Supporting Information for:

Addition of Dihydrogen to a Borylborenium Center

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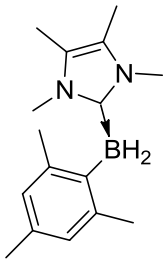
Supporting Information Contents:

I. Experimental methods

General

Solvents were dried by reflux under N_2 over sodium or CaH_2 and freshly distilled prior to use. Air-sensitive compounds were handled under a N_2 atmosphere using standard Schlenk and glovebox techniques. NMR spectra were recorded on Bruker SPECT NMR (400 MHz for ^{1}H, 376 MHz for ^{19}F, 100 MHz for ^{13}C) and Bruker DMX500 NMR (500 MHz for ^{1}H, 160 MHz for ^{11}B) spectrometers. Most assignments were based on a series of 2D NMR experiments. HRMS analyses were performed at Bruker micrOTOF II. GC-MS were obtained on a Focus GC-ISQ MS instrument. Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Center: CCDC 1543216 (complex **4**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk/data_request/cif. IMe_4BH_3 (IMe_4 = 1,3,4,5-tetramethylimidazol-2-ylidene),[1] IPrCuBpin (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene, Bpin = pinacolboryl),[2] 2,4,6-trimethylphenyl lithium (MesLi),[3] Pinacol-d_{12},[4] B_2pin_2-d_{24},[4] Mesitylene-d_9,[5] (Mes-d_9)Br [6] and MesBpin [7] were prepared as reported.

Synthesis of 2:



A solution of I_2 (1.23 g, 4.84 mmol) in toluene (15 mL) was added to the suspension of IMe_4BH_3 (1.34 g, 9.67 mmol) in toluene (15 mL). A vigorous evolution of gas was observed. The reaction mixture was stirred at room temperature for 30 min, which was then transferred to a suspension of MesLi (1.27g, 10.0 mmol) in toluene (30 mL). The mixture was stirred at room temperature for 8 h. The resulting suspension was filtered. The filtrate was concentrated in vacuum, affording **2** as a white solid (2.35 g, 95%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 6.77 (s, 2H, C_6H_2), 3.49 (s, 6H, NCH_3), 2.37 (q, $^{1}J_{B-H}$ = 82 Hz, 2H, BH_2), 2.25 (s, 3H, *para*-CH_3), 2.20 (s, 6H, *ortho*-CH_3), 2.12 (s, 6H, =CCH_3).

^{13}C NMR (100 MHz, $CDCl_3$, 25 ℃): δ [ppm] = 170.41 (br m, (IMe^4)*C*B), 146.32 (br m, *ipso*-C_6H_2), 141.91 (*ortho*-C_6H_2), 132.79 (*para*-C_6H_2), 127.49 (*meta*-C_6H_2), 123.08 (=*C*CH_3(N)), 32.07 (NCH_3), 23.90 (*ortho*-*C*H_3), 20.94 (*para*-*C*H_3), 8.79 (=C(N)*C*H_3).

^{11}B NMR (160 MHz, $CDCl_3$, 25 ℃): δ [ppm] = -28.1 (t, $^{1}J_{B-H}$ = 83 Hz).

HRMS (*m/z*): $[M-H]^+$ calcd. for $C_{16}H_{25}BN_2$, 255.2030; found 255.2051.

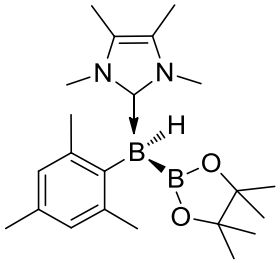
Synthesis of 2-d_9:

A solution of I_2 (673 mg, 2.65 mmol) in toluene (5 mL) was added to the suspension of IMe_4BH_3 (731 mg, 5.30 mmol) in toluene (10 mL). A vigorous evolution of gas was observed. The reaction mixture was stirred at room temperature for 30 min, then transferred to a suspension of (Mes-d_9)Li (715 mg, 5.30 mmol) in toluene (10 mL) which was prepared from (Mes-d_9)Br[6] with *n*-BuLi. The mixture was stirred at room temperature for 6 h. The suspension was filtered before the removal of solvents under vacuum. The residue was purified by column chromatography (PE : EA = 10 : 1). Complex **2**-d_9 was obtained as a white solid (1.10 g, 79%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 6.74 (s, 2H, C_6H_2), 3.47 (s, 6H, NCH_3), 2.33 (q, $^{1}J_{B-H}$ = 83 Hz, 2H, BH_2), 2.10 (s, 6H, =CCH_3).

^{2}H NMR (500 MHz, $CHCl_3$, 25 °C): δ [ppm] = 2.23 (br s, 9D, *para*-C*D*$_3$ & *ortho*-*CD*$_3$).
HRMS (*m/z*): $[M-H]^+$ calcd. for $C_{16}H_{16}D_9BN_2$, 264.2595; found 264.2570.

Synthesis of 3:



A solution of I_2 (130 mg, 0.51 mmol) in toluene (5.0 mL) was added to the solution of **2** (260 mg, 1.02 mmol) in toluene (5.0 mL). A vigorous evolution of gas was observed. The reaction mixture was stirred at room temperature for 30 min. Then a solution of IPrCuBpin (636 mg, 1.10 mmol) in toluene (10 mL) was slowly added to the solution of $IMe_4B(H)(I)(Mes)$ at -40 ^{o}C over 10 min. The resulting mixture was slowly warmed to room temperature and stirred for 2 h. The suspension was filtered before removal of solvents under vacuum. The residue was purified by column chromatography (PE : EA = 10 : 1). Complex **3** was obtained as a white solid (198 mg, 52%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 6.69 (s, 2H, C_6H_2), 3.38 (s, 6H, NC*H*$_3$), 2.19 (s, 3H, *para*-C*H*$_3$), 2.12 (s, 6H, *ortho*-*CH*$_3$), 2.06 (s, 6H, =CC*H*$_3$), 1.17 (s, 6H, C*H*$_3$(pin)), 1.15 (s, 6H, C*H*$_3$(pin)).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ [ppm] = 142.16 (*ortho*-C_6H_2), 132.13 (*para*- C_6H_2), 127.44 (*meta*-C_6H_2), 122.91 (=*C*CH_3(N)), 80.91 (O*C*Me_2), 32.49 (N*C*H_3), 25.26 (*C*H_3(pin)), 25.12 (*C*H_3(pin)), 24.65 (*ortho*-*C*H_3), 21.02 (*para*-*C*H_3), 9.09 (=C(N)*C*H_3).

^{11}B NMR (160 MHz, $CDCl_3$, 25 °C): δ [ppm] = 40.9 (br s, *B*pin), -29.5 (d, *B*H, $^{1}J_{B-H}$ = 56 Hz).
HRMS (*m/z*): $[M-H]^+$ calcd. for $C_{22}H_{35}B_2N_2O_2$, 381.2887; found 381.2880.

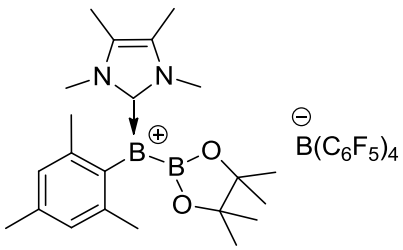
Synthesis of 3-*d*$_{21}$:

A solution of I_2 (254 mg, 1.00 mmol) in toluene (5.0 mL) was added to the solution of **2**-*d*$_9$ (530 mg, 2.00 mmol) in toluene (5.0 mL). A vigorous evolution of gas was observed. The reaction mixture was stirred at room temperature for 30 min. Then a solution of IPrCu(Bpin-*d*$_{12}$) (1156 mg, 2.00 mmol) in toluene (10 mL) which was generated from IPrCuO^{t}Bu with B_2(Pin-*d*$_{24}$)[4] was slowly added to the solution of $IMe_4B(H)(I)$(Mes-*d*$_9$) at -40 ^{o}C over 10 min. The resulting mixture was slowly warmed to room temperature and stirred for 2 h. The suspension was filtered before the removal of solvents under vacuum. The residue was purified by column chromatography (PE : EA = 10 : 1). Complex **3**-*d*$_{21}$ was obtained as a white solid (448 mg, 56%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 6.68 (s, 2H, C_6H_2), 3.38 (s, 6H, NC*H*$_3$), 2.06 (s, 6H, =CC*H*$_3$).

^{2}H NMR (500 MHz, $CHCl_3$, 25 °C): δ [ppm] = 2.18 (br s, 9D, *para*-C*D*$_3$ & *ortho*-*CD*$_3$), 1.22 (br s, 12D, C*D*$_3$(pin)).
HRMS (*m/z*): $[M-H]^+$ calcd. for $C_{22}H_{15}D_{21}B_2N_2O_2$, 402.4205; found 402.4203.

Synthesis of 1:



A suspension of $[Ph_3C][B(C_6F_5)_4]$ (145 mg, 0.157 mmol) in toluene (1.5 mL) was added to the solution of **3** (60 mg, 0.16 mmol) in toluene (1.0 mL). The reaction mixture was stirred at room temperature for 10 min. Addition of hexane (6.0 mL) to the reaction mixture resulted in formation of a

brown oil. The supernatant was discarded. To the brown oil hexane (3.0 mL) was added, and a yellow solid appeared after standing in an ultrasonic bath for 20 min. Then the supernatant was removed by filtration. The resulting yellow solid was washed with hexane (2 x 1.0 mL) and pumped to dryness to give complex **1** (159 mg, 96%).

^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 6.90 (s, 2H, C_6H_2), 3.67 (s, 6H, NCH_3), 2.35 (s, 6H, =CCH_3), 2.31 (s, 3H, *para*-CH_3), 2.07 (s, 6H, *ortho*-CH_3), 1.26 (s, 12H, CH_3(pin)).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 148.57 (dm, $^{1}J_{C\text{-}F}$ = 240 Hz, *o*-C_6F_5), 142.49 (*para*-C_6H_2), 138.65 (dm, $^{1}J_{C\text{-}F}$ = 245 Hz, *p*-C_6F_5), 137.76 (*ortho*-C_6H_2), 136.69 (dm, $^{1}J_{C\text{-}F}$ = 250 Hz, *m*-C_6F_5), 134.69 (=*C*CH$_3$(N)),129.40 (*meta*-C_6H_2), 124.98-123.82 (br m, ipso-C_6F_5), 85.20 (O*C*Me$_2$), 34.75 (N*C*H$_3$), 24.91 (*C*H$_3$(pin)), 22.49 (*ortho*-*C*H$_3$), 21.40 (*para*-*C*H$_3$), 9.68 (=C(N)*C*H$_3$).

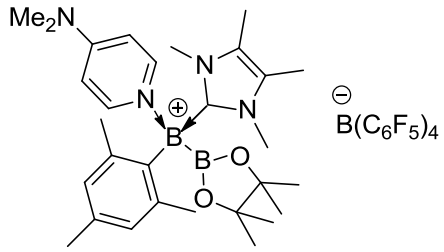
^{11}B NMR (160 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 78.0 (br s, *B*Mes), 32.8 (br s, *B*pin), -16.6 (s, *B*(C_6F_5)$_4$).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -133.15 (br s, 6F, *ortho*-C_6F_5), -163.68 (t, 3F, $^{3}J_{F\text{-}F}$ = 20 Hz, *para*-C_6F_5), -167.57 (t, 6F, $^{3}J_{F\text{-}F}$ = 17 Hz, *meta*-C_6F_5).

HRMS (*m/z*): $[M]^+$ calcd. for $C_{22}H_{35}B_2N_2O_2$, 381.2887; found 381.2888.

Analysis (calcd., found for $C_{46}H_{35}B_3F_{20}N_2O_2$): C (52.11, 52.00), H (3.33, 3.36), N (2.64, 2.78).

Synthesis of 4:



A solution of $[Ph_3C][B(C_6F_5)_4]$ (145 mg, 0.16 mmol) in CH_2Cl_2 (1 mL) was added to the solution of **3** (60 mg, 0.16 mmol) in CH_2Cl_2 (0.5 mL). The reaction mixture was stirred at room temperature for 1 min. To the resulting solution 4-dimethylaminopyridine (DMAP) (20 mg, 0.16 mmol) in CH_2Cl_2 (0.5 mL) was added, and the mixture was concentrated (about 0.5 mL solution). Addition of hexane (4.0 mL) to the reaction mixture resulted in formation of a brown oil. The supernatant was discarded. To the brown oil hexane (2.0 mL) was added, and a yellow solid appeared after standing in an ultrasonic bath for 20 min. Then the supernatant was removed by filtration. The resulting yellow solid was washed with hexane (2 x 1.0 mL) and pumped to dryness to give complex **4** (161 mg, 87%). X-ray quality crystals were obtained by evaporation of saturated solution in toluene/CH_2Cl_2.

^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 9.50 - 7.30 (br, 2H, *H*2(py)), 6.80 (s, 2H, C_6H_2), 6.60 (br s, 2H, *H*3(py)), 3.14 (s, 6H, NCH_3), 3.10 (s, 6H, N(CH_3)$_2$), 2.23 (s, 3H, *para*-CH_3), 2.11 (s, 6H, =CCH_3), 1.86 (s, 6H, *ortho*-CH_3), 1.13 (s, 6H, CH_3(pin)), 1.12 (s, 6H, CH_3(pin)).

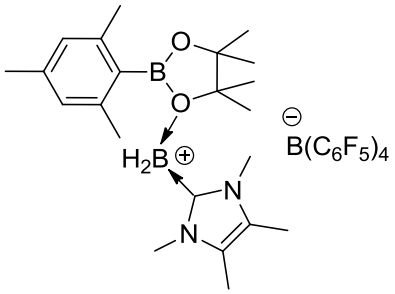
^{13}C NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 155.87 (*C*4(py)), 148.59 (dm, $^{1}J_{C\text{-}F}$ = 240 Hz, *o*-C_6F_5), 147.74 (br, *C*2(py)), 142.21 (*ortho*-C_6H_2), 138.68 (dm, $^{1}J_{C\text{-}F}$ = 245 Hz, *p*-C_6F_5), 136.59 (*para*-C_6H_2), 136.76 (dm, $^{1}J_{C\text{-}F}$ = 250 Hz, *m*-C_6F_5), 130.02 (*meta*-C_6H_2), 126.75 (=*C*CH$_3$(N)), 125.32 - 123.06 (br m, ipso-C_6F_5), 107.79 (*C*3(py)), 83.26 (O*C*Me$_2$), 39.80 (N(*C*H$_3$)$_2$), 33.65 (N*C*H$_3$), 25.07 (*C*H$_3$(pin)), 24.94 (*C*H$_3$(pin)), 23.68 (*ortho*-*C*H$_3$), 20.86 (*para*-*C*H$_3$), 9.17 (=C(N)*C*H$_3$).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 36.8 (br s, *B*pin), -7.8 (br s, *B*Mes), -16.7 (s, *B*(C_6F_5)$_4$).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -133.10 (br s, 6F, *ortho*-C_6F_5), -163.78 (t, 3F,

$^{3}J_{F-F}$ = 20 Hz, *para*-C_6F_5), -167.62 (t, 6F, $^{3}J_{F-F}$ = 17 Hz, *meta*-C_6F_5).
HRMS (*m/z*): $[M]^+$ calcd. for $C_{29}H_{45}B_2N_4O_2$, 503.3733; found 503.3730.

Synthesis of 5:



A solution of **1** (160 mg, 0.151 mmol) in toluene (2.0 mL) was degassed twice and backfilled with 1.5 bar H_2. After stirring at room temperature for one minute, the reaction mixture was dried under vacuum. The residue was washed with hexane (1.0 mL) and again dried under vacuum to give complex **5** (134 mg, 84%).

^{1}H NMR (400 MHz, C_6D_5Br, 25 °C): δ [ppm] = 6.45 (s, 2H, C_6H_2), 2.60 - 3.05 (br s, 2H, BH_2), 2.78 (s, 6H, NCH_3), 2.09 (s, 3H, *para*-CH_3), 1.85 (br s, 6H, *ortho*-CH_3), 1.53 (s, 6H, =CCH_3), 1.26 (br s, 12H, CH_3(pin)).

^{1}H{^{11}B} NMR (500 MHz, C_6D_5Br, 25 °C): δ [ppm] = 6.45 (s, 2H, C_6H_2), 2.87 (s, 2H, BH_2), 2.78 (s, 6H, NCH_3), 2.09 (s, 3H, *para*-CH_3), 1.85 (br s, 6H, *ortho*-CH_3), 1.53 (s, 6H, =CCH_3), 1.26 (br s, 12H, CH_3(pin)).

^{13}C NMR (100 MHz, C_6D_5Br, 25 °C): δ [ppm] = 148.56 (dm, $^{1}J_{C-F}$ = 241 Hz, *o*-C_6F_5), 140.40 (*para*-C_6H_2), 140.18 (*ortho*-C_6H_2), 138.39 (dm, $^{1}J_{C-F}$ = 245 Hz, *p*-C_6F_5), 136.51 (dm, $^{1}J_{C-F}$ = 250 Hz, *m*-C_6F_5), 127.40 (*meta*-C_6H_2), 126.30 (=CCH_3(N)), 124.92-123.87 (br m, ipso-C_6F_5), 31.95 (NCH_3), 23.22 (CH_3(pin)), 21.54 (*ortho*-CH_3), 21.03 (*para*-CH_3), 7.66 (=C(N)CH_3), ^{13}C for ($OCMe_2$) was not observed.

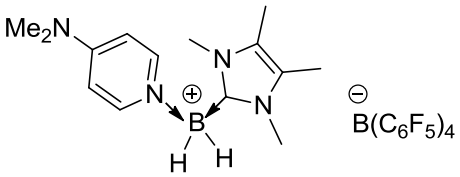
^{11}B NMR (160 MHz, C_6D_5Br, 25 °C): δ [ppm] = 33.3 (br s, *B*pin), -7.6 (br m, BH_2), -15.9 (s, $B(C_6F_5)_4$).

^{19}F NMR (376 MHz, C_6D_5Br, 25 °C): δ [ppm] = -131.58 (br d, 6F, J_{F-F} = 9 Hz, *ortho*-C_6F_5), -161.77 (t, 3F, $^{3}J_{F-F}$ = 21 Hz, *para*-C_6F_5), -165.76 (br t, 6F, $^{3}J_{F-F}$ = 18 Hz, *meta*-C_6F_5).

HRMS (*m/z*): $[IMe^4BH_2]^+$ calcd. for $C_7H_{14}BN_2$, 137.1246; found 137.1248.

HRMS (*m/z*): $[MesBpin+Li]^+$ calcd. for $C_{15}H_{23}BO_2Li$, 253.1949; found 253.1934.

Preparation of $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$ and $[IMe_4B(D)_2(DMAP)][B(C_6F_5)_4]$)



A solution of complex **1** (440 mg, 0.415 mmol) in toluene (5.0 mL) was degassed twice and backfilled with 1.6 atm H_2 (or D_2). After stirring at room temperature for 3 min, the reaction mixture was treated with DMAP (51 mg, 0.42mmol). Addition of hexane (10 mL) to the reaction mixture resulted in formation of a brown oil. The supernatant was discarded. To the brown oil hexane (2.0 mL) was added, and a white solid appeared after standing in an ultrasonic bath for 15 min. Then the supernatant was removed by filtration. The resulting white solid was washed with hexane (2 x 1.0 mL) and pumped to dryness to give $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$[8] (314 mg, 81 %). $[IMe_4B(D)_2(DMAP)][B(C_6F_5)_4]$ was prepared in a similar way with the yield of 80 %.

Additionally, MesBpin was isolated by column chromatography (PE : EA = 100 : 1) with the yield of 91% (93 mg).

$[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$: ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 7.66 (d, $^{3}J_{H-H}$ =

7.6 Hz, 2H, *H*2(py)), 6.49 (d, $^{3}J_{H\text{-}H}$ = 6.8 Hz, 2H, *H*3(py)), 3.59 (s, 6H, NCH_3), 3.20-2.70 (br m, 2H, BH_2), 3.06 (s, 6H, N(CH_3)$_2$), 2.13 (s, 6H, =CCH_3).

^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ [ppm] = 155.55 (*C*4(py)), 148.27 (dm, $^{1}J_{C\text{-}F}$ = 241 Hz, *o*-C_6F_5), 145.36 (*C*2(py)), 138.27 (dm, $^{1}J_{C\text{-}F}$ = 246 Hz, *p*-C_6F_5), 136.34 (dm, $^{1}J_{C\text{-}F}$ = 246 Hz, *m*-C_6F_5), 126.16(=*C*CH$_3$(N)), 125.40-122.99 (br m, ipso-C_6F_5), 107.43 (*C*3(py)), 39.41 (N(*C*H$_3$)$_2$), 32.62 (N*C*H$_3$), 8.53 (=C(N)*C*H$_3$).

^{11}B NMR (160 MHz, $CDCl_3$, 25 °C): δ [ppm] = -14.7 (br s, *B*H$_2$), -16.7 (s, *B*(C_6F_5)$_4$).

^{19}F NMR (376 MHz, $CDCl_3$, 25 °C): δ [ppm] = -131.21 (br s, 6F, *ortho*-C_6F_5), -161.77 (t, 3F, $^{3}J_{F\text{-}F}$ = 20 Hz, *para*-C_6F_5), -165.64 (t, 6F, $^{3}J_{F\text{-}F}$ = 18 Hz, *meta*-C_6F_5).

MesBpin: ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ [ppm] = 6.79 (s, 2H, C_6H_2), 2.39 (s, 6H, ortho-CH_3), 2.26 (s, 3H, para-CH_3), 1.39 (s, 12H, B*pin*).

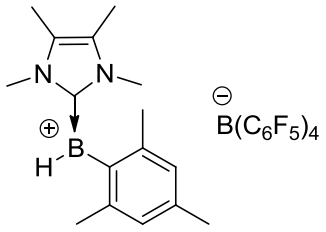
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ [ppm] = 142.26 (*ortho*-C_6H_2), 139.04 (*para*-C_6H_2), 127.58 (*meta*-C_6H_2), 83.57 (*C*(CH$_3$)$_2$), 25.08 (C(*C*H$_3$)$_2$), 22.32 (*ortho*-*C*H$_3$), 21.35 (*para*-*C*H$_3$).

^{11}B NMR (160 MHz, $CDCl_3$, 25 °C): δ [ppm] = 32.3 (s).

[IMe$_4$B(D)$_2$(DMAP)][B(C_6F_5)$_4$]: ^{2}H NMR (500 MHz, $CHCl_3$, 25 °C): δ [ppm] = 3.04 (br s, 2D, BD_2).

HRMS (*m/z*): $[M]^+$ calcd. for $C_{14}H_{22}D_2BN_4$, 261.2217; found 261.2228.

Synthesis of 7:



A solution of [Ph_3C][B(C_6F_5)$_4$] (308 mg, 0.332 mmol) in CH_2Cl_2 (1.5 mL) was added to the solution of **2** (85 mg, 0.33 mmol) in CH_2Cl_2 (0.5 mL). The reaction mixture was stirred at room temperature for 5 min. Addition of hexane (6.0 mL) to the reaction mixture resulted in formation of a brown oil. The supernatant was discarded. To the brown oil hexane (2.0 mL) was added, and a white solid appeared after standing in an ultrasonic bath for 15 min. Then the supernatant was removed by filtration. The resulting white solid was washed with hexane (2 x 1.5 mL) and pumped to dryness to give complex **7** (276 mg, 90%).

^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 6.95 (s, 2H, C_6H_2), 3.73 (s, 6H, NCH_3), 2.34 (s, 6H, =CCH_3), 2.34 (s, 3H, *para*-CH_3), 2.20 (s, 6H, *ortho*-CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 148.56 (dm, $^{1}J_{C\text{-}F}$ = 238 Hz, *o*-C_6F_5), 145.16 (m, (IMe$_4$)*C*B), 143.17 (*ortho*-C_6H_2), 138.94 (*para*-C_6H_2), 138.62 (dm, $^{1}J_{C\text{-}F}$ = 244 Hz, *p*-C_6F_5), 136.68 (dm, $^{1}J_{C\text{-}F}$ = 243 Hz, *m*-C_6F_5), 129.71 (=*C*CH$_3$(N)), 129.54 (*meta*-C_6H_2), 125.53-123.29 (br m, ipso-C_6F_5), 34.22 (N*C*H$_3$), 22.56 (*ortho*-*C*H$_3$), 21.64 (*para*-*C*H$_3$), 9.36 (=C(N)*C*H$_3$).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 60.2 (br s, *B*Mes), -16.7 (s, *B*(C_6F_5)$_4$).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -133.11 (br s, 6F, *ortho*-C_6F_5), -163.58 (t, 3F, $^{3}J_{F\text{-}F}$ = 20 Hz, *para*-C_6F_5), -167.53 (t, 6F, $^{3}J_{F\text{-}F}$ = 18 Hz, *meta*-C_6F_5).

HRMS (*m/z*): $[M]^+$ calcd. for $C_{16}H_{24}BN_2$, 255.2030; found 255.2034.

II. Mechanism studies

Kinetic experiment for the reaction between 1 and H_2

A solution of $[Ph_3C][B(C_6F_5)_4]$ (36 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL) was added to the solution of **3** (15 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL). The resulting solution was transferred to a J. Young NMR tube. After two freeze-pump-thaw cycles, the mixture was subjected to 1.5 atm H_2 at 77 K. ^{1}H NMR analysis was carried out to monitor the disappearance of **1** at 253 K, 258 K, 263 K or 268 K, while Ph_3CH signal was used as the internal standard.

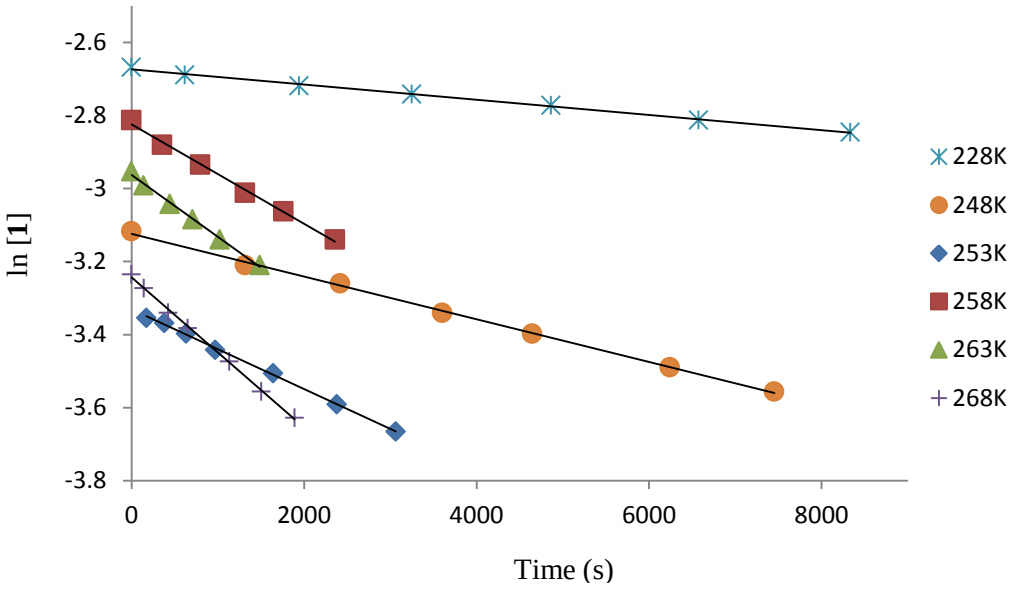


Figure S1. Plots of the reaction between **1** and H_2 (excess) at various temperatures

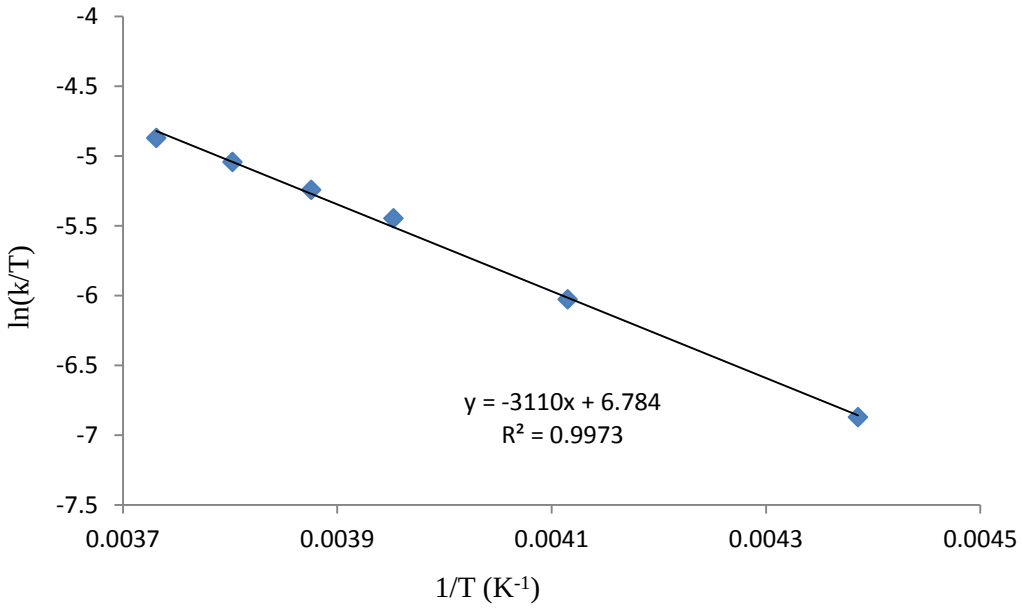


Figure S2. Eyring plot of the reaction between **1** and H_2 (excess)

Enthalpy and entropy values extracted from the plot are $\Delta H^{\neq}$ = 6.2(2) kcal mol^{-1} and $\Delta S^{\neq}$ = -33.8(6) cal mol^{-1} K^{-1} respectively. According to enthalpy and entropy values, Gibbs free energy at 298 K is $\Delta G(298K)^{\neq}$ = 16.3(4) kcal mol^{-1}.

A solution of $[Ph_3C][B(C_6F_5)_4]$ (36 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL) was added to the solution of **3** (15 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL). The resulting solution was transferred to a J. Young NMR tube. After two freeze-pump-thaw cycles, the mixture was subjected to 1.4 atm, 2.0 atm or 5.0 atm H_2 at 258 K. ^{1}H NMR analysis was carried out to monitor the disappearance of **1** at 258K, while Ph_3CH signal was used as the internal standard.

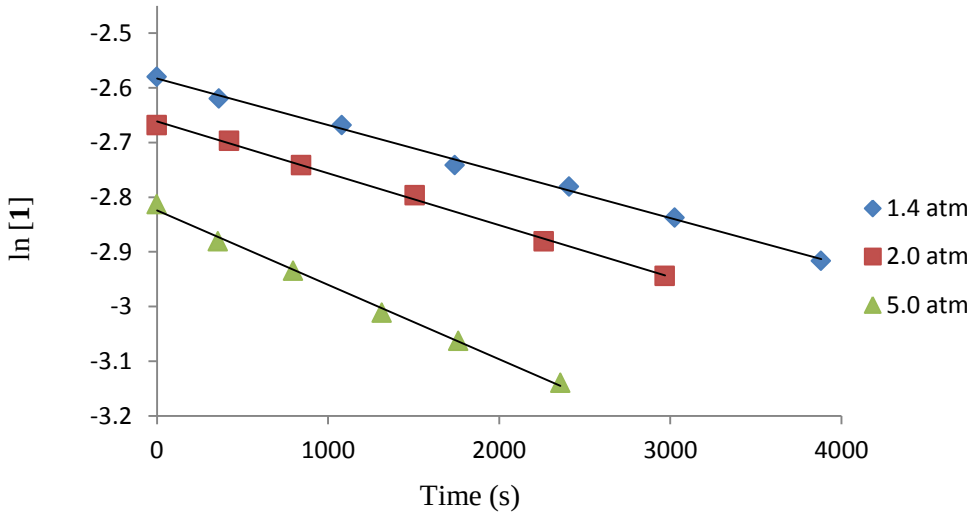


Figure S3. Plots of ln[**1**] against time at various H_2 pressure at 258 K

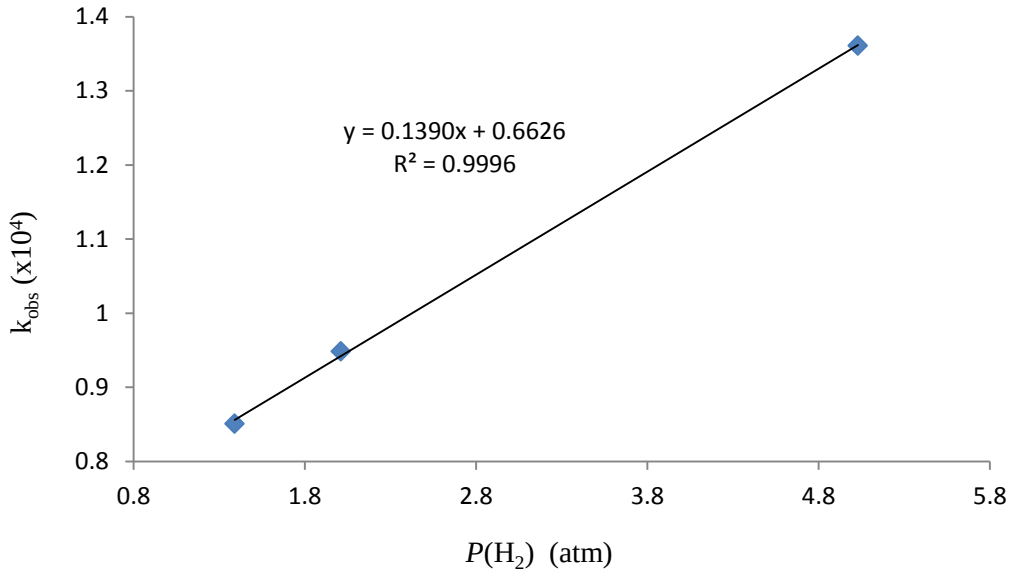


Figure S4. Plot of k_{obs} against H_2 pressure at 258 K

Kinetic experiment for the reaction between 7 and HBpin

A solution of $[Ph_3C][B(C_6F_5)_4]$ (46 mg, 0.050 mmol) in CH_2Cl_2 (0.3 mL) was added to the solution of **2** (13 mg, 0.050 mmol) in CH_2Cl_2 (0.2 mL). The resulting solution was frozen by liquid nitrogen and HBpin (64 mg, 0.50 mmol) in CH_2Cl_2 (0.5 mL) was added. The resulting mixture was stirred at 198 K, 203 K, 208 K or 213 K for varying time, which was then quenched by the solution of DMAP (8.0 mg, 0.066 mmol) in CH_2Cl_2 (0.4 mL). GC-MS analysis was carried out to monitor the yield of MesBpin, while Ph_3CH signal was used as the internal standard.

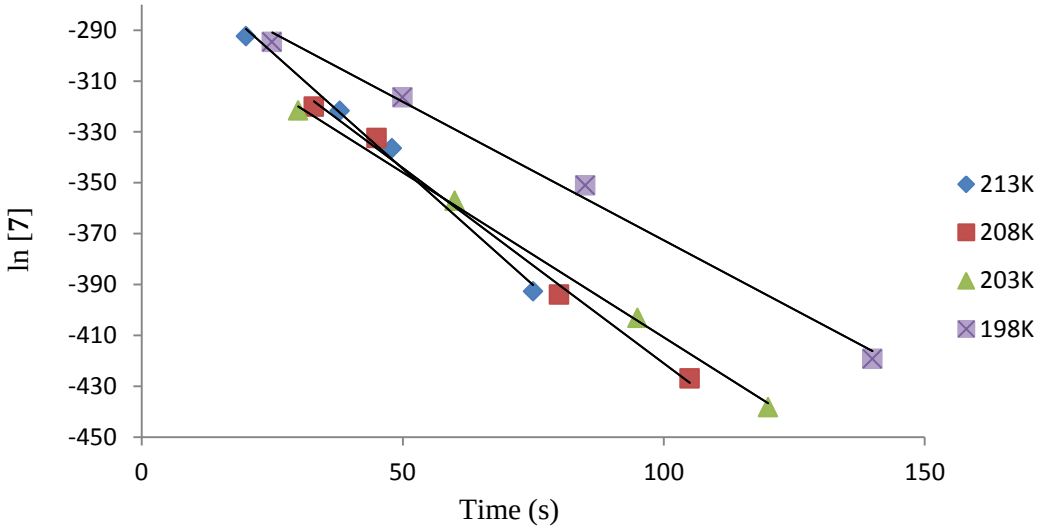


Figure S5. Plots of the reaction between **7** and HBpin at various temperatures

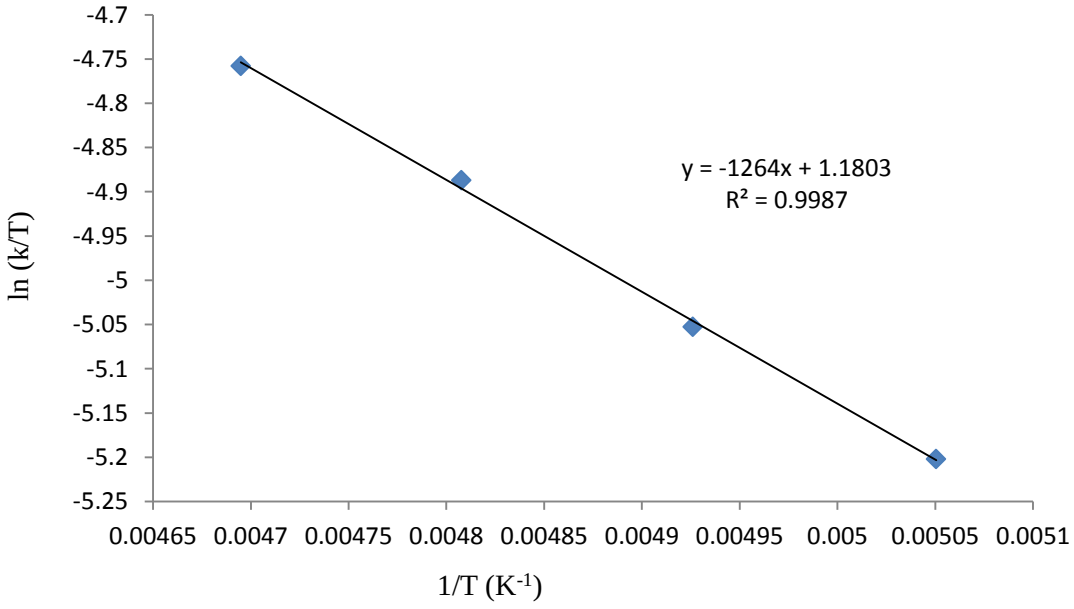


Figure S6. Eyring plot for the reaction between **7** and HBpin

Enthalpy and entropy values extracted from the plot are $\Delta H^{\neq}$ = 2.5(1) kcal mol^{-1} and $\Delta S^{\neq}$ = -44.9(3) cal mol^{-1} K^{-1} respectively. According to enthalpy and entropy values, Gibbs free energy at 298 K is $\Delta G(298K)^{\neq}$ = 15.9(2) kcal mol^{-1}.

Isotopic labelling experiment

A solution of $[Ph_3C][B(C_6F_5)_4]$ (36 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL) was added to the solution of **3** (15 mg, 0.039 mmol) in CD_2Cl_2 (0.2 mL). The resulting solution was transferred to a J. Young NMR tube. After two freeze-pump-thaw cycles, the mixture was subjected to 1.5 atm D_2 at 77 K. ^{1}H NMR analysis was carried out to monitor the disappearance of **1** at 258 K , while Ph_3CH signal was used as the internal standard. A KIE k_H/k_D = 0.80 can be calculated for this reaction.

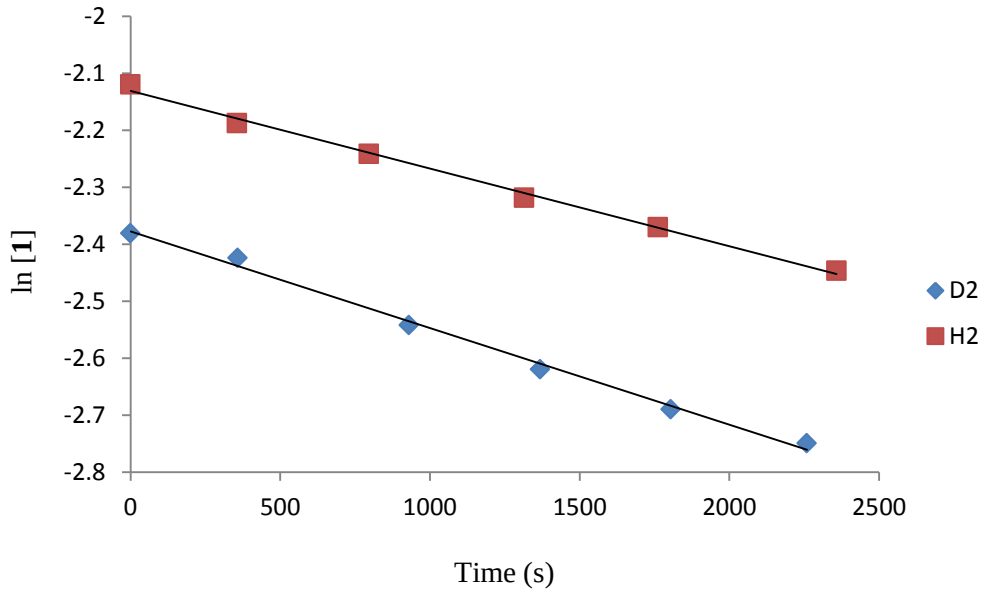


Figure S7. Plots of the reaction between **1** and H_2 or D_2 at 258 K

Crossover experiment

A solution of $[Ph_3C][B(C_6F_5)_4]$ (36 mg, 0.039 mmol) in toluene (0.3 mL) was added to the solution of **3** (7.5 mg, 0.020 mmol) and **3**-d_{21} (8.0 mg, 0.020 mmol) in CH_2Cl_2 (0.3 mL). After two freeze-pump-thaw cycles, the mixture was subjected to 1.8 bar H_2 at 283 K, 273 K, 253K, 233 K, 213 K or 195 K, which was stirred for 1.0, 2.0, 5.0, 15, 50 or 90 min, respectively. Then the reaction solution was quenched with DMAP. GC-MS analysis was carried out to determine the ratio of non-crossover products (MesBpin and (Mes-d_9)(Bpin-d_{12})) to crossover products (Mes(Bpin-d_{12})) and ((Mes-d_9)Bpin).

The ratio of rate constants for path **II** and path **III** (k_{II}/k_{III}) was calculated using the following formula:

$$k_{II}/k_{III} = \frac{(\text{the ratio of crossover products}) \times 2}{(\text{the ratio of non} - \text{crossover products}) - (\text{the ratio of crossover products})}$$

For example, k_{II}/k_{III} (195 K) = (9.7 x 2) / (90.3-9.7) = 0.24.

According to the Eyring-Polanyi equation, the linear dependence of k_{II}/k_{III} on 1/T is showed below:

$$\ln(k_{II}/k_{III}) = -\frac{\Delta\Delta H^{\neq}}{RT} + \frac{\Delta\Delta S^{\neq}}{R}$$

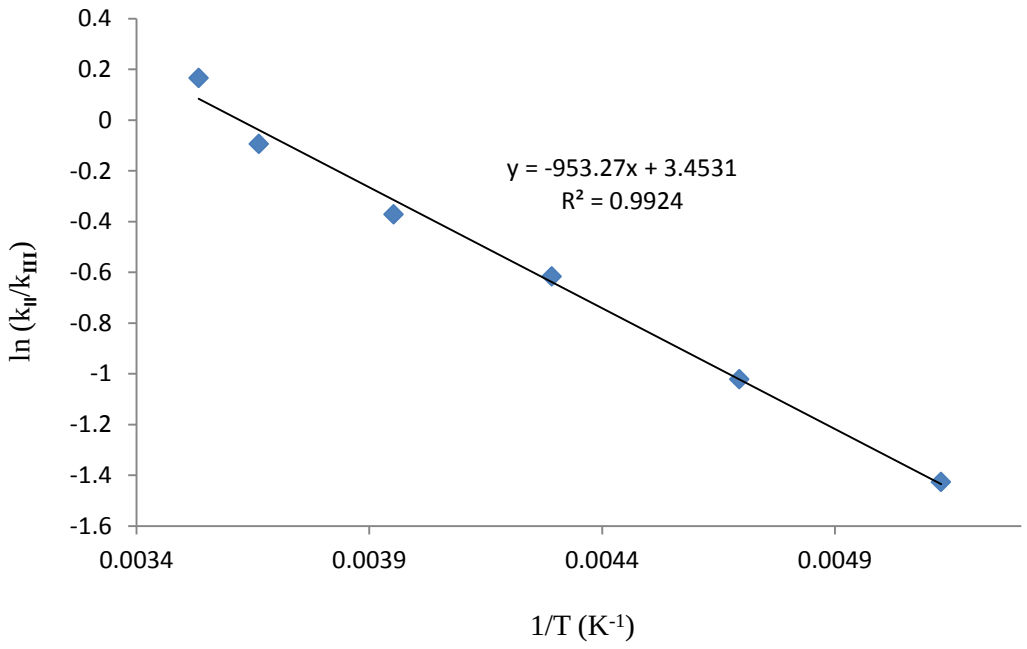


Figure S8. Eyring plot of the ratio of rate constants for path **II** and path **III**

Differences in enthalpy and entropy extracted from the plot are $\Delta\Delta H^{\neq}$ = 1.9(1) kcal mol^{-1}, $\Delta\Delta S^{\neq}$ = 6.9(4) cal mol^{-1} K^{-1} .

III. NMR spectra

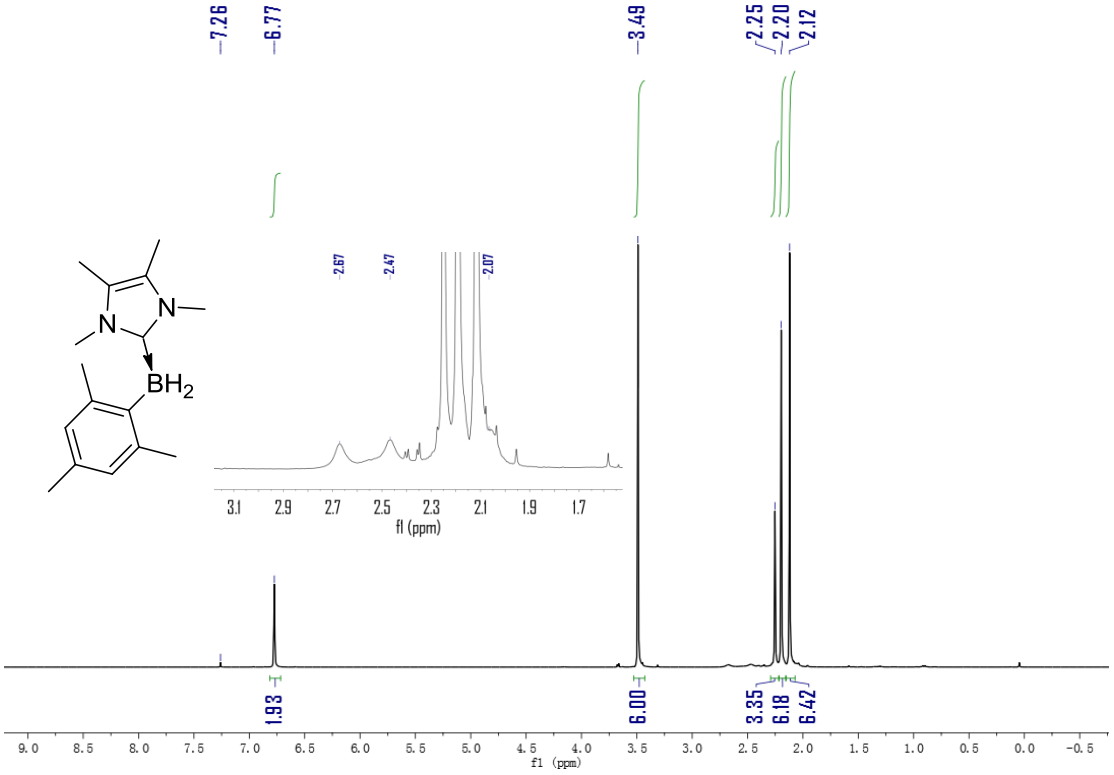


Figure S9. ^{1}H NMR spectrum of **2** in $CDCl_3$

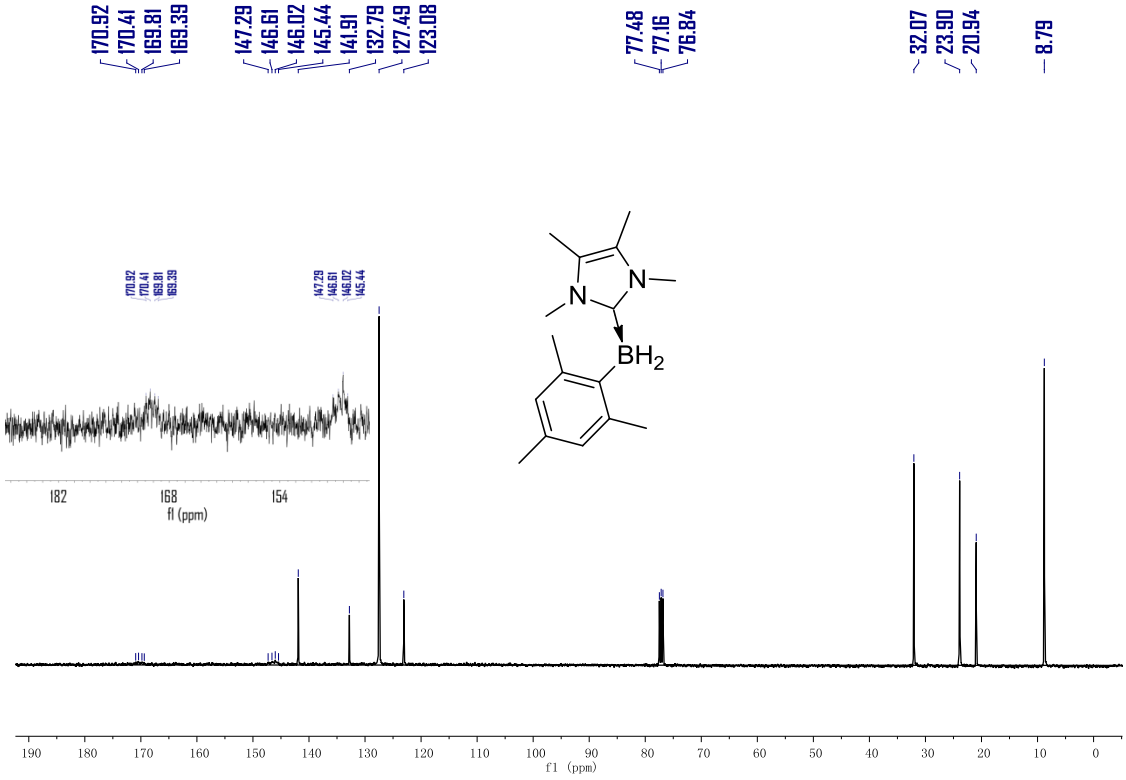


Figure S10. ^{13}C NMR spectrum of **2** in $CDCl_3$

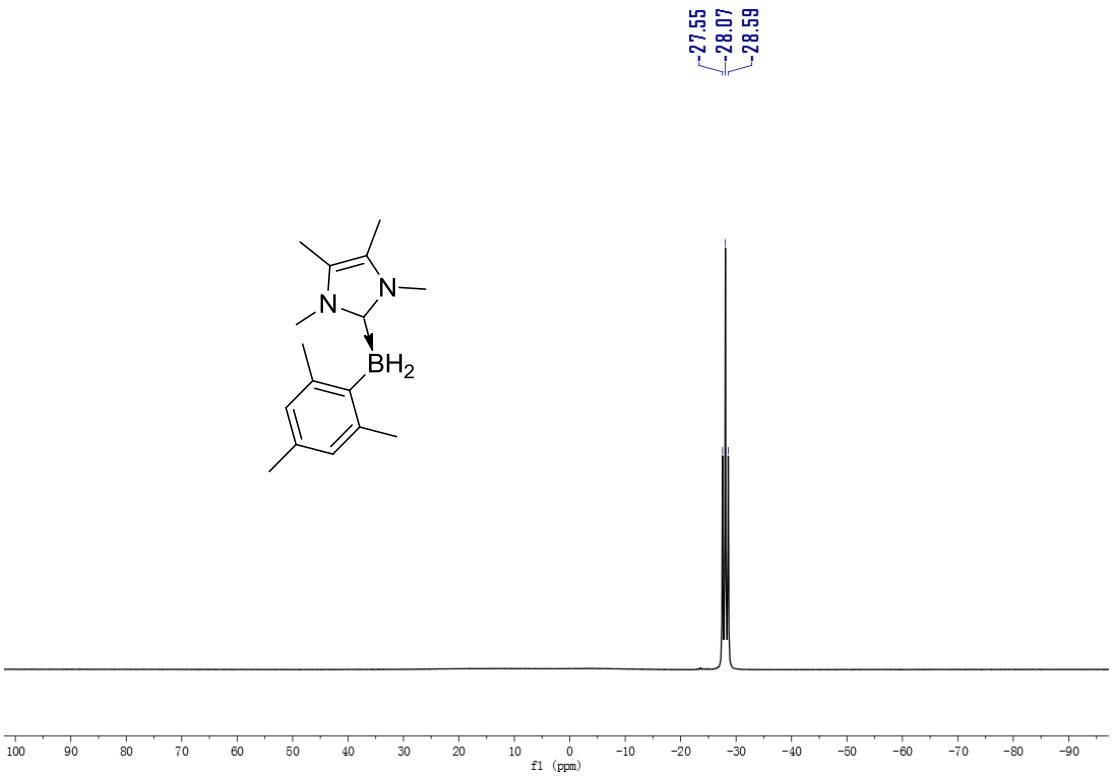


Figure S11. ^{11}B NMR spectrum of **2** in $CDCl_3$

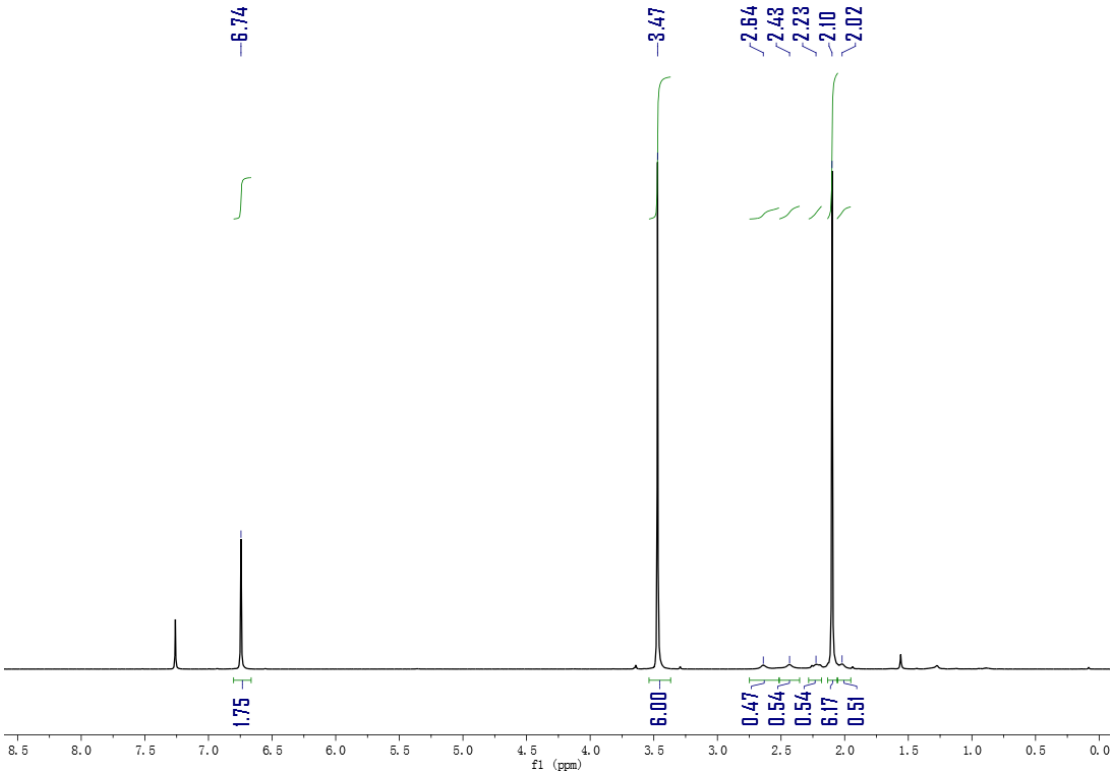


Figure S12. ^{1}H NMR spectrum of **2**-d_9 in $CDCl_3$

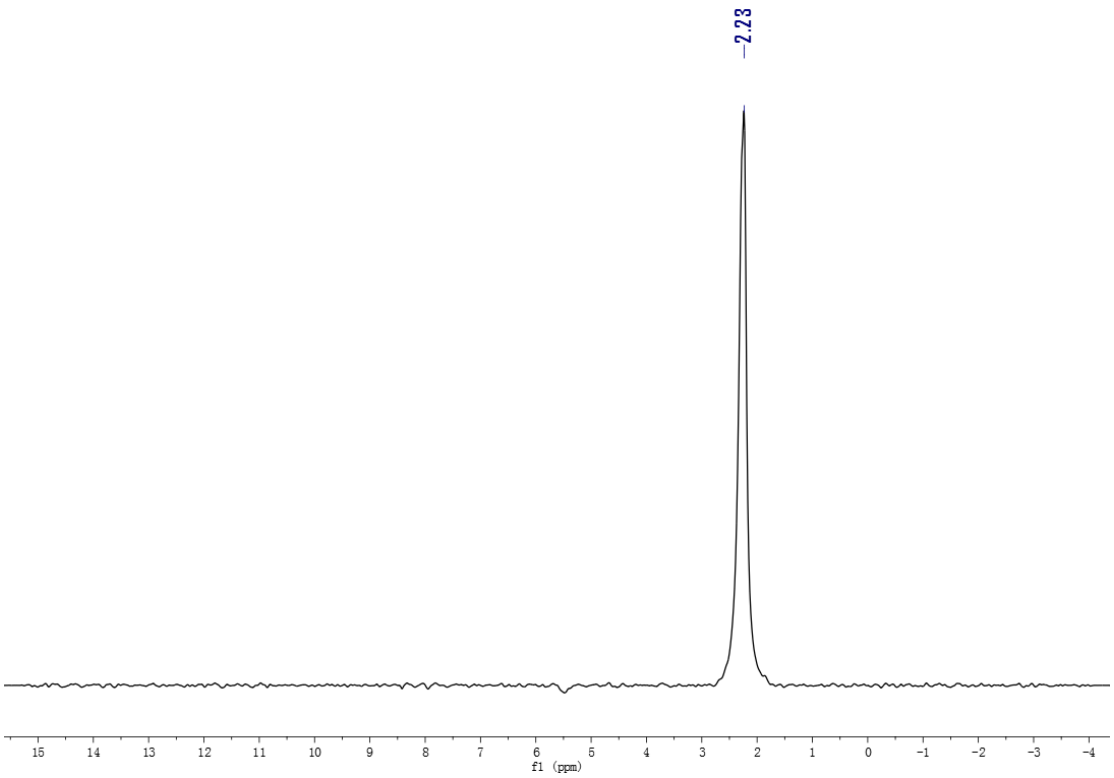


Figure S13. ^{2}H NMR spectrum of **2**-d_9 in $CHCl_3$

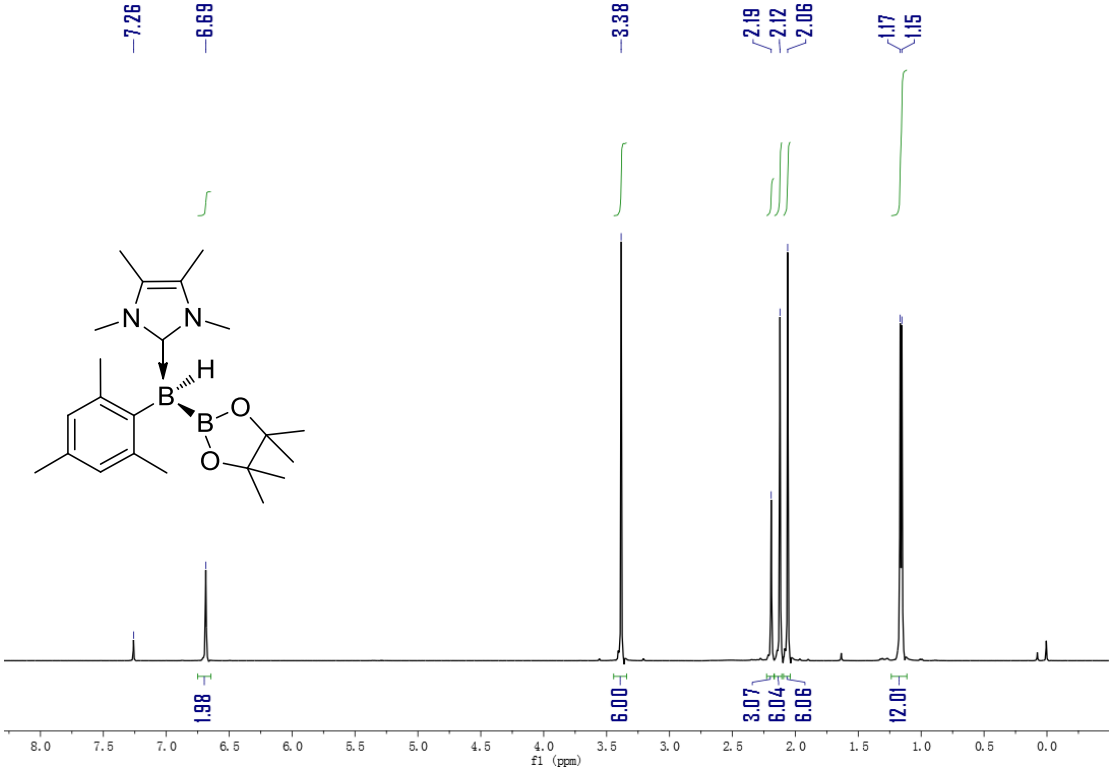


Figure S14. ^{1}H NMR spectrum of **3** in $CDCl_3$

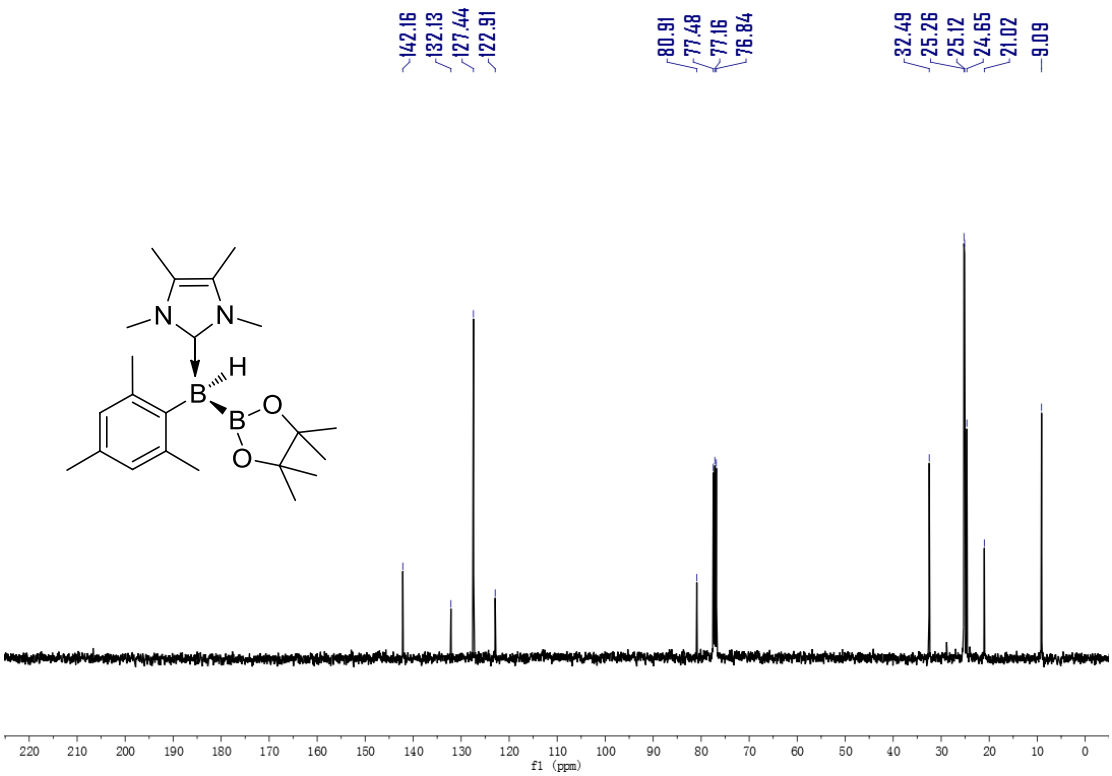


Figure S15. ^{13}C NMR spectrum of **3** in $CDCl_3$

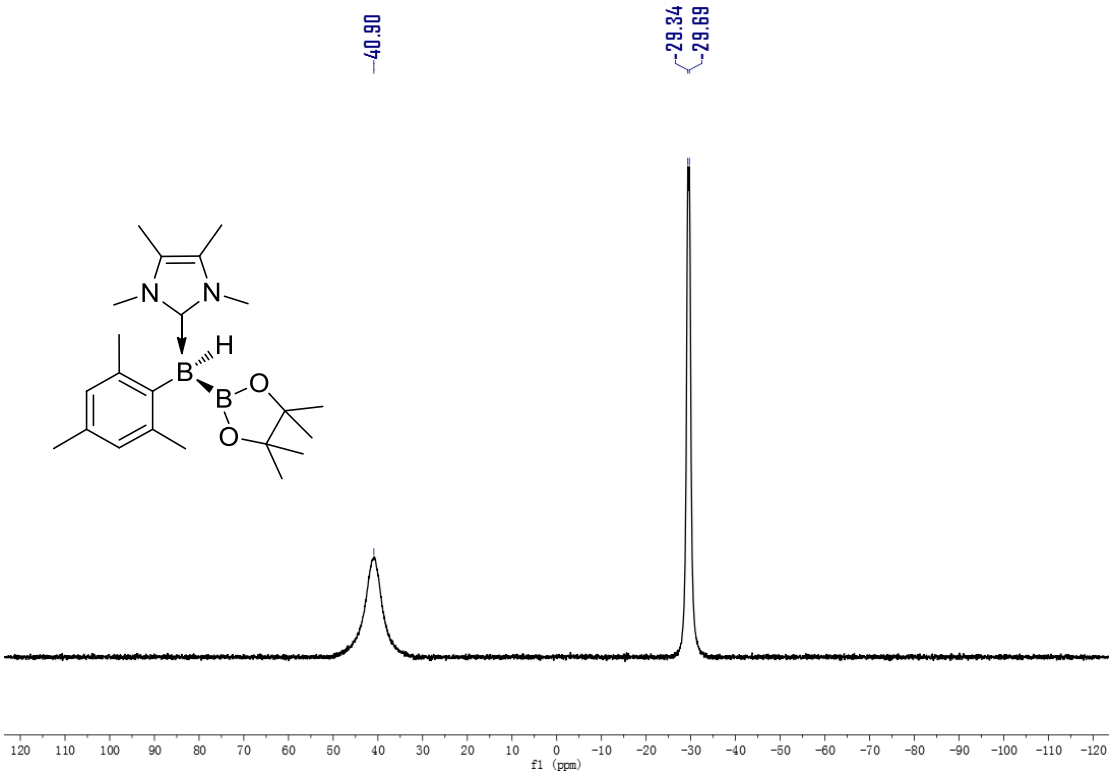


Figure S16. ^{11}B NMR spectrum of **3** in $CDCl_3$

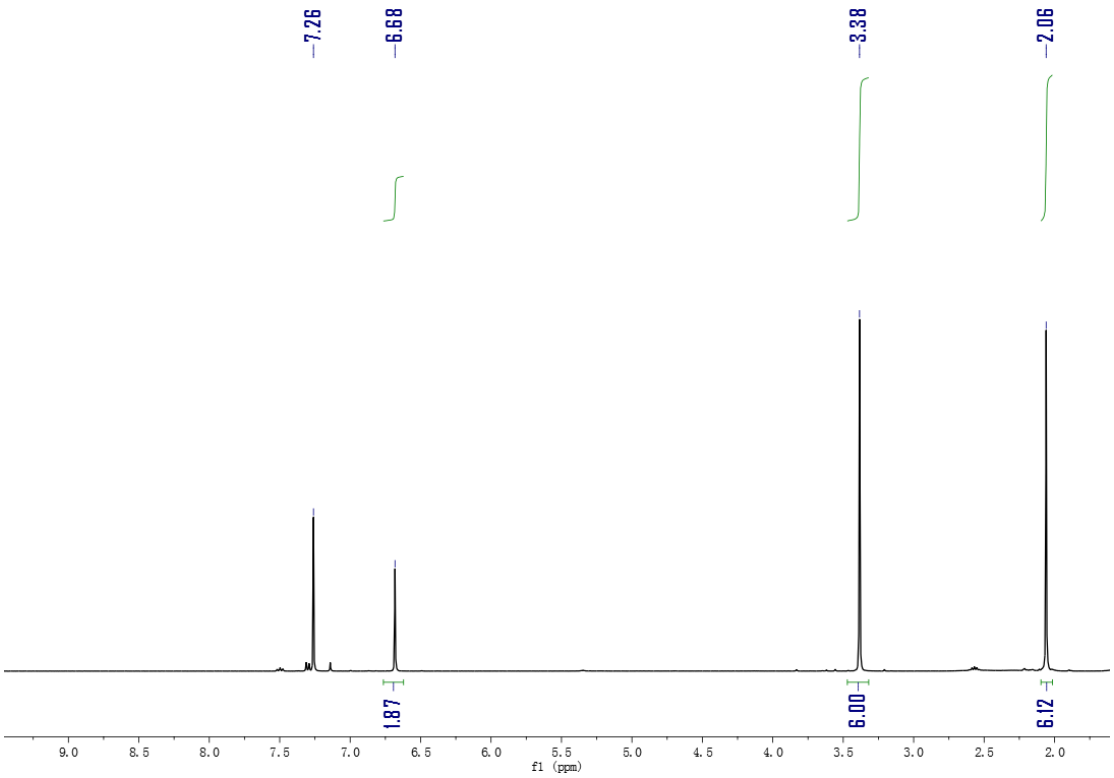


Figure S17. ^{1}H NMR spectrum of **3**-d_{21} in $CDCl_3$

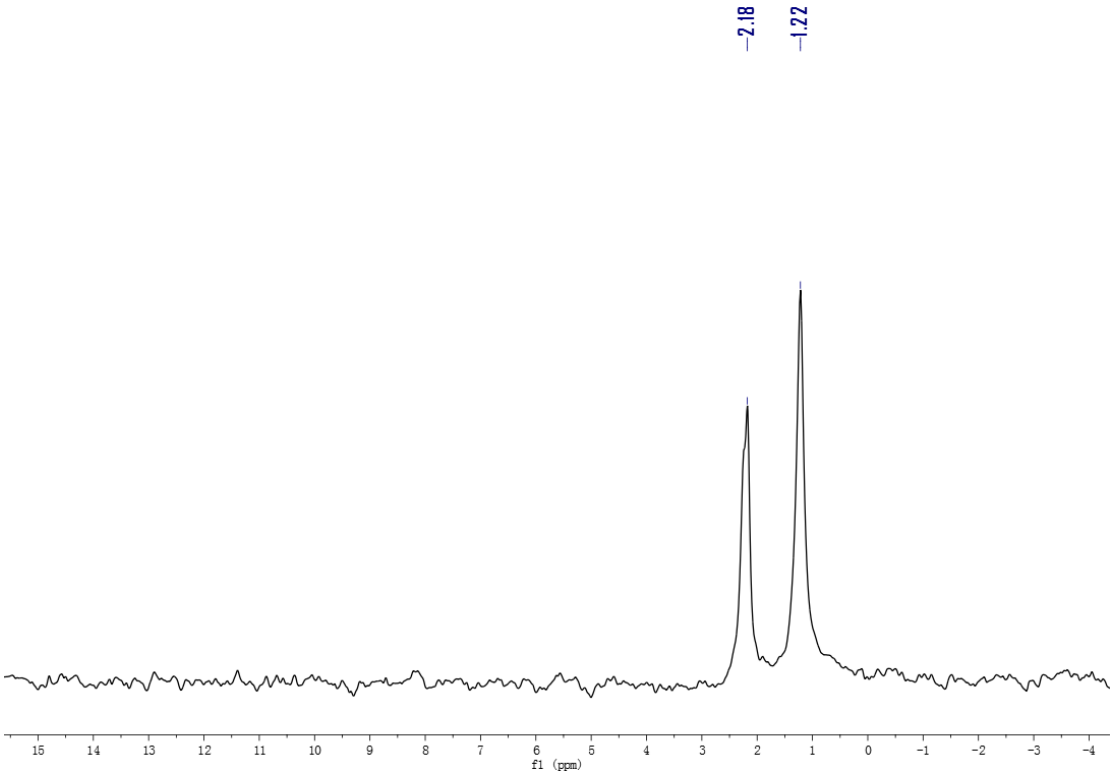


Figure S18. ^{2}H NMR spectrum of **3**-d_{21} in $CHCl_3$

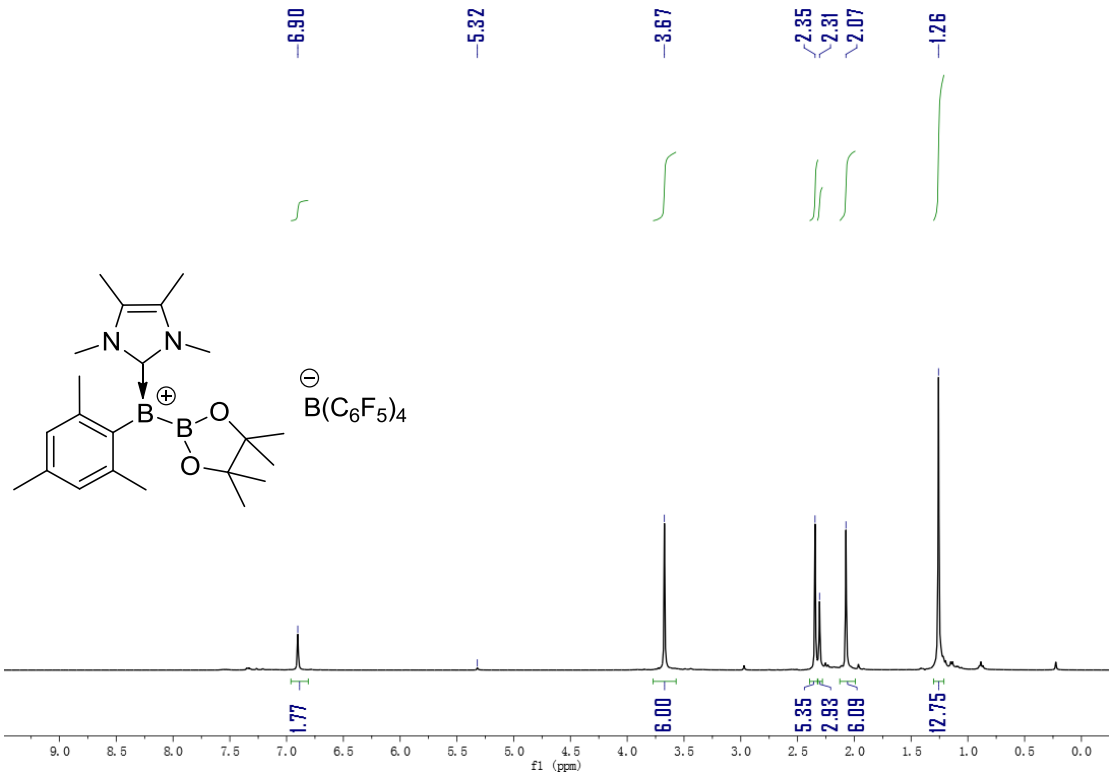


Figure S19. ^{1}H NMR spectrum of **1** in CD_2Cl_2

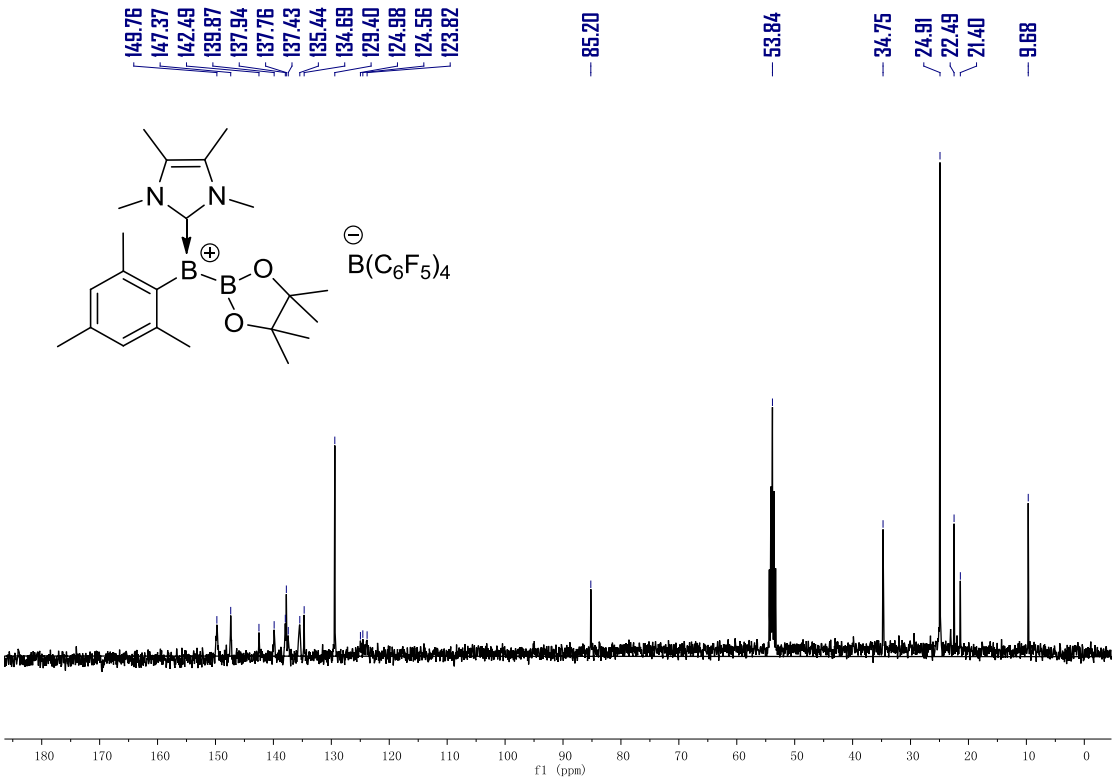


Figure S20. ^{13}C NMR spectrum of **1** in CD_2Cl_2

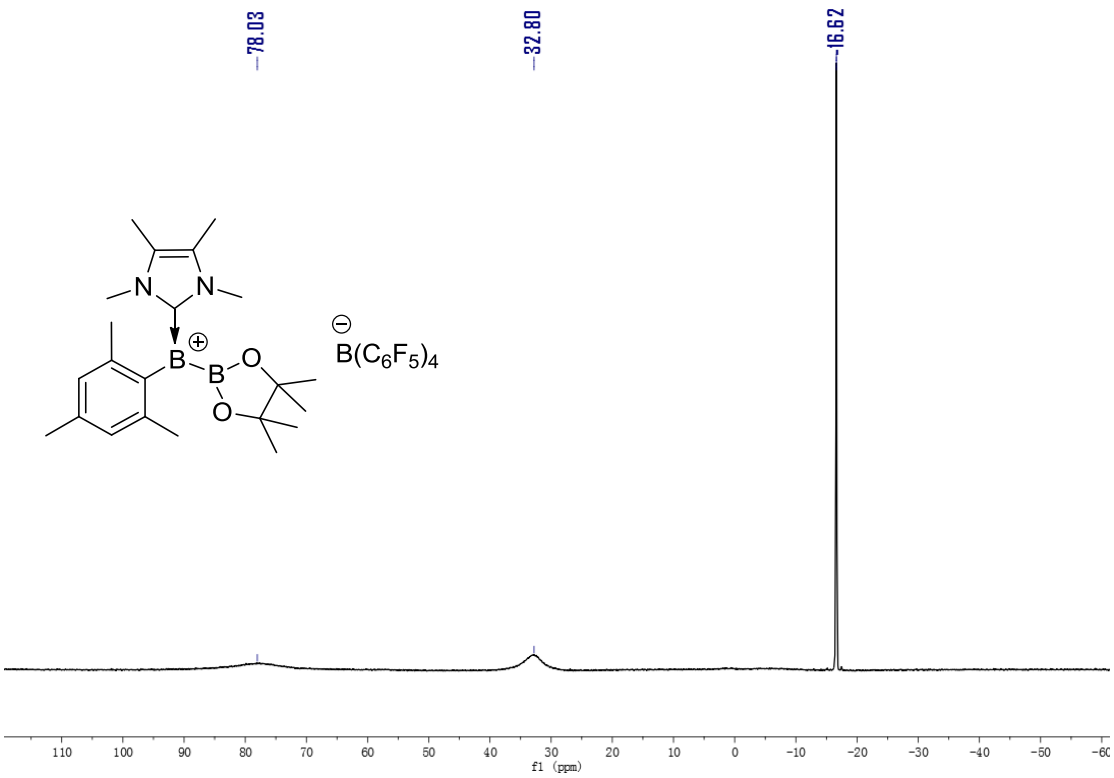


Figure S21. ^{11}B NMR spectrum of **1** in CD_2Cl_2

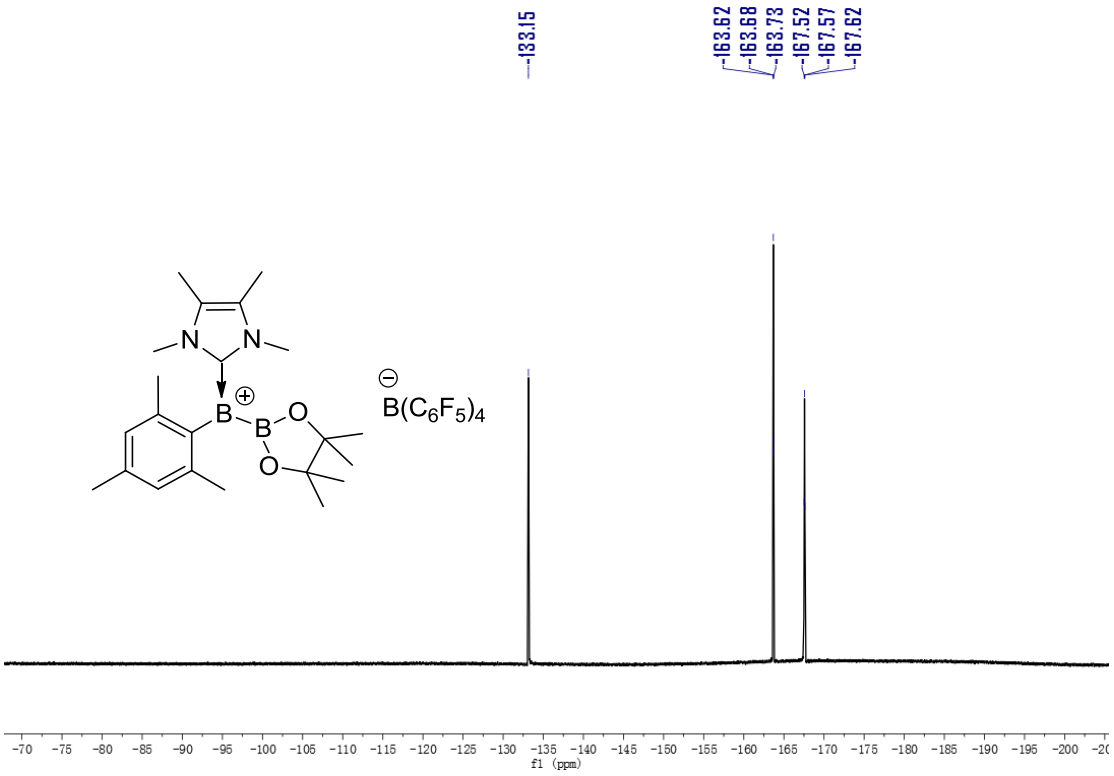


Figure S22. ^{19}F NMR spectrum of **1** in CD_2Cl_2

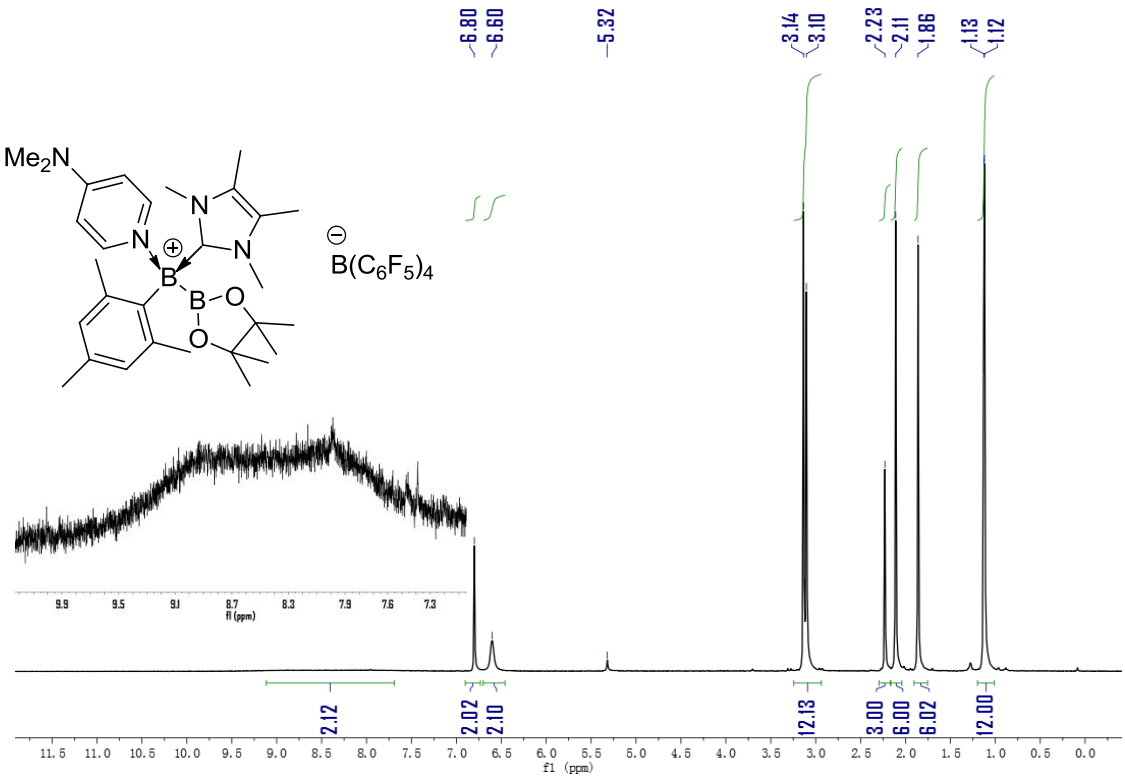


Figure S23. ^{1}H NMR spectrum of **4** in CD_2Cl_2

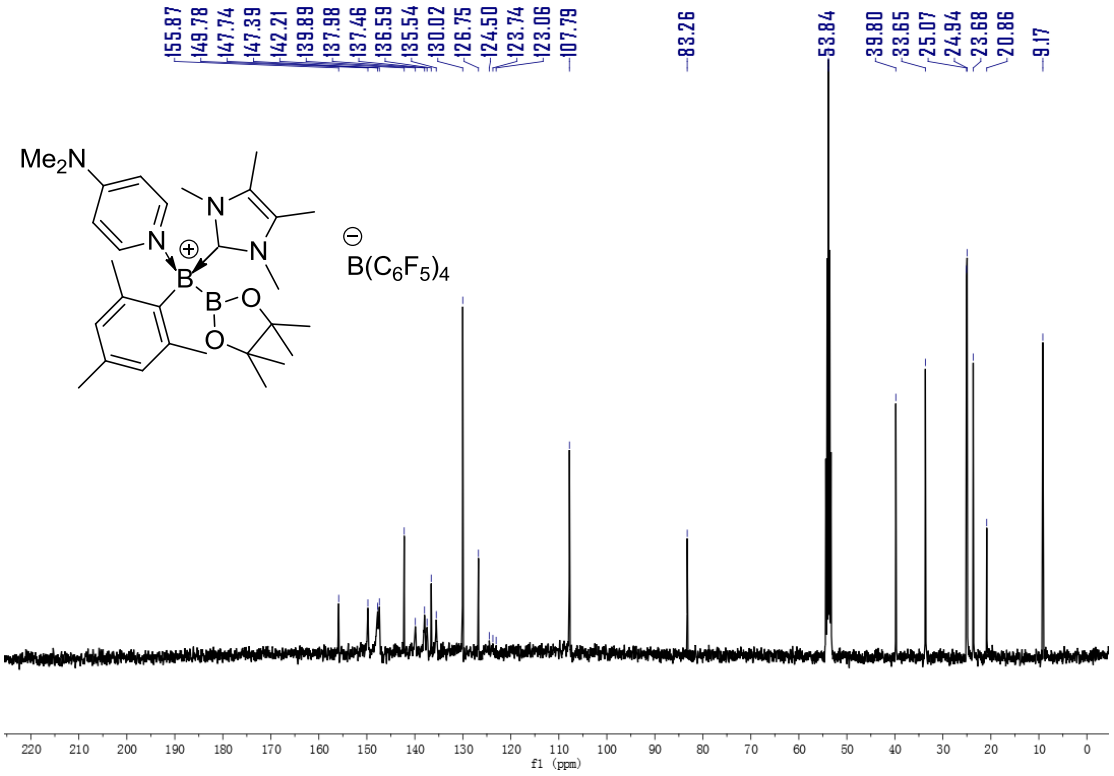


Figure S24. ^{13}C NMR spectrum of **4** in CD_2Cl_2

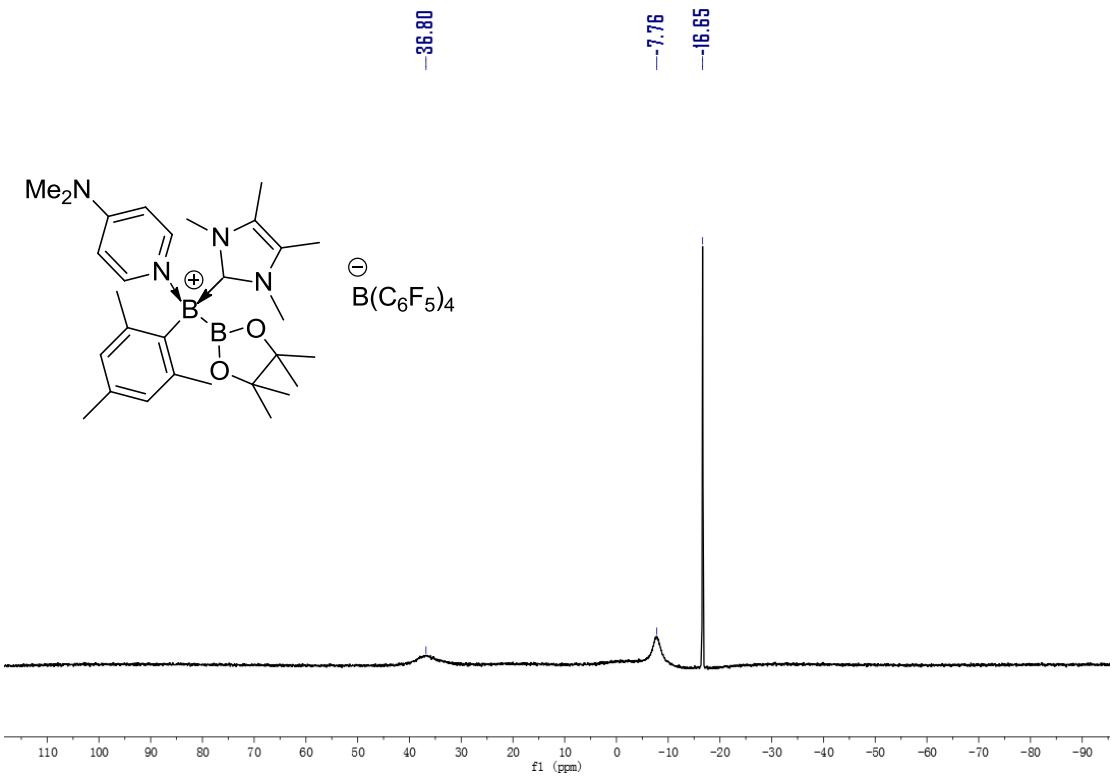


Figure S25. ^{11}B NMR spectrum of **4** in CD_2Cl_2

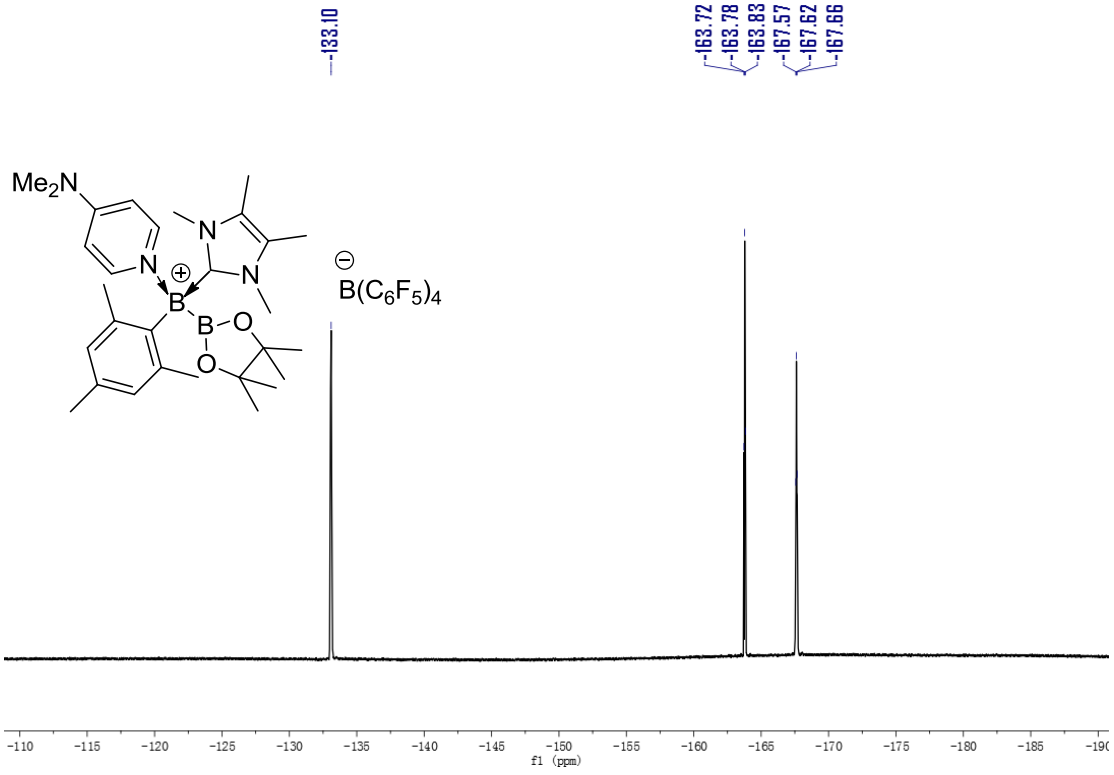


Figure S26. ^{19}F NMR spectrum of **4** in CD_2Cl_2

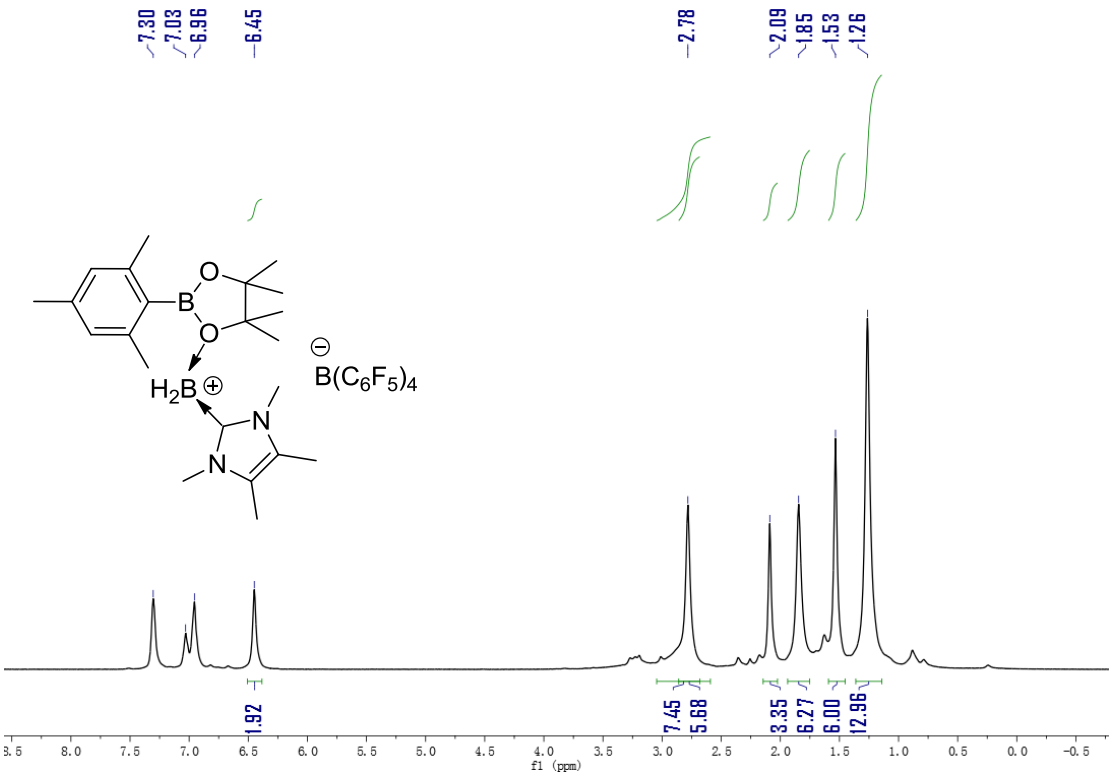


Figure S27. ^{1}H NMR spectrum of **5** in C_6D_5Br

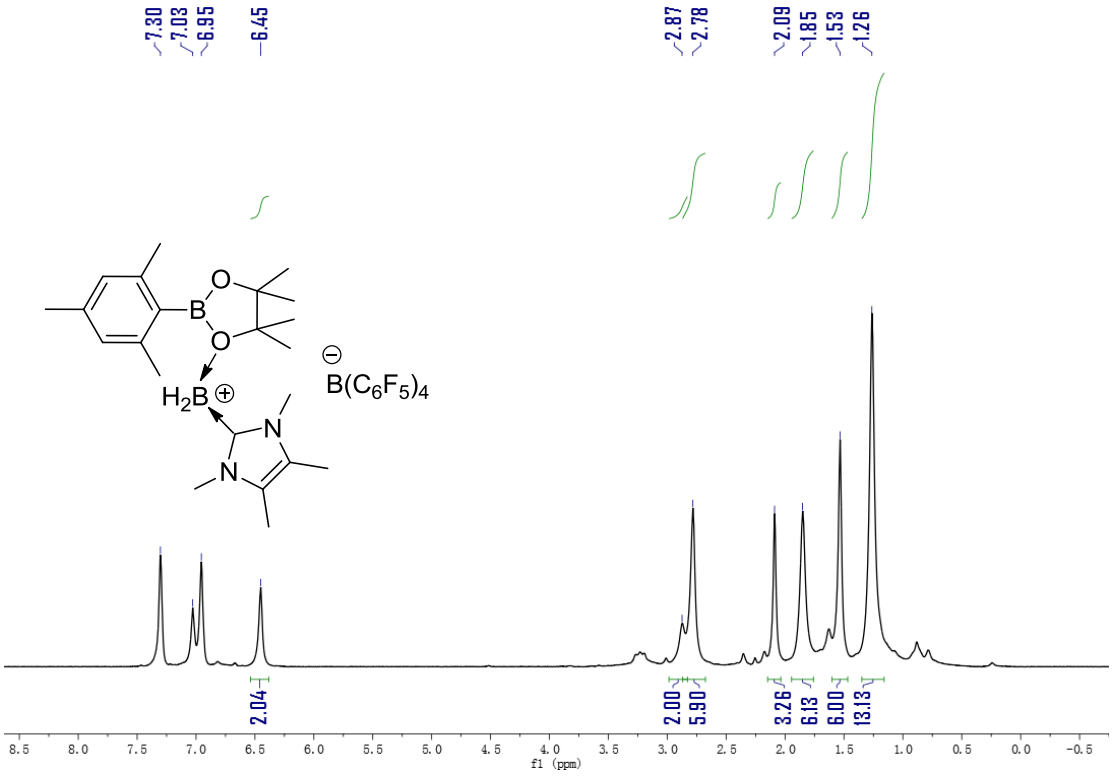


Figure S28. ^{1}H {^{11}B} NMR spectrum of **5** in C_6D_5Br

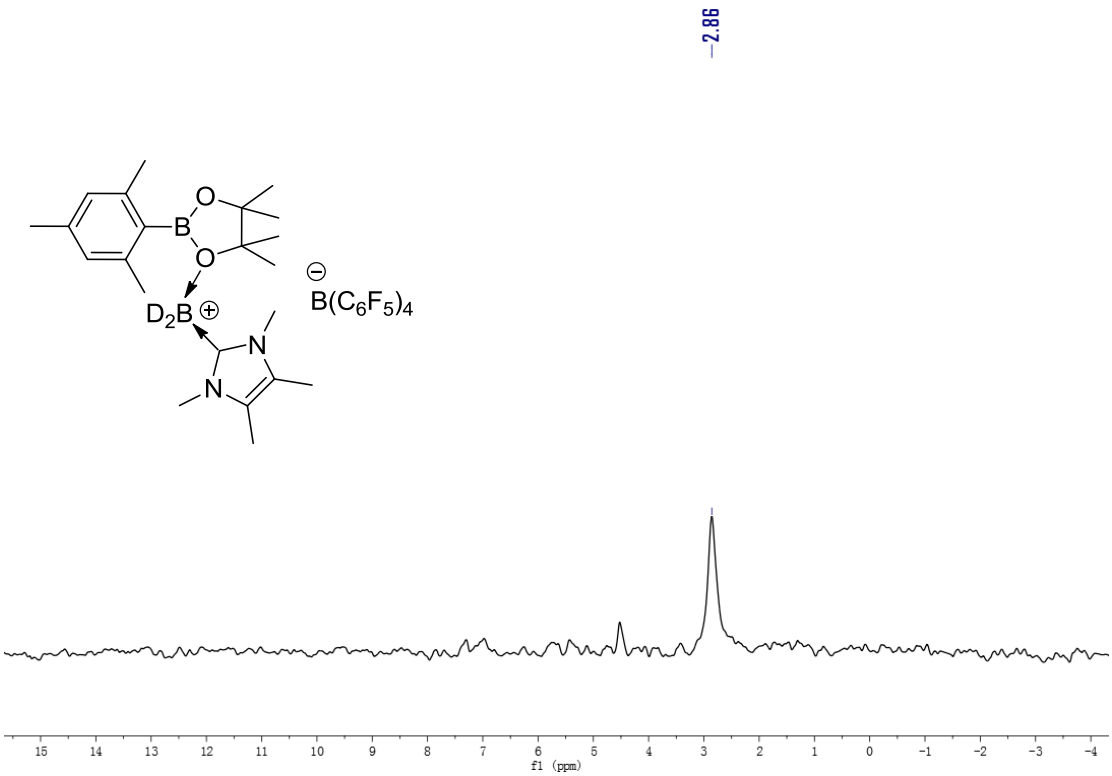


Figure S29. ^{2}D NMR spectrum of **5-D$_2$** in C_6H_5Br

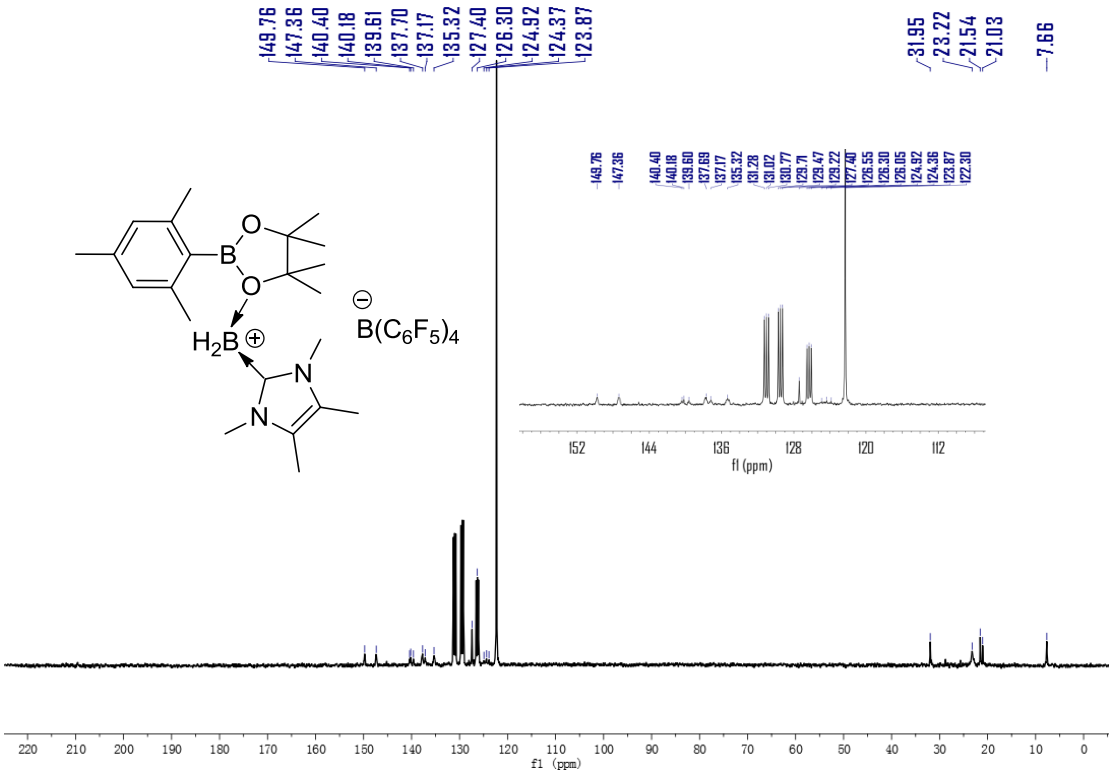


Figure S30. ^{13}C NMR spectrum of **5** in C_6D_5Br

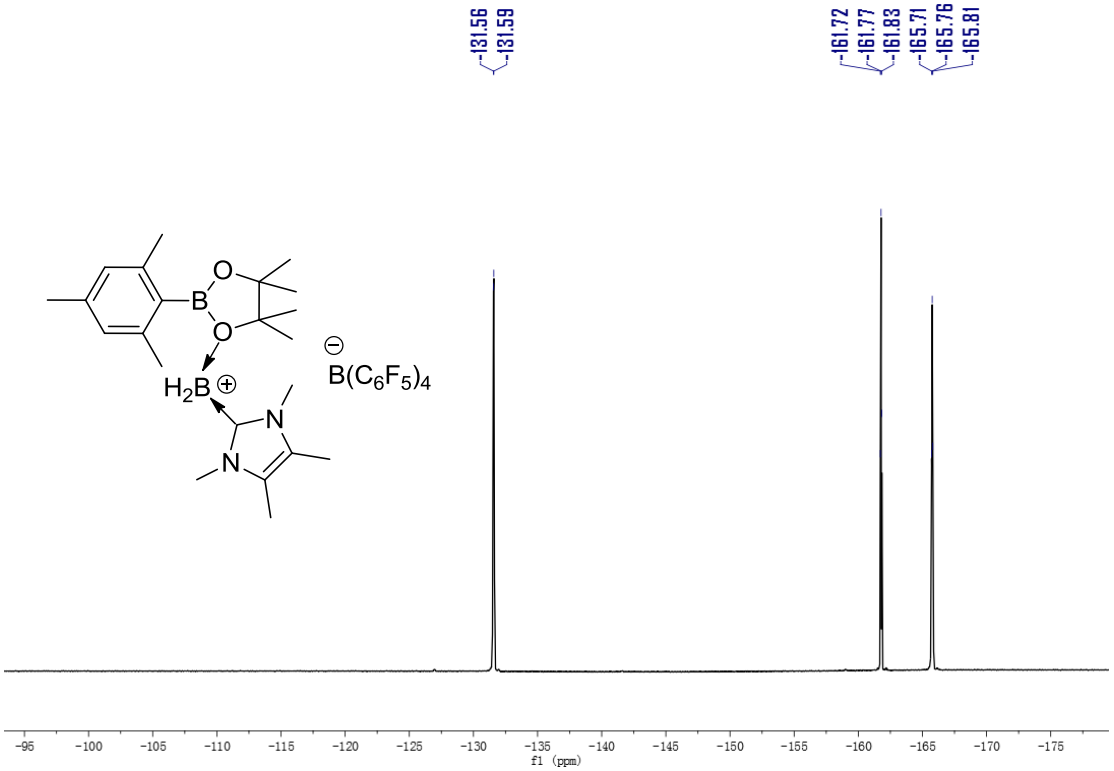


Figure S31. ^{19}F NMR spectrum of **5** in C_6D_5Br

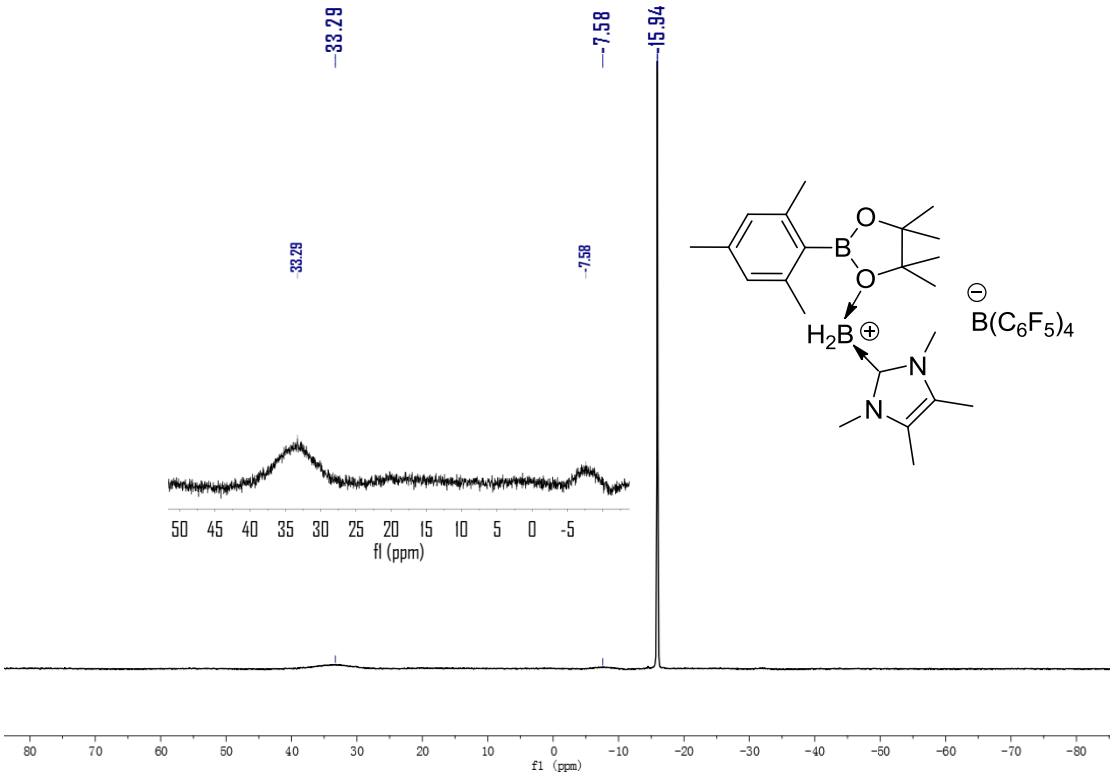


Figure S32. ^{11}B NMR spectrum of **5** in C_6D_5Br

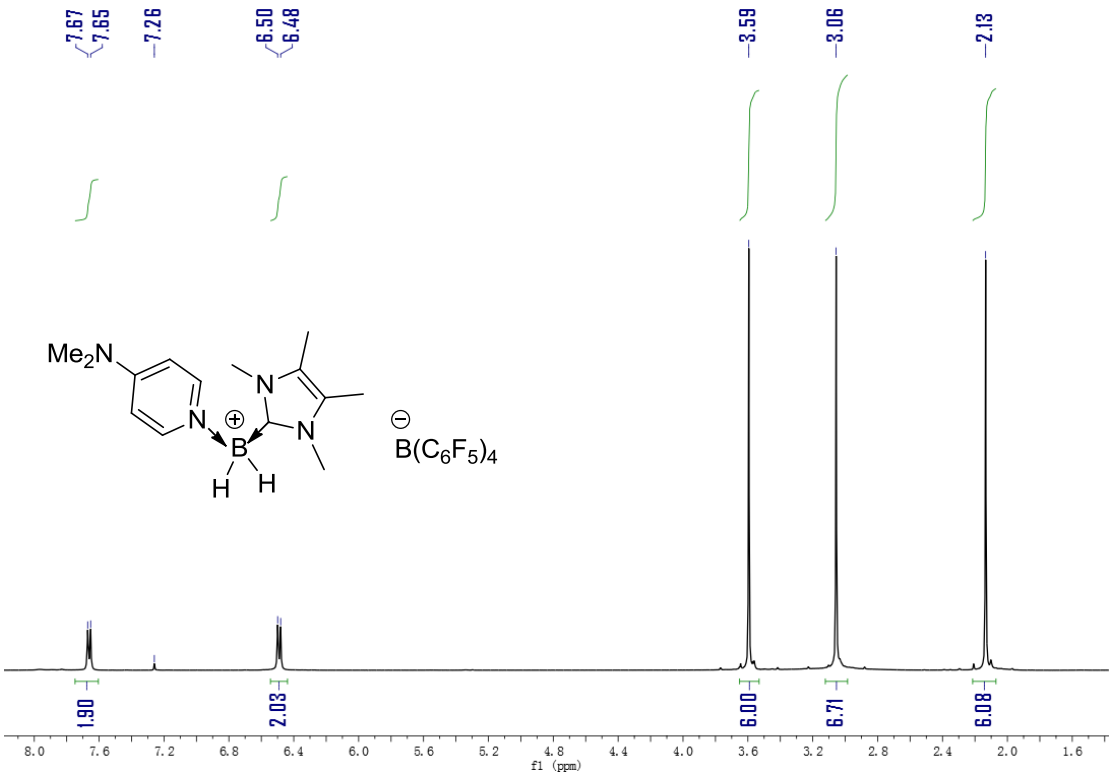


Figure S33. ^{1}H NMR spectrum of $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$ in $CDCl_3$

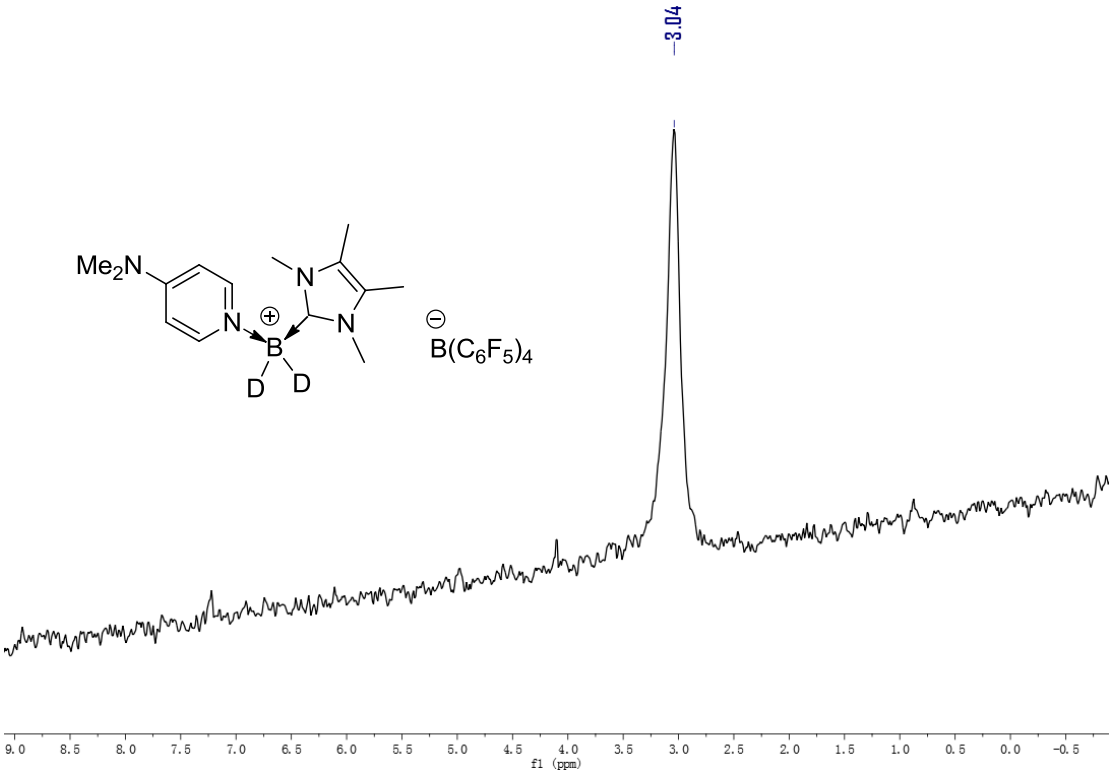


Figure S34. ^{2}H NMR spectrum of $[IMe_4B(D)_2(DMAP)][B(C_6F_5)_4]$ in $CHCl_3$

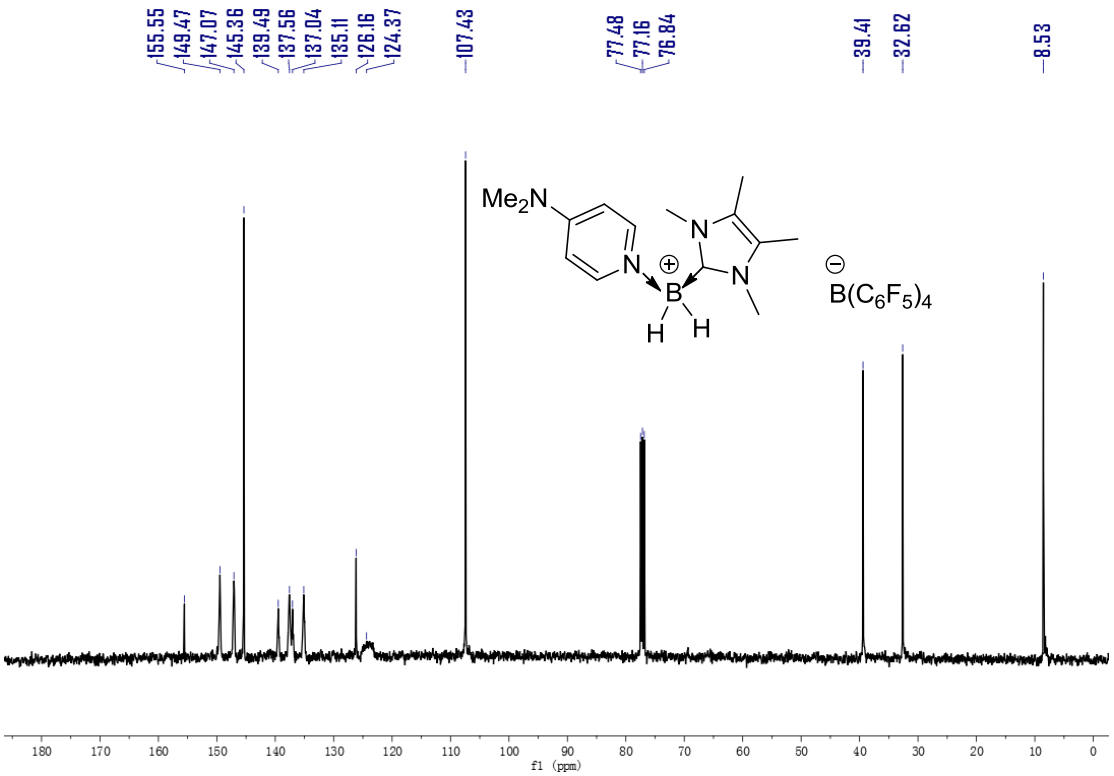


Figure S35. ^{13}C NMR spectrum of $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$ in $CDCl_3$

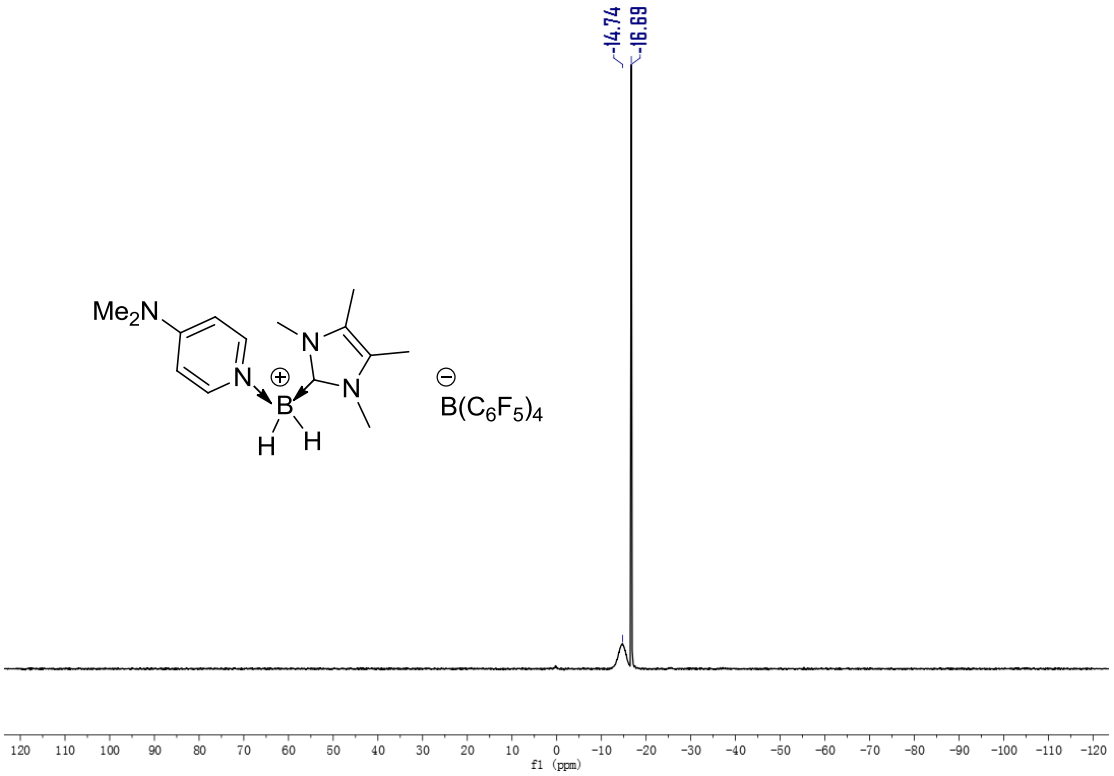


Figure S36. ^{11}B NMR spectrum of $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$ in $CDCl_3$

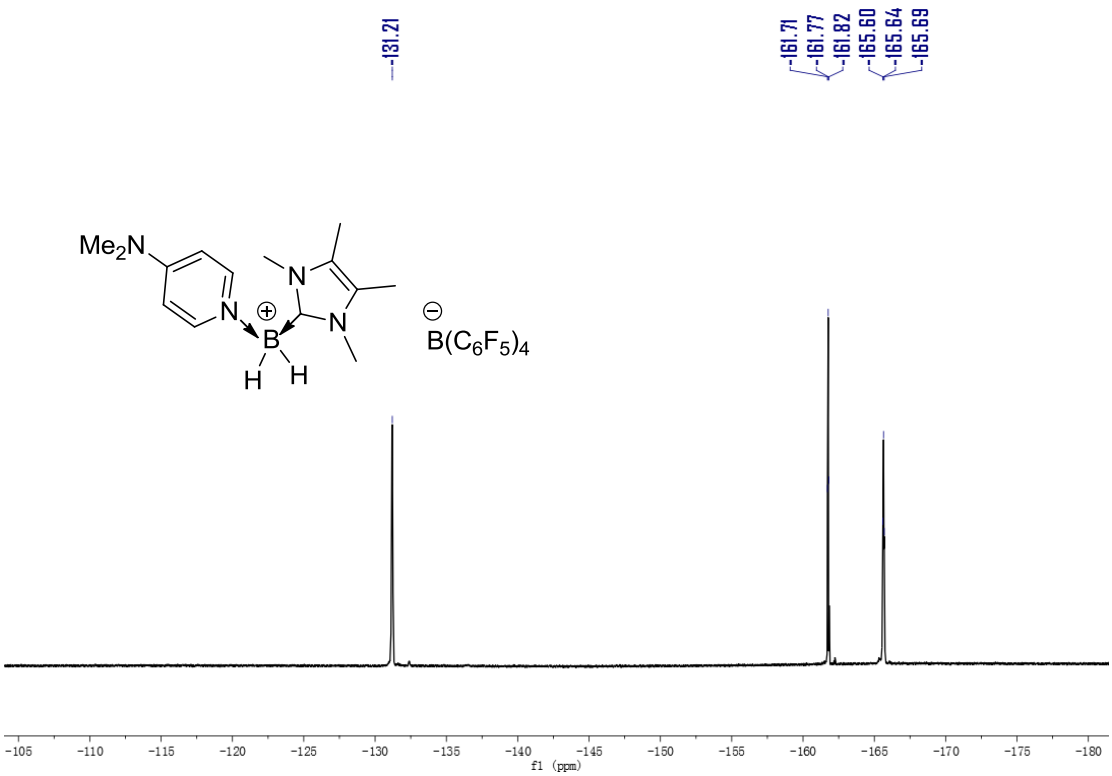


Figure S37. ^{19}F NMR spectrum of $[IMe_4B(H)_2(DMAP)][B(C_6F_5)_4]$ in $CDCl_3$

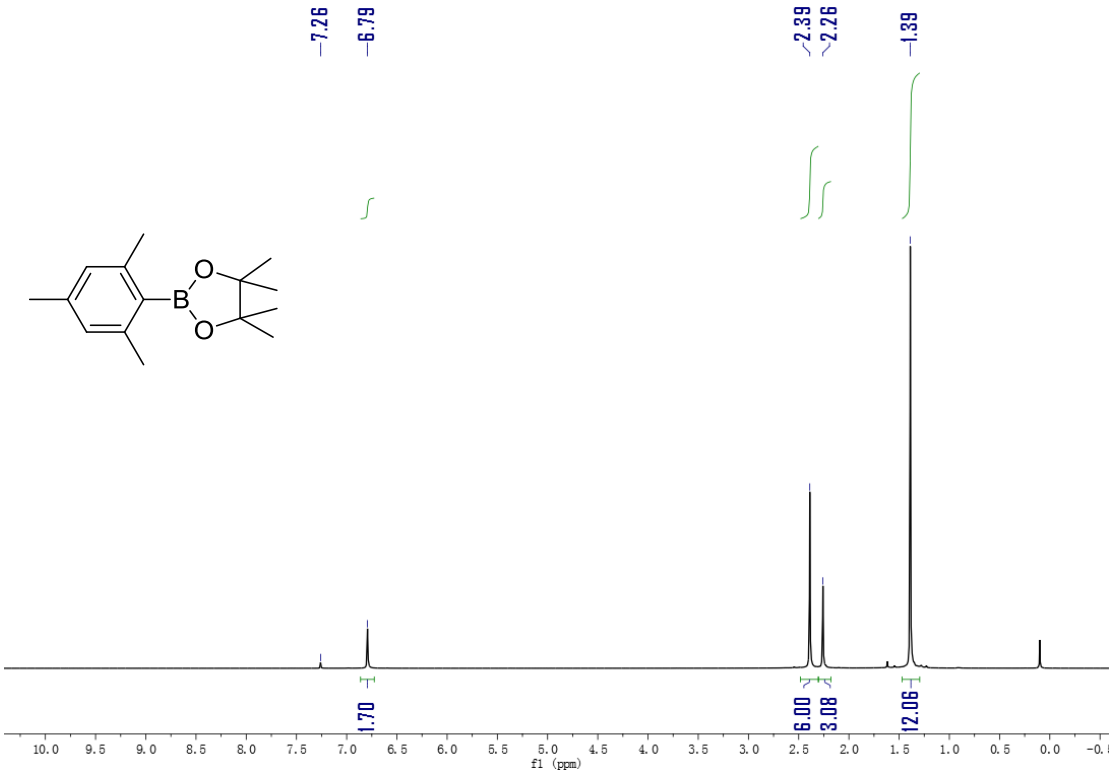


Figure S38. ^{1}H NMR spectrum of MesBpin in $CDCl_3$

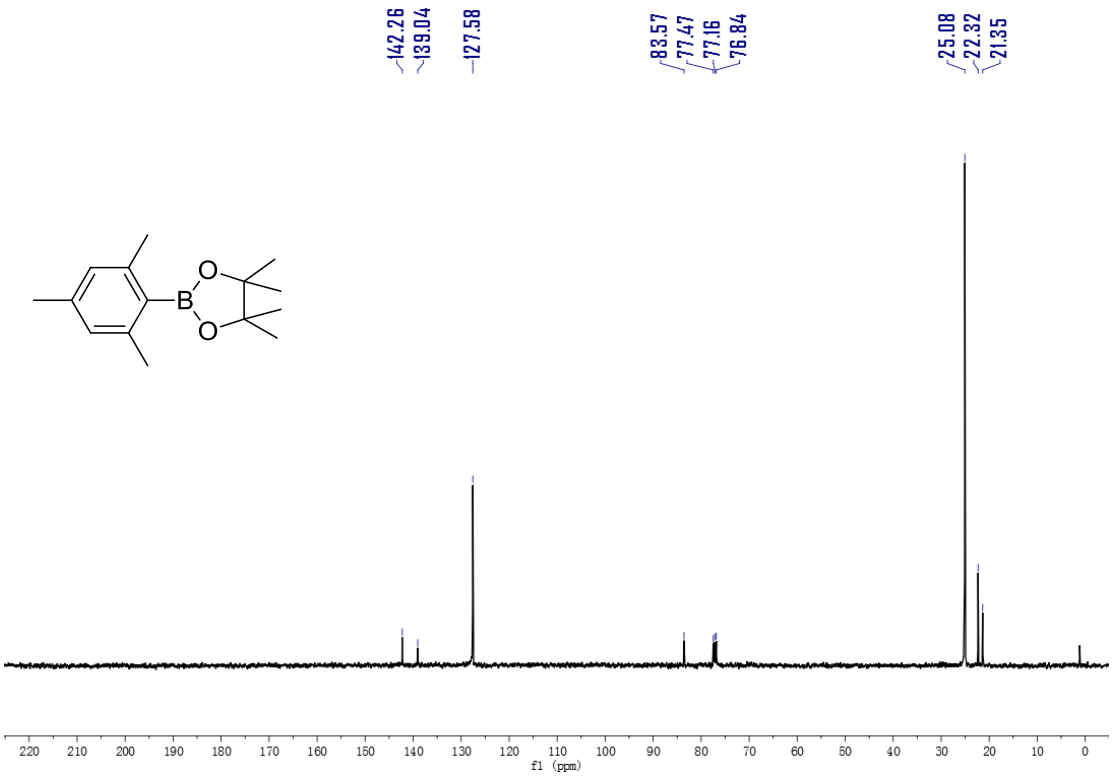


Figure S39. ^{13}C NMR spectrum of MesBpin in $CDCl_3$

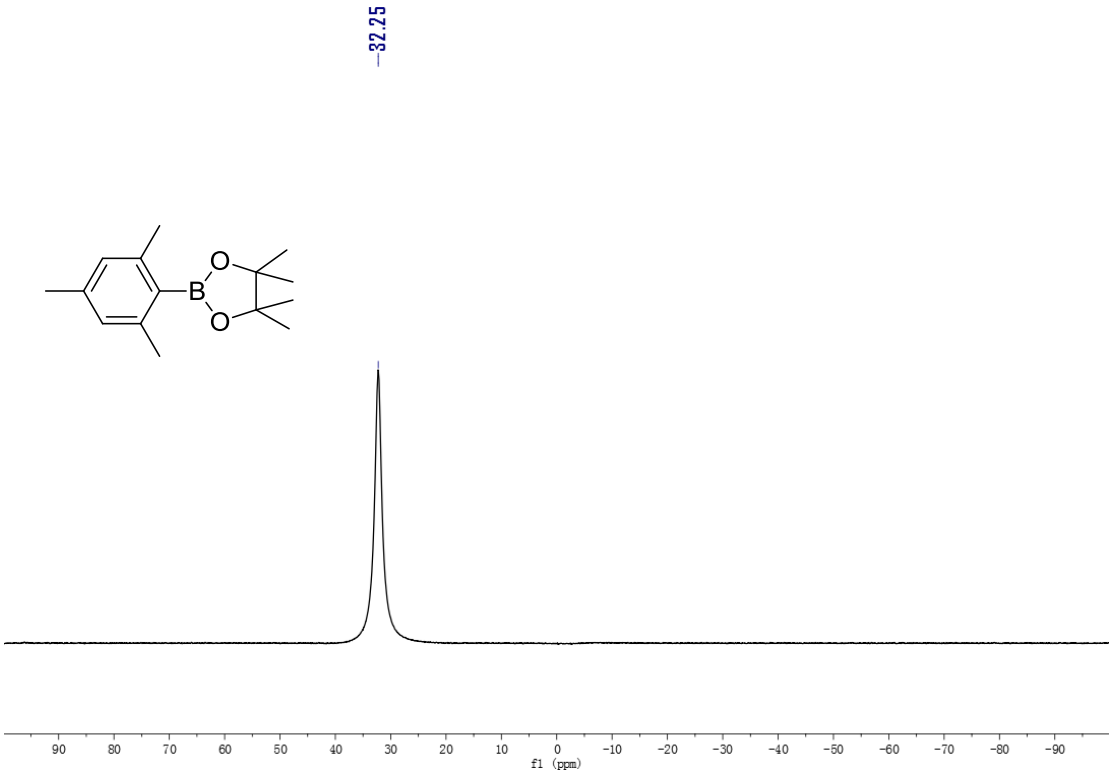


Figure S40. ^{11}B NMR spectrum of MesBpin in $CDCl_3$

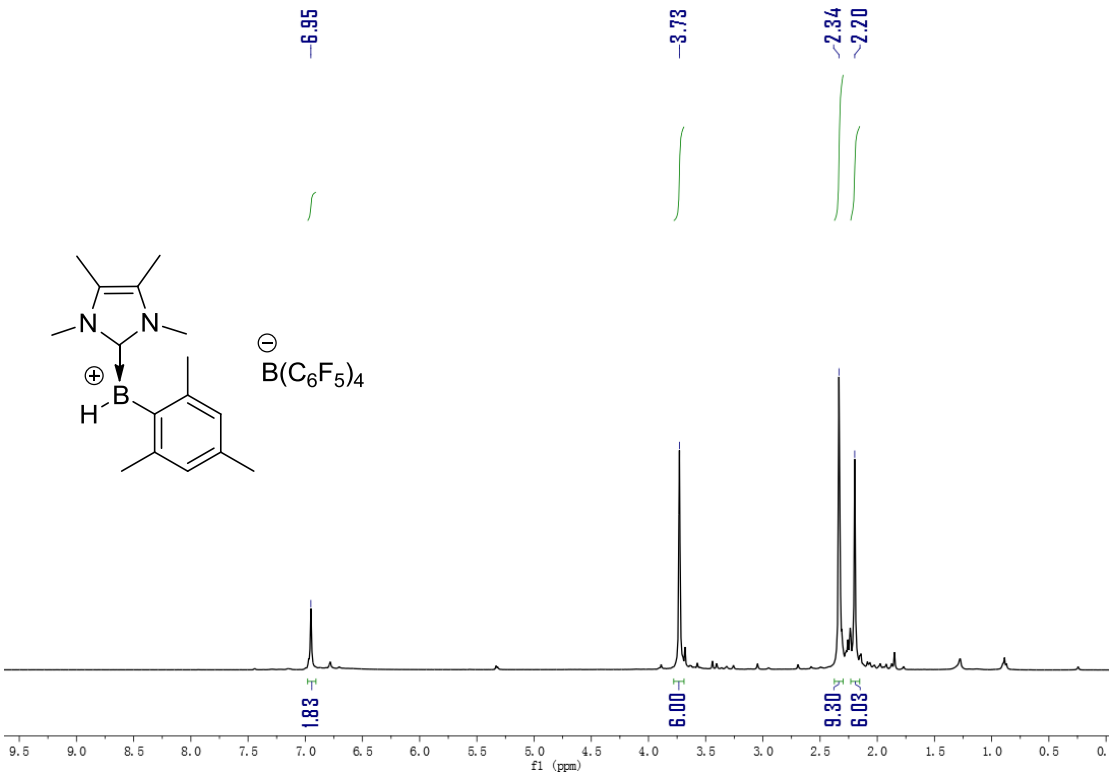


Figure S41. ^{1}H NMR spectrum of **7** in CD_2Cl_2

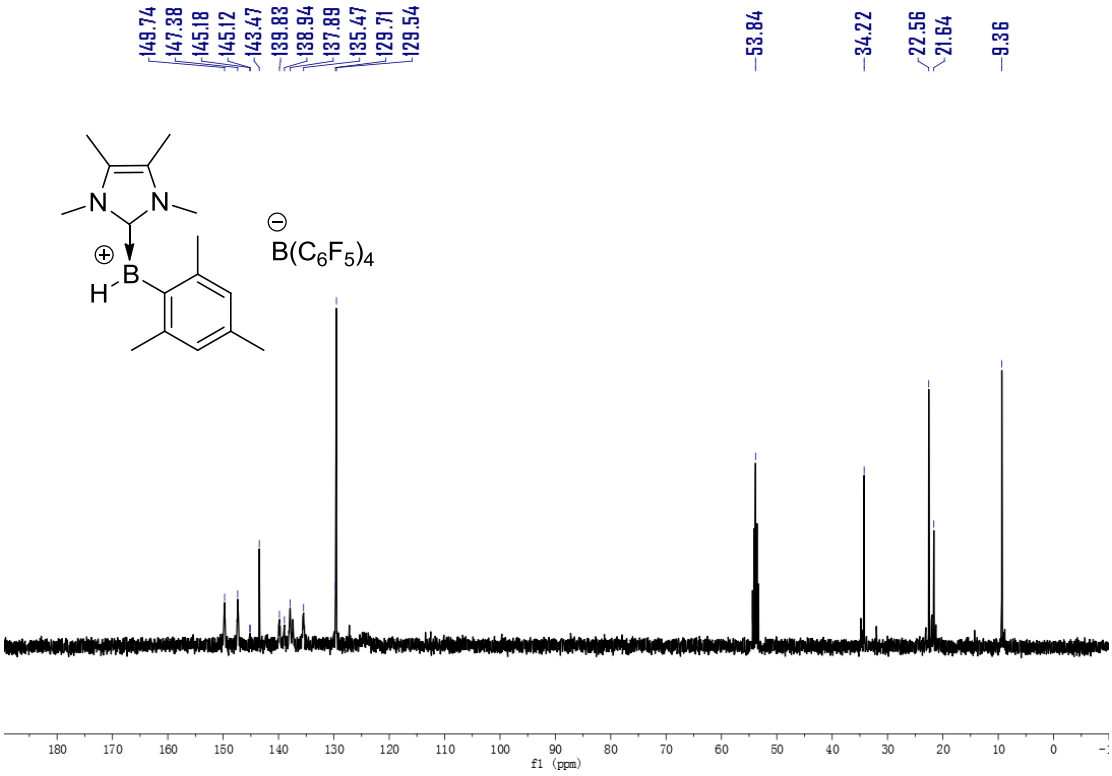


Figure S42. ^{13}C NMR spectrum of **7** in CD_2Cl_2

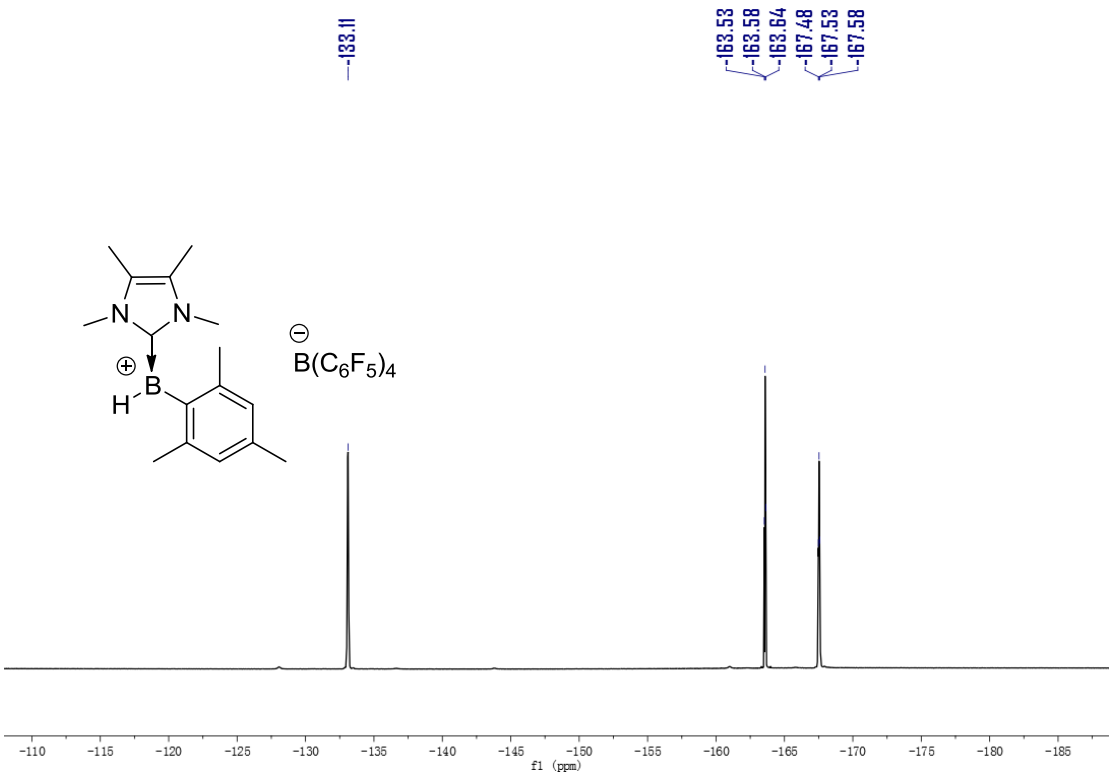


Figure S43. ^{19}F NMR spectrum of **7** in CD_2Cl_2

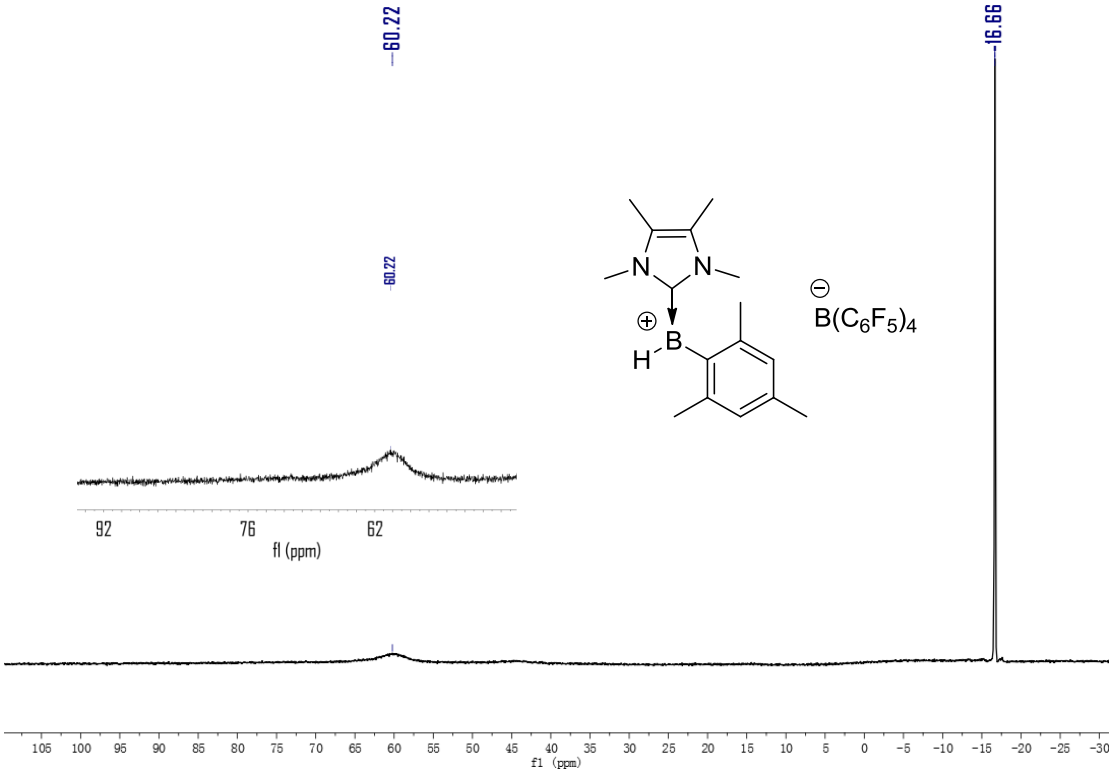


Figure S44. ^{11}B NMR spectrum of **7** in CD_2Cl_2

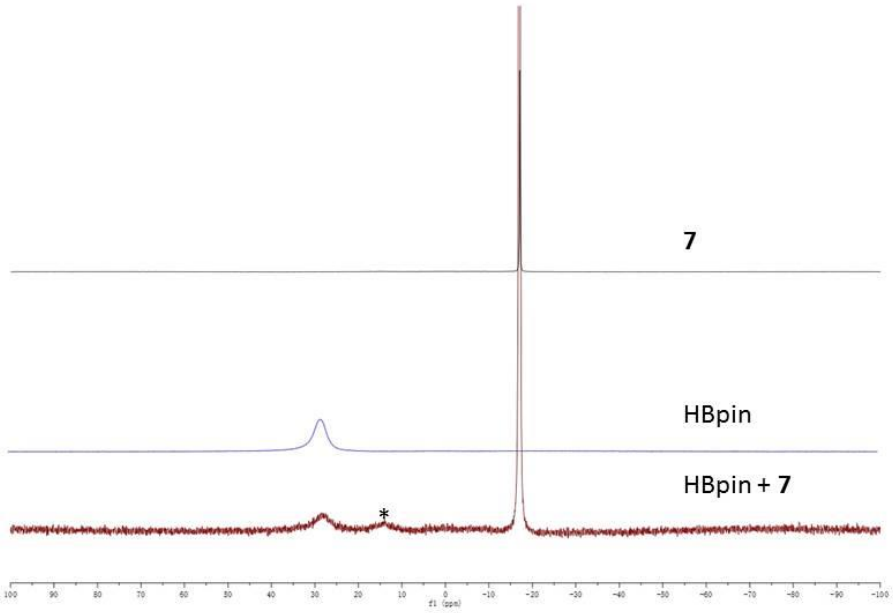


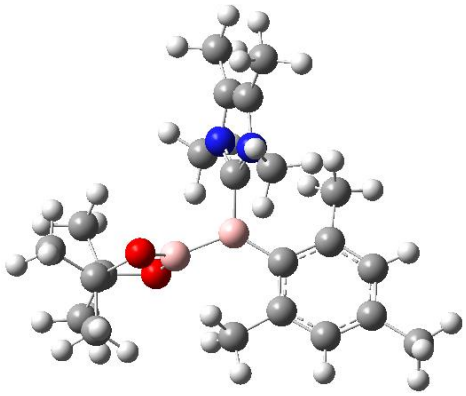
Figure S45. ^{11}B NMR spectrum of an equimolar mixture of HBpin and **7** in CD_2Cl_2 at -78 °C (*: hydrolysis product from **7**)

IV. Computation details

Quantum chemical calculations were all performed at the density functional theory (DFT) level using the hybrid meta-GGA M06-2x functional,[9] which has been proven to give reliable results to the structural and energetic properties of non-covalent systems and reaction energy barriers.[10] The M06-2x functional has a mean absolute error in energy barriers of about 1.3 kcal/mol. The 6-31+G(d,p) basis set[10] was employed in all the calculations. All the DFT calculations were performed with a pruned (99,590) integration grid.

Full geometry optimization were carried out in the dichloromethane solution which was modelled by the polarizable continuum solvation model (IEFPCM)[12] with radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.[13] This solvation model is by far the most reliable one in predicting solvation free energies. The convergence criteria used for the geometry optimization are 4.50×10^{-4} au. for gradients, and 1.80×10^{-3} au. for displacements. Harmonic vibrational analyses were carried out to confirm if the optimized structure is a local minima or a first order transition state and to provide zero-point vibrational energy corrections and thermal corrections to various thermodynamic properties. Transition states were further confirmed by IRC calculations.[14] All the calculations were performed by using the Gaussian 09 program.[15]

Geometries and Cartesian coordinates of the important intermediates and transition states involved in the reaction



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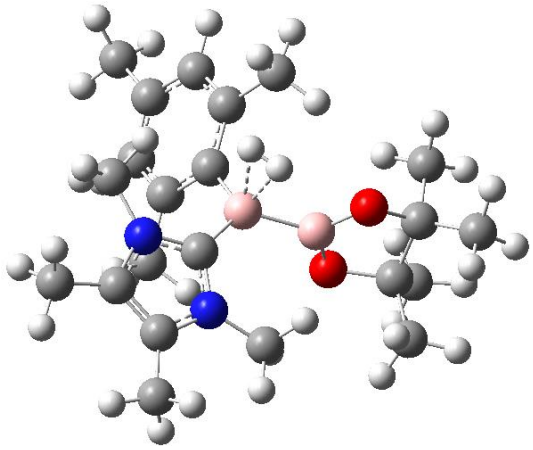

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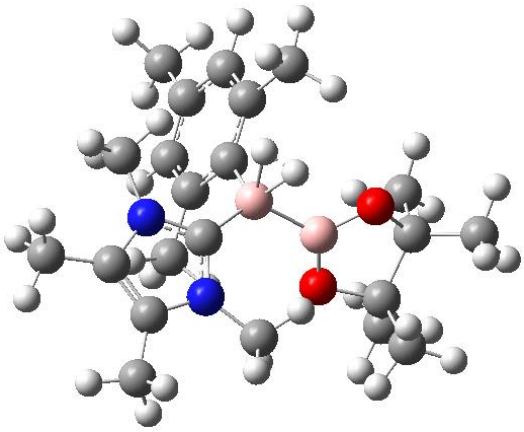

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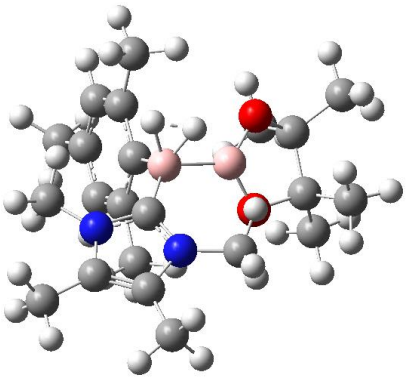

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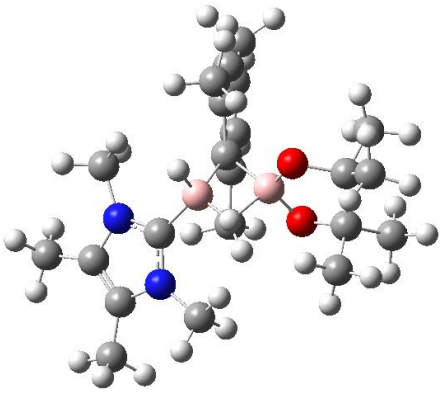
H,0,0.4965347965,2.0116873122,3.1891076661
C,0,-0.6896292051,0.8589763874,-1.8996059195
H,0,-1.7175694832,1.2325210299,-1.8058244111
H,0,-0.390344653,0.9975678611,-2.9418493737
H,0,-0.7005994574,-0.2145448636,-1.6954226088
C,0,-4.8441728727,-2.0553521797,-0.6637181931
H,0,-5.1050483233,-2.7549291655,0.1370544255
H,0,-5.7651135275,-1.6000612142,-1.0310368619
H,0,-4.3947435805,-2.6253587497,-1.4823531373
C,0,-5.2940524235,1.2149207035,-0.2794646304
H,0,-5.6920610185,1.6380754628,0.648451903
H,0,-5.040583039,2.0415256602,-0.950316625
H,0,-6.0828279759,0.6233891214,-0.7471002588
B,0,0.7636309252,-1.0236657968,0.6488395293
O,0,1.9206161816,-1.1918393454,1.3594712209
O,0,0.7593887257,-1.6683847512,-0.5527816174
B,0,-0.5009316711,0.1357303861,1.0469352741
C,0,-2.0106483494,-0.1301825136,0.6200084103
H,0,-0.1093824516,-0.5020646619,2.0400036292
C,0,0.3641413781,1.3356878371,0.396370066
H,0,-0.5738953811,0.4013344707,2.2840093586



IM1

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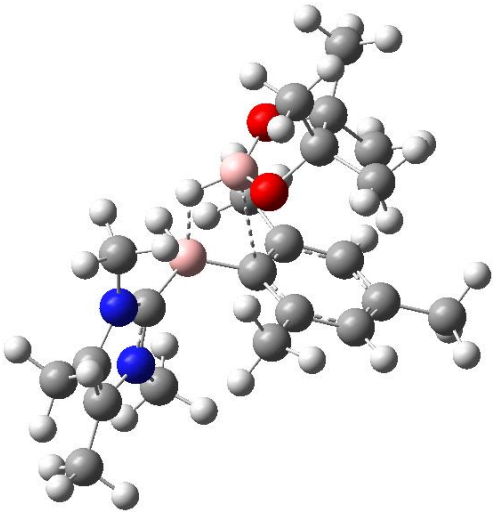
C,0,4.3265496624,-1.9349727293,1.3208399394
C,0,4.1452837115,0.0749962722,-0.1637086464
C,0,3.349682238,-2.0598883142,-1.9879635223
C,0,2.2256091005,-3.3312954469,-0.1464492667
H,0,5.1023459052,-2.4212759079,0.7203304123
H,0,4.8167143832,-1.2739041053,2.0417857668

H,0,3.7763701189,-2.7001503512,1.8729531805
H,0,4.4686344215,0.7270509549,0.6534420497
H,0,5.0284085015,-0.2410770135,-0.726882299
H,0,3.4951818999,0.653417181,-0.829671004
H,0,4.3204487113,-2.5514508515,-1.8648716836
H,0,2.7470265169,-2.6615946887,-2.6749692049
H,0,3.5073789576,-1.0765131024,-2.4363981252
H,0,1.5187384721,-3.7675573496,-0.8587215851
H,0,3.0882331091,-3.9990171691,-0.0638153016
H,0,1.7413320933,-3.2684446421,0.8345238734
C,0,-3.8200835981,-1.4057514782,-0.14847457
C,0,-4.0899658521,-0.10829688,0.1849588315
C,0,-2.7554638061,1.783731676,1.1745972794
H,0,-1.9778102541,1.8209452878,1.937657078
H,0,-2.4770473013,2.4227943935,0.331174534
H,0,-3.6941932728,2.1311726226,1.6058363493
C,0,-1.8018481266,-2.8904817635,-0.0660601576
H,0,-1.5257560373,-2.9474217248,-1.1227261975
H,0,-0.9077342465,-2.9487364824,0.5517205163
H,0,-2.4598618129,-3.7221123898,0.1872559872
N,0,-2.9216736773,0.4056839801,0.7250658752
N,0,-2.4952356261,-1.6342770249,0.1979427692
C,0,0.9188181221,2.0558612947,1.068073931
C,0,-0.1175763905,1.2576106043,-1.0171766098
C,0,1.1160962956,3.2892487904,0.4626450021
C,0,0.1048005035,2.5136212611,-1.5756496
C,0,0.7286822251,3.5358878494,-0.8601121427
H,0,1.5856904184,4.0885055565,1.0317802001
H,0,-0.2141196872,2.6979062667,-2.5989221193
C,0,0.9825764541,4.8788693228,-1.4804619093
H,0,0.5048019163,5.669218232,-0.8924366982
H,0,2.0565786982,5.0918451381,-1.4946811459
H,0,0.6046575978,4.9257797178,-2.5036494939
C,0,1.3074911046,1.9222259098,2.5145567846
H,0,1.7877776778,0.9676661111,2.7273047939
H,0,1.9800386352,2.734716027,2.7979920778
H,0,0.41148205,1.991542883,3.1436838084
C,0,-0.8535668123,0.2608950231,-1.8761667643
H,0,-1.9340801277,0.4453602816,-1.8016143571
H,0,-0.574617768,0.3969456974,-2.9241883024
H,0,-0.6576439777,-0.7739549204,-1.6032737652
C,0,-4.6806360386,-2.4642688519,-0.7463120381
H,0,-4.8405775314,-3.289320742,-0.0448119713
H,0,-5.6549544091,-2.0447157881,-1.0018391895

H,0,-4.2336129423,-2.8720426351,-1.6583336084
C,0,-5.3327798976,0.7030546527,0.0597817923
H,0,-5.743202215,0.9578936398,1.0423338307
H,0,-5.1418519319,1.6345105708,-0.4821348241
H,0,-6.0884352254,0.1386801633,-0.4889483433
B,0,1.2175865364,-0.5085163586,0.3808799532
O,0,2.3155517813,-0.6047250788,1.2304756137
O,0,1.4355947282,-1.1670762537,-0.8251609733
B,0,-0.4641785534,-0.2448866835,1.2238772173
C,0,-1.9487326972,-0.5216459362,0.717577731
H,0,0.1731390976,-1.3021643352,1.1099604425
C,0,0.3204697831,0.9819638725,0.3190385131
H,0,-0.404144707,0.0356407617,2.3814669599



TS3’

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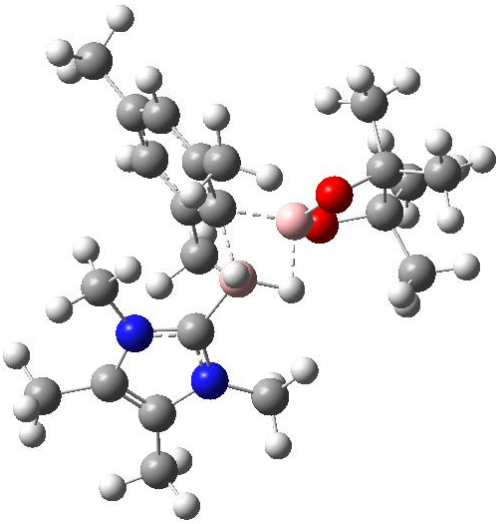
C,0,4.6365015727,-1.6574711785,1.0844930334
C,0,3.5762535013,0.3185559605,-0.0283338716
C,0,3.0996962906,-1.650630389,-2.0899119795
C,0,3.0257781047,-3.5245667016,-0.430347513
H,0,5.4201449625,-1.7834525338,0.3304222686
H,0,4.9962585846,-0.9461119852,1.8335600755
H,0,4.4630955383,-2.6177812088,1.5744351738
H,0,3.8183834555,0.9407498031,0.8383131252
H,0,4.399825745,0.385271131,-0.7453735946
H,0,2.6679021244,0.7129197829,-0.4949846633
H,0,4.1834332834,-1.6866256084,-2.2408507838
H,0,2.6345623937,-2.355787959,-2.7849545706
H,0,2.7439996283,-0.6447271781,-2.3257631958

H,0,2.4139236551,-4.111193183,-1.1214960827
H,0,4.0775563366,-3.7632387195,-0.612340969
H,0,2.7714130359,-3.8202271655,0.5924408774
C,0,-3.9786216371,-1.4044978115,-0.1760455125
C,0,-4.3497498908,-0.0922103262,-0.0917228909
C,0,-3.2483761428,2.0193119715,0.7207603312
H,0,-2.587160982,2.2359343525,1.5603208716
H,0,-2.8950636615,2.5385260516,-0.1742505924
H,0,-4.2534318534,2.3571774547,0.972069945
C,0,-1.930670538,-2.7290596707,0.4594714064
H,0,-1.1231382989,-2.7262017566,-0.2772289172
H,0,-1.5251077707,-2.8297586609,1.4661985561
H,0,-2.5973042097,-3.5660710129,0.2630391425
N,0,-3.2833315863,0.5779609396,0.4858667133
N,0,-2.7013330511,-1.4901957665,0.3651828654
C,0,0.7919320859,2.1945880098,1.2016223288
C,0,-0.0821238536,1.3488562625,-0.9157288804
C,0,1.4834724229,3.181152219,0.5005127217
C,0,0.6426892215,2.3401136966,-1.5824757394
C,0,1.419586414,3.2724390887,-0.8926326186
H,0,2.1042828313,3.886709751,1.0493734199
H,0,0.6049645436,2.3829640411,-2.6692076519
C,0,2.2115534508,4.3211729099,-1.6252084913
H,0,2.0897213614,5.3030813599,-1.1582972395
H,0,3.2800976391,4.0785336356,-1.5999763465
H,0,1.9054485842,4.3909719863,-2.6717580418
C,0,0.9674201786,2.1308314214,2.7004246091
H,0,1.3472132817,1.150067575,3.0056972761
H,0,1.6803117823,2.8896716707,3.0317023568
H,0,0.0253963158,2.2970069642,3.2321108348
C,0,-0.8724040839,0.3765384723,-1.7631054122
H,0,-1.9458746674,0.6041849749,-1.7536928531
H,0,-0.5387722974,0.4333645706,-2.8024349184
H,0,-0.7392872773,-0.6571583561,-1.43052243
C,0,-4.709665822,-2.5870417974,-0.7119332344
H,0,-4.9060366908,-3.3270019493,0.0702624799
H,0,-5.6683204951,-2.2658957977,-1.1223387613
H,0,-4.143957842,-3.0731043487,-1.5125240579
C,0,-5.6093522216,0.6048838853,-0.4734745547
H,0,-6.1167588986,1.0130433127,0.4067609345
H,0,-5.4111779084,1.4284816253,-1.1661978782
H,0,-6.288593954,-0.0969754677,-0.9589915245
B,0,1.1654015913,-1.3808954681,0.7960796469
O,0,2.3141397889,-1.0752261967,1.4474709734

O,0,1.3175150142,-1.8490490265,-0.4692969472
B,0,-0.8871084616,0.2641514395,1.3285475361
C,0,-2.2768415265,-0.2739923745,0.7426853807
H,0,0.0886711604,-1.3094087561,1.326594049
C,0,-0.0322226915,1.2709385515,0.5010306813
H,0,-0.7746797368,0.1912060732,2.5097169932



TS3

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C,0,-4.2483089032,0.5069980493,0.1088246319
C,0,-3.7241559799,-1.7017061047,1.9435935234
C,0,-2.638618123,-3.0547763931,0.1393087323
H,0,-5.3592829264,-1.8962150375,-0.8626946627
H,0,-4.9207441849,-0.752695253,-2.14405308
H,0,-4.0051096676,-2.2602436197,-1.956385363
H,0,-4.4809496893,1.1901204466,-0.7136960623
H,0,-5.1797955531,0.2600936359,0.6269241568
H,0,-3.5840682073,1.0241250395,0.8101242984
H,0,-4.7268014488,-2.1076107655,1.7727863793
H,0,-3.2077060923,-2.3579920471,2.6507871524
H,0,-3.8168852297,-0.7116078328,2.3952307071
H,0,-2.0132940576,-3.5630232469,0.8795117012
H,0,-3.555949259,-3.6359006815,0.0065407768
H,0,-2.1037615953,-3.0323294809,-0.8166068893
C,0,3.6948665582,-1.7572535766,0.080860163
C,0,4.0466463706,-0.4944522188,-0.3056939505
C,0,2.8118614195,1.456373065,-1.3189407333
H,0,2.0546474579,1.4998056175,-2.1029144273

H,0,2.545966913,2.1406791116,-0.5072532075
H,0,3.7764144184,1.7399156164,-1.7391876889
C,0,1.5769962463,-3.0893035556,0.1292285515
H,0,1.4598426716,-3.165982088,1.2136548641
H,0,0.5979865687,-3.0317192796,-0.3422293102
H,0,2.1040096961,-3.9686059124,-0.2443044738
N,0,2.8979921018,0.0897402102,-0.8149645858
N,0,2.342721989,-1.893343619,-0.2007470824
C,0,-0.6286361606,2.1230048354,-0.9742011268
C,0,0.2795119297,1.1195505158,1.0843147917
C,0,-0.568312276,3.3648895974,-0.357693239
C,0,0.3212309905,2.3873163114,1.653188212
C,0,-0.1093527931,3.5180320241,0.9566054368
H,0,-0.8791860763,4.2462593458,-0.9136883441
H,0,0.6997694523,2.4976984026,2.6667244372
C,0,-0.0907285375,4.875246285,1.596458184
H,0,0.3156497876,5.6232782329,0.9096840014
H,0,-1.1129703822,5.1824946708,1.8445761541
H,0,0.4978580656,4.8766657392,2.5162626653
C,0,-1.0562451524,2.0867867195,-2.4150616758
H,0,-1.6809030801,1.2248175802,-2.6454795308
H,0,-1.5950754161,3.0020865868,-2.6696192489
H,0,-0.1657524084,2.0328884621,-3.0539362954
C,0,0.8229406073,-0.0130862735,1.9171094134
H,0,1.9211644857,0.0250892412,1.9051238166
H,0,0.5050459414,0.1059591361,2.9564259138
H,0,0.5042703889,-0.9954238432,1.5755672134
C,0,4.4956796912,-2.8612967252,0.6790046292
H,0,4.5198725799,-3.7358913205,0.0212219534
H,0,5.522917764,-2.5283179351,0.8359493509
H,0,4.0840594557,-3.1731067631,1.6442312584
C,0,5.3496403261,0.2250958988,-0.2476250483
H,0,5.7502324397,0.4101355573,-1.2496117896
H,0,5.2428419515,1.1880000254,0.261227845
H,0,6.0768123103,-0.3721080587,0.3048285547
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O,0,-2.4108712614,-0.3067730129,-1.1983172911
O,0,-1.6856726836,-0.9759728709,0.8820688687
B,0,0.3780372469,-0.3777326233,-1.185507354
C,0,1.8579934376,-0.7594017467,-0.7353545101
H,0,-0.3572441027,-1.3492968635,-1.0172029753
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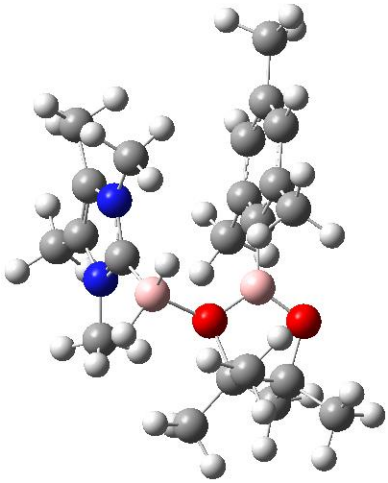

Complex **5**

Charge = 1 Multiplicity = 1

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C,0,0.5671498982,3.2904962152,0.1774193712
H,0,1.3128072876,3.2732580301,-0.6163951272
H,0,0.2710254979,4.3225665054,0.3656355899
H,0,0.9863545333,2.8590206381,1.0920241984
C,0,-2.3165745427,-0.0351280206,-2.0473321323
H,0,-3.0332175373,0.3381554447,-2.7819367173
H,0,-1.4769249094,-0.4992591929,-2.5579250498
H,0,-2.7991062844,-0.7663574472,-1.3950678567
N,0,-0.5972899479,2.5311955414,-0.2573578833
N,0,-1.833824197,1.0772216525,-1.2382153558
C,0,-4.1470332756,1.6075663051,-0.4045525329
H,0,-4.3669158938,0.5911505462,-0.0591539347
H,0,-4.6131347934,2.3125379726,0.2855153957
H,0,-4.607696497,1.7369239069,-1.3892909268
C,0,-2.223449285,3.8349850445,1.1588785585
H,0,-1.6399671632,3.7140870118,2.0777379502
H,0,-2.0229165593,4.8334423424,0.7571421565
H,0,-3.2821634967,3.7794058399,1.4178019605
B,0,0.7717665771,0.844725392,-1.7490583345
C,0,-0.5583216469,1.4831714292,-1.1057628046
H,0,0.5334411293,-0.0696753505,-2.4889591511
H,0,1.4639402515,1.6893383907,-2.2469292936
O,0,1.6260753279,0.2527055092,-0.526544595
B,0,1.2071439281,-0.8458865178,0.2851123597
C,0,3.1361897766,0.2156571604,-0.560736423
O,0,2.2522020154,-1.3153622835,0.9943421862
C,0,-0.2334760274,-1.4420722537,0.3480231475

C,0,3.4015921346,-0.441754017,0.824137561
C,0,3.7125281178,1.6085954137,-0.6918632616
C,0,3.5151244483,-0.663095666,-1.7407208336
C,0,-1.1667712414,-0.9485029108,1.2796466539
C,0,-0.5606417875,-2.5536054531,-0.4489981604
C,0,4.6632925601,-1.2839085471,0.8666085303
C,0,3.3658827153,0.5547860287,1.9778391596
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H,0,3.5696767062,2.0017457871,-1.6995664073
H,0,3.2883588121,2.3023234579,0.0351719154
H,0,3.1136281592,-0.2349105339,-2.6627453574
H,0,4.6036237332,-0.7033617725,-1.8312070979
H,0,3.1336228104,-1.6821483891,-1.6264949706
C,0,-2.4243802821,-1.5458347408,1.3712346639
C,0,-0.7956666681,0.1763038671,2.2161821233
C,0,-1.8211330225,-3.1443039851,-0.3184106567
C,0,0.4466594179,-3.1150111624,-1.4232954091
H,0,5.5366451403,-0.6658853282,0.635845479
H,0,4.7875471988,-1.6950340009,1.8718392006
H,0,4.6155906545,-2.1101702235,0.1545211781
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H,0,4.2526624436,1.1938484742,1.973270083
H,0,2.4732828742,1.1888146783,1.9311321335
C,0,-2.7671145167,-2.6505019373,0.5825167738
H,0,-3.1468742572,-1.1538033007,2.0857560551
H,0,-0.2274967943,-0.2116768839,3.070263613
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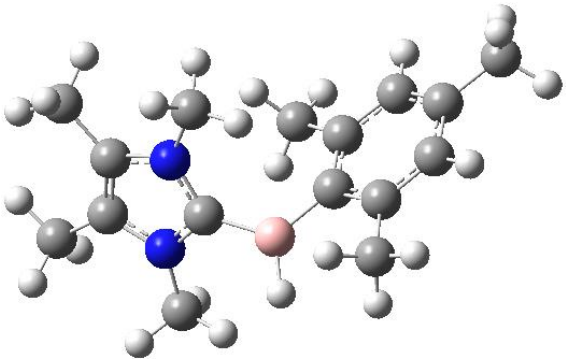
H,0,1.3006971844,-3.5533817429,-0.8936625652
H,0,0.0007487833,-3.8965018285,-2.0431741706
C,0,-4.1350741851,-3.2721640639,0.6938339574
H,0,-4.3851307058,-3.4891905049,1.7367565113
H,0,-4.9026093637,-2.5911888211,0.308693854
H,0,-4.1930532634,-4.2030393168,0.1244764159

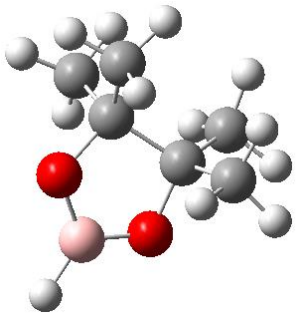


Complex **7**

Charge = 1 Multiplicity = 1

B,0,-0.5875509575,0.428721678,-0.0593842441
C,0,-0.6990912037,4.1635013284,0.3376964486
C,0,-1.7513129639,3.9858713991,-0.5278414259
C,0,-2.8057192688,2.048255783,-1.6950564723
H,0,-2.6255258048,0.9788125423,-1.7826041532
H,0,-3.8121132787,2.2208755763,-1.3073807729
H,0,-2.7040536552,2.5169370829,-2.6755687136
C,0,0.9682445473,2.6693444622,1.4502650039
H,0,1.3581237818,1.6686923674,1.2711300466
H,0,1.7488116525,3.4040570482,1.2505806809
H,0,0.6352313568,2.7544036925,2.4868385986
N,0,-1.8250915633,2.6337131201,-0.7827454882
N,0,-0.1545516317,2.9172499627,0.5490537458
C,0,-0.8524219122,1.9768283308,-0.1195149489
C,0,-1.7089325705,-0.621430156,0.0630465366
C,0,-1.5366809437,-1.8798784699,-0.5778588715
C,0,-2.8881653463,-0.3948538409,0.8179982415
C,0,-2.543252154,-2.8382516564,-0.5026519986
C,0,-3.8612973115,-1.3943603272,0.893342074
C,0,-3.7156603843,-2.6122859728,0.2276492671
H,0,-2.4130149699,-3.7896951332,-1.0150425551
H,0,-4.7522887138,-1.2206236068,1.4932954224
C,0,-0.1588828441,5.389231651,0.9872542921
H,0,-0.815072335,6.2359076377,0.7817706591
H,0,-0.0955554285,5.2599511304,2.0720365785
H,0,0.8409851594,5.6301873791,0.6130950063
C,0,-2.6821517865,4.9634380175,-1.1547997358
H,0,-2.5868722442,4.9491449615,-2.2453632095
H,0,-3.7221487922,4.7361791445,-0.901367974
H,0,-2.4543460843,5.9715834261,-0.8063790115
C,0,-4.7804512079,-3.6729248421,0.2975470039
H,0,-5.1684702714,-3.8972346542,-0.7014744158
H,0,-4.3734049712,-4.6044316456,0.7042008562

H,0,-5.6148879983,-3.3579070506,0.9282456729
C,0,-0.2894793274,-2.1947570563,-1.3699282234
H,0,-0.1213453733,-1.4688796221,-2.1713925939
H,0,0.5979022198,-2.1823550737,-0.7278850467
H,0,-0.3659338127,-3.1857695664,-1.8232493142
C,0,-3.1346476462,0.8801482392,1.595120664
H,0,-2.2227144564,1.2789998957,2.0479327019
H,0,-3.5642456652,1.6631646225,0.9597098474
H,0,-3.8508209272,0.6929620157,2.3991648526
H,0,0.5554618684,0.1041193798,-0.1124186118



HBpin
Charge = 0 Multiplicity = 1
B,0,0.,0.,1.2524073263
O,0,1.0128879047,0.529604958,0.5033478386
O,0,-1.0128879047,-0.529604958,0.5033478386
C,0,0.5531861887,0.5533270812,-0.8765812655
C,0,-0.5531861887,-0.5533270812,-0.8765812655
C,0,1.7308958891,0.2738780105,-1.7930705109
C,0,-0.0003308083,1.9528357609,-1.1307159093
C,0,-1.7308958891,-0.2738780105,-1.7930705109
C,0,0.0003308083,-1.9528357609,-1.1307159093
H,0,1.3930931722,0.1988718365,-2.8320413973
H,0,2.4483081964,1.0971839953,-1.7266266242
H,0,2.24198287,-0.6517768609,-1.5208531497
H,0,0.7863551801,2.6851901694,-0.9276029007
H,0,-0.3209599385,2.067598091,-2.1702507368
H,0,-0.8501702885,2.1701114831,-0.4755308875
H,0,-1.3930931722,-0.1988718365,-2.8320413973
H,0,-2.4483081964,-1.0971839953,-1.7266266242
H,0,-2.24198287,0.6517768609,-1.5208531497
H,0,-0.7863551801,-2.6851901694,-0.9276029007
H,0,0.3209599385,-2.067598091,-2.1702507368
H,0,0.8501702885,-2.1701114831,-0.4755308875
H,0,0.,0.,2.439071761

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