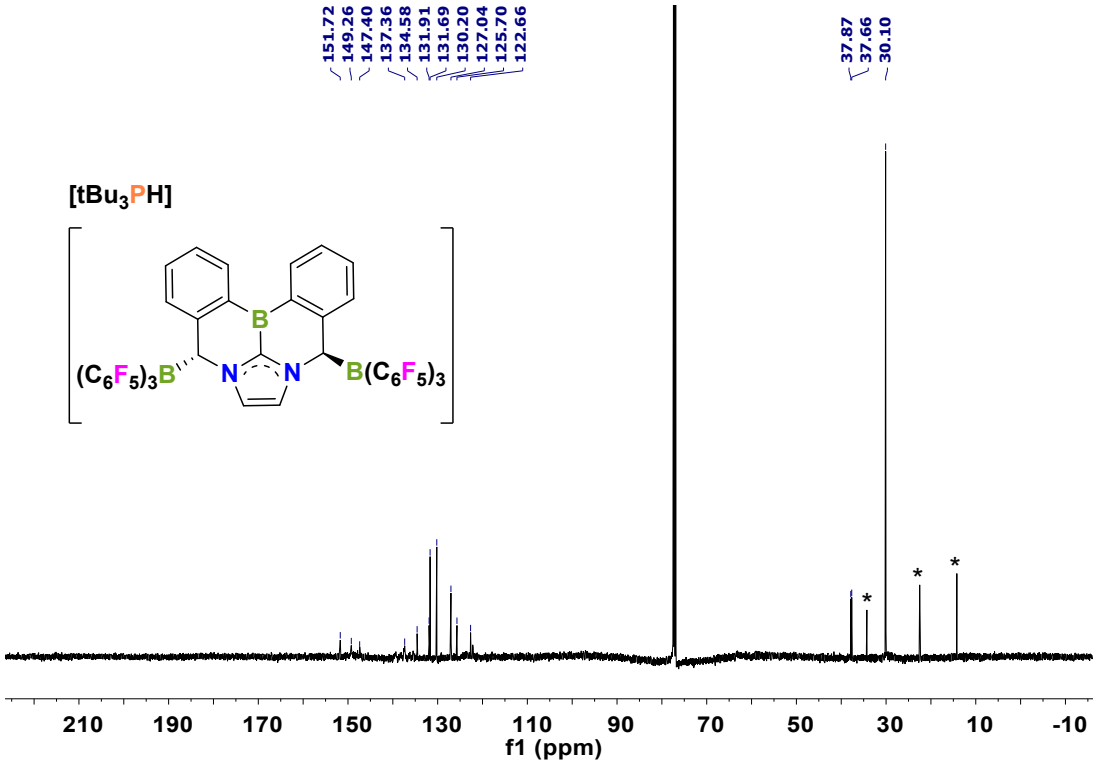

Figure S45. $^{13}C\{H\}$ NMR spectrum of **13**. (* residual pentane)

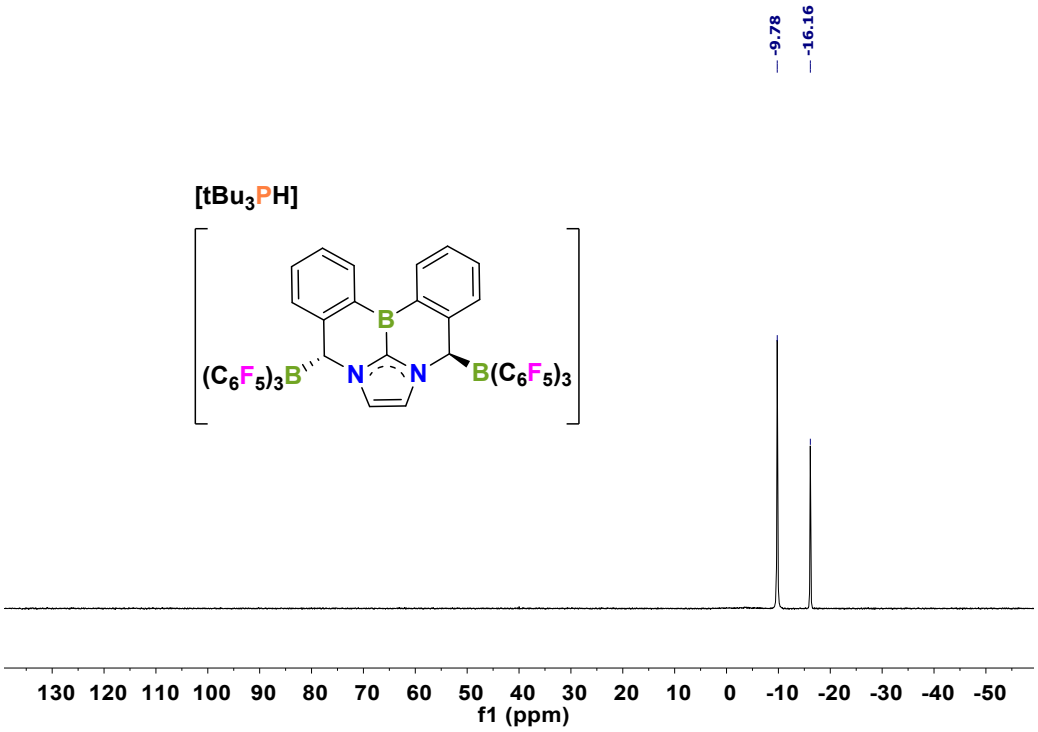

Figure S46. ^{11}B NMR spectrum of **13**.

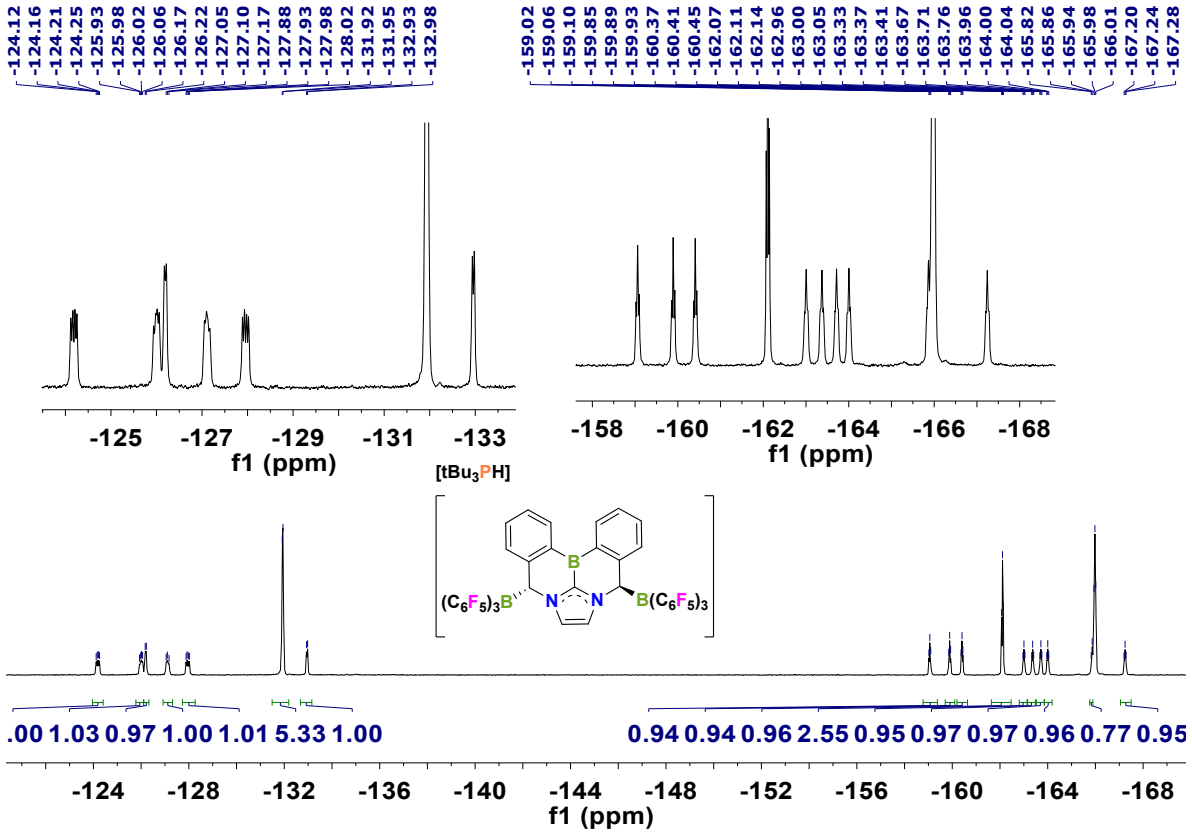

Figure S47. ^{19}F NMR spectrum of **13**.

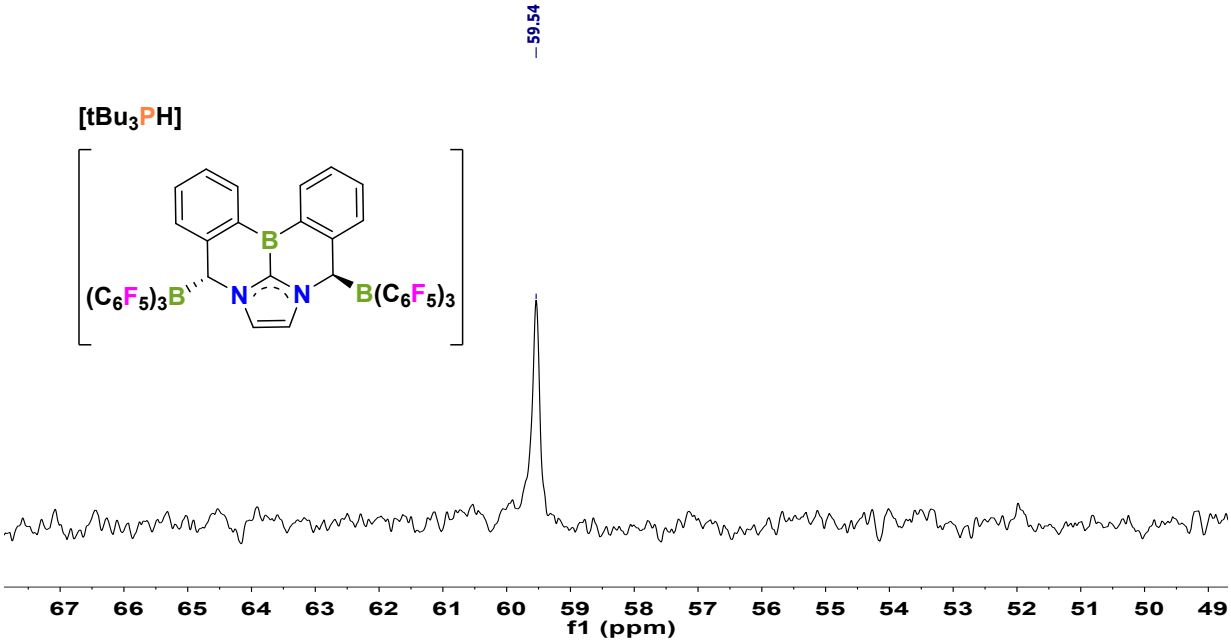

Figure S48. $^{31}P\{H\}$ NMR spectrum of **13**.

Computational Details

Table S1. Isotropic shift of the boron centre.

	δ (absolute) $_{comp}$	δ (referenced) $_{comp}$	δ ($CDCl_3$) $_{expt}$
2	-59.4461	48.1	48.1
11 [a]	-1091.43	-1.5966	-1.8

[a] Isotropic shift calculated for both isomers were identical.

Table S2. Isotropic shift of the phosphorus centre.

	δ (absolute) $_{comp}$	δ (referenced) $_{comp}$	δ ($CDCl_3$) $_{expt}$
$H_2CC(Ph)PMes_2$	-227.545	40.3	40.3
11 [a]	-243.33	26.6	33

[a] Isotropic shift calculated for both isomers were identical.

Tables of Optimized Coordinates

The following tables contain the optimized coordinates of the compounds. All calculations were carried out in the gas phase.

Table S3. Optimized Cartesian coordinates of **2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954465	0.576459	-3.640107
2	6	0	1.782385	1.265427	-4.494492
3	6	0	1.381343	2.581345	-2.728578
4	7	0	0.720379	1.397288	-2.565778
5	1	0	0.524485	-0.415656	-3.726373
6	1	0	2.191165	0.984862	-5.458843
7	7	0	2.033358	2.486661	-3.922927
8	6	0	-0.128064	1.069845	-1.411620
9	1	0	-1.138642	0.858194	-1.798208
10	1	0	0.254214	0.129742	-0.982127
11	6	0	-0.203987	2.133372	-0.337982
12	6	0	0.461533	3.385597	-0.450857
13	6	0	-0.974739	1.845979	0.792275
14	6	0	0.318109	4.319511	0.607495
15	6	0	-1.094649	2.787453	1.817953
16	1	0	-1.487666	0.884950	0.882532
17	6	0	-0.448218	4.028663	1.728999
18	1	0	0.826477	5.282524	0.527063
19	1	0	-1.698514	2.549527	2.695564
20	1	0	-0.548791	4.756283	2.535448
21	6	0	2.931689	3.529039	-4.501991
22	1	0	2.683893	4.463395	-3.983213
23	1	0	3.962834	3.254499	-4.235395
24	6	0	2.779906	3.654595	-5.997922
25	6	0	1.655180	4.289519	-6.549393
26	6	0	3.770641	3.146602	-6.850854
27	6	0	1.521406	4.405002	-7.933803
28	1	0	0.885708	4.706663	-5.894258
29	6	0	3.637327	3.265422	-8.237826
30	1	0	4.660112	2.670368	-6.429499
31	6	0	2.511718	3.891465	-8.779294
32	1	0	0.648765	4.906612	-8.355204
33	1	0	4.417346	2.875579	-8.893685
34	1	0	2.408968	3.989106	-9.861241
35	5	0	1.306565	3.707388	-1.677018
36	1	0	1.878387	4.745500	-1.836967

Table S4. Optimized Cartesian coordinates of dimesityl(1-phenylvinyl)phosphane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.371462	-2.479575	-1.243612
2	1	0	-0.691990	-2.392382	-1.473783
3	1	0	0.921298	-3.305252	-1.703390
4	6	0	0.989170	-1.636616	-0.398575
5	6	0	2.446072	-1.773606	-0.112860
6	6	0	2.982622	-1.477379	1.148325
7	6	0	3.324923	-2.186754	-1.127296
8	6	0	4.350941	-1.599743	1.388157
9	1	0	2.318922	-1.155555	1.952532
10	6	0	4.689450	-2.310939	-0.887173
11	1	0	2.931916	-2.379443	-2.127417
12	6	0	5.210067	-2.016953	0.374061
13	1	0	4.745941	-1.366872	2.378246
14	1	0	5.353733	-2.625663	-1.693658
15	1	0	6.281046	-2.106536	0.561564
16	15	0	0.031548	-0.488124	0.678325
17	6	0	0.370487	1.293695	0.301622
18	6	0	1.283768	1.835664	-0.631776
19	6	0	-0.378992	2.181290	1.117463
20	6	0	1.398568	3.225723	-0.743961
21	6	0	-0.232926	3.561363	0.957184
22	6	0	0.651645	4.110089	0.031204
23	1	0	2.099207	3.629088	-1.479992
24	1	0	-0.830417	4.226879	1.585934
25	6	0	-1.708411	-0.753826	0.110597
26	6	0	-2.279467	-0.171637	-1.040555
27	6	0	-2.503727	-1.583839	0.936612
28	6	0	-3.636208	-0.391498	-1.311126
29	6	0	-3.848926	-1.780070	0.622246
30	6	0	-4.440957	-1.179143	-0.491030
31	1	0	-4.071301	0.062872	-2.205300
32	1	0	-4.453051	-2.425047	1.265977
33	6	0	-1.493550	0.662924	-2.019723
34	1	0	-1.373818	1.698336	-1.666301
35	1	0	-0.486056	0.254492	-2.172147
36	1	0	-2.008058	0.689947	-2.989329
37	6	0	-1.933312	-2.282576	2.147302
38	1	0	-1.073364	-2.912556	1.875788
39	1	0	-1.572506	-1.560276	2.893826
40	1	0	-2.693555	-2.920726	2.615931
41	6	0	-5.903846	-1.378948	-0.786207
42	1	0	-6.148034	-1.083600	-1.814919
43	1	0	-6.196521	-2.429197	-0.648045
44	1	0	-6.523609	-0.773772	-0.106806
45	6	0	2.164577	1.013287	-1.537926
46	1	0	3.030800	0.612639	-0.991060
47	1	0	1.638047	0.157527	-1.978325
48	1	0	2.547429	1.638235	-2.355160
49	6	0	-1.358027	1.700563	2.162528
50	1	0	-2.259520	1.262382	1.707167
51	1	0	-0.910337	0.924328	2.801533
52	1	0	-1.671921	2.536261	2.800803
53	6	0	0.820145	5.600313	-0.101395
54	1	0	1.124470	5.877807	-1.119597
55	1	0	-0.111788	6.129750	0.138608
56	1	0	1.596531	5.967339	0.587933

Table S5. Optimized Cartesian coordinates of **11(R)**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.989407	1.363575	-2.853952
2	6	0	3.608842	0.161232	-2.705709
3	6	0	2.054939	0.319730	-1.113278
4	7	0	2.043625	1.440921	-1.856440
5	1	0	3.149630	2.162533	-3.571206
6	1	0	4.428790	-0.291471	-3.255149
7	7	0	3.018282	-0.462792	-1.626306
8	6	0	1.241715	2.608370	-1.473424
9	1	0	1.622326	3.472751	-2.030052
10	1	0	0.198995	2.437156	-1.778205
11	6	0	1.333138	2.825960	0.022252
12	6	0	1.292021	1.697195	0.863568
13	6	0	1.484669	4.110632	0.541462
14	6	0	1.486038	1.904698	2.235379
15	6	0	1.631900	4.293860	1.916662
16	1	0	1.506801	4.973460	-0.127932
17	6	0	1.654573	3.186688	2.761918
18	1	0	1.509227	1.048166	2.915167
19	1	0	1.756676	5.298642	2.321941
20	1	0	1.805564	3.320706	3.834086
21	6	0	3.528389	-1.694453	-1.020343
22	1	0	2.752657	-2.059635	-0.336934
23	1	0	3.662432	-2.439722	-1.815697
24	6	0	4.822308	-1.451416	-0.277122
25	6	0	4.884679	-0.461345	0.710787
26	6	0	5.954185	-2.217283	-0.557868
27	6	0	6.069185	-0.244528	1.408516
28	1	0	4.003565	0.148918	0.935326
29	6	0	7.140342	-2.002112	0.145492
30	1	0	5.911584	-2.991454	-1.327543
31	6	0	7.198705	-1.016232	1.127285
32	1	0	6.112250	0.528444	2.176700
33	1	0	8.020627	-2.605730	-0.078433
34	1	0	8.125964	-0.845910	1.675608
35	5	0	1.117672	0.237121	0.181880
36	6	0	0.948303	-1.013865	1.206718
37	1	0	0.924922	-1.996789	0.710390
38	1	0	1.666217	-1.086731	2.039854
39	6	0	-0.486508	-0.678528	1.696406
40	1	0	-0.426490	0.175893	2.375420
41	6	0	-1.314395	-1.758440	2.333383
42	6	0	-1.933919	-1.515902	3.567291
43	6	0	-1.476394	-3.018668	1.741620
44	6	0	-2.718461	-2.490903	4.180288
45	1	0	-1.788795	-0.553112	4.063389
46	6	0	-2.262733	-3.993614	2.351543
47	1	0	-0.994741	-3.245128	0.788505
48	6	0	-2.892216	-3.731009	3.568174
49	1	0	-3.189071	-2.282936	5.142063
50	1	0	-2.381926	-4.966803	1.873375
51	1	0	-3.506414	-4.496299	4.044342
52	15	0	-0.932834	0.045644	-0.000924
53	6	0	-1.967684	1.551999	-0.197631
54	6	0	-2.284661	1.920411	-1.527218
55	6	0	-2.416020	2.356359	0.876107
56	6	0	-3.041603	3.074650	-1.751281
57	6	0	-3.171606	3.495113	0.592772
58	6	0	-3.501787	3.875773	-0.708976
59	1	0	-3.278595	3.351547	-2.781389
60	1	0	-3.518120	4.108572	1.427876
61	6	0	-1.828242	-1.288820	-0.890604

62	6	0	-3.180194	-1.513288	-0.539550
63	6	0	-1.217621	-2.096229	-1.876712
64	6	0	-3.882709	-2.535922	-1.185410
65	6	0	-1.965073	-3.102244	-2.489014
66	6	0	-3.302278	-3.340741	-2.162684
67	1	0	-4.922911	-2.710381	-0.900693
68	1	0	-1.484853	-3.723859	-3.248459
69	6	0	0.216264	-1.933292	-2.307482
70	1	0	0.418642	-0.926125	-2.701736
71	1	0	0.904054	-2.106877	-1.470343
72	1	0	0.460384	-2.654209	-3.097074
73	6	0	-3.931653	-0.709512	0.491649
74	1	0	-4.328399	0.220436	0.055520
75	1	0	-4.776196	-1.295028	0.876216
76	1	0	-3.307484	-0.434874	1.350133
77	6	0	-4.088477	-4.415420	-2.861032
78	1	0	-4.469277	-4.045612	-3.825356
79	1	0	-3.463590	-5.294031	-3.068941
80	1	0	-4.951049	-4.732888	-2.261813
81	6	0	-1.860758	1.134259	-2.747251
82	1	0	-0.851435	0.707477	-2.652507
83	1	0	-2.544137	0.293349	-2.939031
84	1	0	-1.867703	1.784172	-3.631860
85	6	0	-2.143499	2.051340	2.326085
86	1	0	-2.447074	1.029544	2.592472
87	1	0	-1.077122	2.172516	2.565665
88	1	0	-2.706476	2.740937	2.966077
89	6	0	-4.337909	5.099112	-0.964473
90	1	0	-4.339100	5.370392	-2.027444
91	1	0	-5.380147	4.922838	-0.659029
92	1	0	-3.968608	5.956852	-0.385671

Table S6. Optimized Cartesian coordinates of **11(S)**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.989407	1.363575	-2.853952
2	6	0	-3.608842	0.161232	-2.705709
3	6	0	-2.054939	0.319730	-1.113278
4	7	0	-2.043625	1.440921	-1.856440
5	1	0	-3.149630	2.162533	-3.571206
6	1	0	-4.428790	-0.291471	-3.255149
7	7	0	-3.018282	-0.462792	-1.626306
8	6	0	-1.241715	2.608370	-1.473424
9	1	0	-1.622326	3.472751	-2.030052
10	1	0	-0.198995	2.437156	-1.778205
11	6	0	-1.333138	2.825960	0.022252
12	6	0	-1.292021	1.697195	0.863568
13	6	0	-1.484669	4.110632	0.541462
14	6	0	-1.486038	1.904698	2.235379
15	6	0	-1.631900	4.293860	1.916662
16	1	0	-1.506801	4.973460	-0.127932
17	6	0	-1.654573	3.186688	2.761918
18	1	0	-1.509227	1.048166	2.915167
19	1	0	-1.756676	5.298642	2.321941
20	1	0	-1.805564	3.320706	3.834086
21	6	0	-3.528389	-1.694453	-1.020343
22	1	0	-2.752657	-2.059635	-0.336934
23	1	0	-3.662432	-2.439722	-1.815697
24	6	0	-4.822308	-1.451416	-0.277122
25	6	0	-4.884679	-0.461345	0.710787
26	6	0	-5.954185	-2.217283	-0.557868
27	6	0	-6.069185	-0.244528	1.408516
28	1	0	-4.003565	0.148918	0.935326
29	6	0	-7.140342	-2.002112	0.145492
30	1	0	-5.911584	-2.991454	-1.327543
31	6	0	-7.198705	-1.016232	1.127285
32	1	0	-6.112250	0.528444	2.176700
33	1	0	-8.020627	-2.605730	-0.078433
34	1	0	-8.125964	-0.845910	1.675608
35	5	0	-1.117672	0.237121	0.181880
36	6	0	-0.948303	-1.013865	1.206718
37	1	0	-0.924922	-1.996789	0.710390
38	1	0	-1.666217	-1.086731	2.039854
39	6	0	0.486508	-0.678528	1.696406
40	1	0	0.426490	0.175893	2.375420
41	6	0	1.314395	-1.758440	2.333383
42	6	0	1.933919	-1.515902	3.567291
43	6	0	1.476394	-3.018668	1.741620
44	6	0	2.718461	-2.490903	4.180288
45	1	0	1.788795	-0.553112	4.063389
46	6	0	2.262733	-3.993614	2.351543
47	1	0	0.994741	-3.245128	0.788505
48	6	0	2.892216	-3.731009	3.568174
49	1	0	3.189071	-2.282936	5.142063
50	1	0	2.381926	-4.966803	1.873375
51	1	0	3.506414	-4.496299	4.044342
52	15	0	0.932834	0.045644	-0.000924
53	6	0	1.967684	1.551999	-0.197631
54	6	0	2.284661	1.920411	-1.527218
55	6	0	2.416020	2.356359	0.876107
56	6	0	3.041603	3.074650	-1.751281
57	6	0	3.171606	3.495113	0.592772
58	6	0	3.501787	3.875773	-0.708976
59	1	0	3.278595	3.351547	-2.781389
60	1	0	3.518120	4.108572	1.427876
61	6	0	1.828242	-1.288820	-0.890604

62	6	0	3.180194	-1.513288	-0.539550
63	6	0	1.217621	-2.096229	-1.876712
64	6	0	3.882709	-2.535922	-1.185410
65	6	0	1.965073	-3.102244	-2.489014
66	6	0	3.302278	-3.340741	-2.162684
67	1	0	4.922911	-2.710381	-0.900693
68	1	0	1.484853	-3.723859	-3.248459
69	6	0	-0.216264	-1.933292	-2.307482
70	1	0	-0.418642	-0.926125	-2.701736
71	1	0	-0.904054	-2.106877	-1.470343
72	1	0	-0.460384	-2.654209	-3.097074
73	6	0	3.931653	-0.709512	0.491649
74	1	0	4.328399	0.220436	0.055520
75	1	0	4.776196	-1.295028	0.876216
76	1	0	3.307484	-0.434874	1.350133
77	6	0	4.088477	-4.415420	-2.861032
78	1	0	4.469277	-4.045612	-3.825356
79	1	0	3.463590	-5.294031	-3.068941
80	1	0	4.951049	-4.732888	-2.261813
81	6	0	1.860758	1.134259	-2.747251
82	1	0	0.851435	0.707477	-2.652507
83	1	0	2.544137	0.293349	-2.939031
84	1	0	1.867703	1.784172	-3.631860
85	6	0	2.143499	2.051340	2.326085
86	1	0	2.447074	1.029544	2.592472
87	1	0	1.077122	2.172516	2.565665
88	1	0	2.706476	2.740937	2.966077
89	6	0	4.337909	5.099112	-0.964473
90	1	0	4.339100	5.370392	-2.027444
91	1	0	5.380147	4.922838	-0.659029
92	1	0	3.968608	5.956852	-0.385671

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