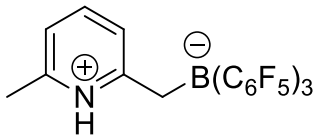
I. Experimental Section

General:

Solvents were dried by reflux under N2 over sodium or CaH_2 and freshly distilled prior to use. Air-sensitive compounds were handled under a N2 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, 471 MHz for ^{19}F) spectrometers. Most assignments were based on a series of 2D NMR experiments. Elemental analyses were performed at VARIO EL III in Shanghai Institute of Organic Chemistry, CAS. HRMS analyses were performed at Bruker micrOTOF II. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Center: CCDC 1445374 (**1a**) and 1445373 (**2**) contain 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.



Synthesis of 1a: A solution of 2,6-lutidine (42 mg, 0.39 mmol) and HBcat (4.8 mg, 0.040 mmol) in CH_2Cl_2 (1 mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. Then the volatile was removed under vacuum. The resulting solid was washed with toluene/hexane (2mL/3mL) and pumped to dryness to give compound **1a** (205mg, 85%).

X-ray quality crystals were grown by slow evaporation of a THF solution.

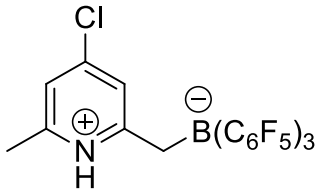
^{1}H NMR (400 MHz, THF-d_8, 25 ℃): δ [ppm] = 12.98 (br s, 1H, N*H*), 8.01 (t, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.36(d, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*5(py)), 7.31 (d, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*3(py)), 3.30 (q, 2H, $^{2}J_{B\text{-}H}$ = 6.1 Hz, CH_2), 2.52 (s, 3H, CH_3).

^{13}C NMR (100 MHz, THF-d_8, 25 ℃): δ [ppm] = 166.10 (*C2*(py)), 151.19 (*C*6(py)), 148.93 (dm, $^{1}J_{C\text{-}F}$ = 241 Hz, *C*F), 145.20 (*C*4(py)), 139.13 (dm, $^{1}J_{C\text{-}F}$ = 241 Hz, *C*F), 137.42 (dm, $^{1}J_{C\text{-}F}$ = 245 Hz, *C*F), 124.75 (*C*3(py)), 122.59 (*C*5(py)), 32.43 (q, $^{1}J_{C\text{-}B}$ = 38 Hz, *C*H_2), 18.78 (*C*H_3).

^{19}F NMR (376 MHz, THF-d_8, 25 ℃): δ [ppm] = -134.07 (d, 6F, $^{3}J_{F\text{-}F}$= 21 Hz, *ortho*-C_6F_5), -164.93 (t, 3F, $^{3}J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -168.81 (t, 6F, $^{3}J_{F\text{-}F}$= 21 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, THF-d_8, 25 ℃): δ [ppm] = -13.1 (s).

HRMS (ESI, m/z): calcd for $C_{25}H_9BF_{15}N$ [M+Na^+] 642.0481, found 642.0485.



Synthesis of 1d: A solution of 4-chloro-2,6-lutidine (110 mg, 0.78 mmol) and HBcat (4.8mg, 0.040 mmol) in CH_2Cl_2 (1 mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39 mmol) in CH_2Cl_2 (1 mL). The reaction mixture was stirred at 25 ℃ for 24h. After removal of the volatile under vacuum, the resulting solid was dissolved in CH_2Cl_2 again. The dichloromethane solution was concentrated to ~3mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1d** (184mg, 72%).

^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 10.92 (br s, 1H, N*H*), 7.23 (s, 1H, *H*5(py)), 6.96 (d, 1H, *H*3(py)), 3.27 (q, 2H, $^{2}J_{B\text{-}H}$ = 5.7 Hz, CH_2), 2.55 (s, 3H, CH_3).

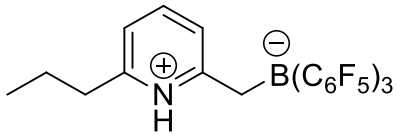
^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 167.79 (*C2*(py)), 154.38 (*C*6(py)),

151.09 (*C*4(py)), 148.30 (dm, $^{1}J_{C\text{-}F}$ = 234 Hz, *C*F), 139.05 (dm, $^{1}J_{C\text{-}F}$ = 245 Hz, *C*F), 137.34 (dm, $^{1}J_{C\text{-}F}$ = 242 Hz, *C*F), 125.14 (*C*3(py)), 122.74 (*C*5(py)), 32.75 (q, $^{1}J_{C\text{-}B}$ = 37 Hz, *C*H_2), 20.22 (*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.38 (d, 6F, $^{3}J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -160.73 (t, 3F, $^{3}J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.14 (t, 6F, $^{3}J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -13.1 (s).

HRMS (ESI, m/z): calcd for $C_{25}H_8BF_{15}N$ [M+Na^+] 676.0097, found 676.0095.



Synthesis of 1e: A solution of 6-propyl-2-methylpyridine (47mg, 0.39mmol) and HBcat (4.8mg, 0.040mmol) in CH_2Cl_2 (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. Then the volatile was removed under vacuum. The resulting solid was washed with toluene/hexane (2ml/3ml) and again pumped to dryness to give compound **1e** (200mg, 81%).

^{1}H NMR (400 MHz, THF-d_8, 25 ℃): δ [ppm] = 12.94 (br s, 1H, N*H*), 8.04 (t, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.37(d, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*5(py)), 7.31 (d, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*3(py)), 3.31 (q, 2H, $^{2}J_{B\text{-}H}$ = 6.1 Hz, C*H*$_2$), 2.74 (t, 2H, $^{3}J_{H\text{-}H}$= 7.6 Hz, C*H*$_2$CH_2), 1.64 (m, 2H, $^{3}J_{H\text{-}H}$= 7.4 Hz, CH_2C*H*$_2$), 0.95 (t, 3H, $^{3}J_{H\text{-}H}$= 7.4 Hz, C*H*$_3$CH_2).

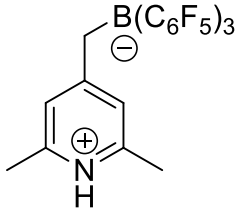
^{13}C NMR (100 MHz, THF-d_8, 25 ℃): δ [ppm] = 166.38 (*C2*(py)), 154.87 *(C*6(py)), 148.89 (dm, $^{1}J_{C\text{-}F}$ = 238 Hz, *C*F), 145.26 (*C*4(py)), 139.13 (dm, $^{1}J_{C\text{-}F}$ = 247 Hz, *C*F), 137.41 (dm, $^{1}J_{C\text{-}F}$ = 250 Hz, *C*F_5), 125.10 (*C*3(py)), 121.96 (*C*5(py)), 35.42 (*C*H_2CH_2),

32.36 (q, $^{1}J_{C\text{-}B}$ = 38 Hz *C*H_2B(C_6F_5)$_3$), 23.26 (CH_3*C*H_2), 13.31 (*C*H_3).

^{19}F NMR (376 MHz, THF-d_8, 25 ℃): δ [ppm] = -132.23 (d, 6F, $^{3}J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -163.08 (t, 3F, $^{3}J_{F\text{-}F}$= 20 Hz, *para*-C_6F_5), -166.82 (t, 6F, $^{3}J_{F\text{-}F}$= 19 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, THF-d_8, 25 ℃): δ [ppm] = -13.2 (s).

HRMS (ESI, m/z): calcd for $C_{27}H_{13}BF_{15}N$ [M+NH_4^+] 651.1245, found 651.1245.



Synthesis of 1f: A solution of 2,4,6-collidine (48mg, 0.40mmol) and HBcat (4.8mg, 0.040mmol) in CH_2Cl_2 (1mL) was added to the solution of B(C_6F_5)$_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. After removal of the volatile under vacuum, the resulting solid was dissolved in CH_2Cl_2. The dichloromethane solution was concentrated to ~2mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1f** (94mg, 38%).

^{1}H NMR (400 MHz, THF-d_8, 25 ℃): δ [ppm] = 13.13 (br s, 1H, N*H*), 6.88 (s, 2H, *H*3(py)), 3.16 (q, 2H, $^{2}J_{B\text{-}H}$ = 7.1 Hz, CH_2), 2.45 (s,6H, CH_3).

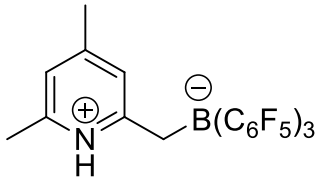
^{13}C NMR (100 MHz, THF-d_8, 25 ℃): δ [ppm] = 174.31 (*C*4(py)), 150.07 (*C*2(py)), 148.80 (dm, $^{1}J_{C\text{-}F}$ = 249 Hz, *C*F), 138.82 (dm, $^{1}J_{C\text{-}F}$ = 249 Hz, *C*F), 137.37 (dm, $^{1}J_{C\text{-}F}$ = 249 Hz, *C*F), 124.87 (*C*3(py)), 35.93 (q, $^{1}J_{C\text{-}B}$ = 39 Hz, *C*H_2), 18.63 (*C*H_3).

^{19}F NMR (376 MHz, THF-d_8, 25 ℃): δ [ppm] = -133.24 (d, 6F, $^{3}J_{F\text{-}F}$= 21Hz, *ortho*-

C_6F_5), -165.88 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -169.26 (t, 6F, $^3J_{F\text{-}F}$= 19 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, THF-d_8, 25 ℃): δ [ppm] = -12.4 (s).

HRMS (ESI, m/z): calcd for $C_{26}H_{11}BF_{15}N$ [M+Na^+] 656.0643, found 656.0642.



Synthesis of 1f': A solution of 2,4,6-collidine (48mg, 0.40mmol) and HBcat (4.8mg, 0.040mmol) in toluene (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in toluene (2mL). The reaction mixture was stirred at 50 ℃ for 24h. After removal of the volatile under vacuum, the resulting solid was dissolved in CH_2Cl_2. The dichloromethane solution was concentrated to ~2mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1f'** (188mg, 76%).

^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 10.47 (br s, 1H, N*H*), 7.01 (s, 1H, *H*5(py)), 6.74 (d, 1H, *H*3(py)), 3.21 (q, 2H, $^2J_{B\text{-}H}$ = 5.2 Hz, CH_2), 2.50 (s, 3H, C5(py)CH_3), 2.33 (s, 3H, C4(py)CH_3).

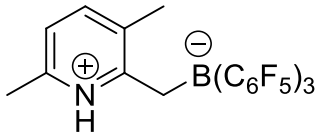
^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 165.24 (*C2*(py)), 159.58 *(C*6(py)), 149.09 (*C*4(py)), 148.36 (dm, $^1J_{C\text{-}F}$ = 238 Hz, *C*F), 138.94 (dm, $^1J_{C\text{-}F}$ = 250 Hz, *C*F), 137.25 (dm, $^1J_{C\text{-}F}$ = 255 Hz, *C*F), 125.37(*C*3(py)), 123.04 (*C*5(py)), 31.86 (q, $^1J_{C\text{-}B}$ = 37 Hz, *C*H_2), 22.18 (C4(py)*C*H_3), 20.07 (C5(py)*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.39 (d, 6F, $^3J_{F\text{-}F}$= 21 Hz, *ortho*-C_6F_5), -161.33 (t, 3F, $^3J_{F\text{-}F}$= 21 Hz, *para*- C_6F_5), -165.53 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz,

meta-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -13.3 (s).

HRMS (ESI, m/z): calcd for $C_{26}H_{11}BF_{15}N$ [M+Na^+] 656.0643, found 656.0642.



Synthesis of 1g: A solution of 3-methyl-2,6-lutidine (47mg, 0.39mmol) and HBcat (4.8mg, 0.040mmol) in CH_2Cl_2 (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. After removal of the volatile under vacuum, the resulting solid was dissolved in CH_2Cl_2 again. The dichloromethane solution was concentrated to ~1mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1g** (168mg, 68%).

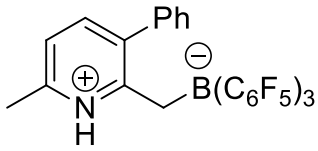
^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 10.75 (br s, 1H, N*H*), 7.82 (d, 1H, $^3J_{H\text{-}H}$ = 7.9 Hz, *H*4(py)), 7.15 (d, 1H, $^3J_{H\text{-}H}$ = 7.9 Hz, *H*5(py)), 3.27 (q, 2H, $^2J_{B\text{-}H}$ = 6.1 Hz, CH_2) , 2.46 (s, 3H, C6(py)CH_3), 2.16 (s, 3H, C3(py)CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 165.17 (*C*2(py)), 148.38 (dm, $^1J_{C\text{-}F}$ = 238 Hz, *C*F), 147.80 (*C*6(py)), 146.44 *(C*4(py)), 139.12 (dm, $^1J_{C\text{-}F}$ = 246 Hz, *C*F), 137.25 (dm, $^1J_{C\text{-}F}$ = 245 Hz, *C*F), 135.33 (*C*3(py)), 122.03 (*C*5(py)), 28.06 (q, $^1J_{C\text{-}B}$ = 37 Hz, *C*H_2), 19.78 (C6(py)*C*H_3) , 18.23 (C3(py)*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.44 (d, 6F, $^3J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -160.66 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.08 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -14.1 (s).

HRMS (ESI, m/z): calcd for $C_{26}H_{11}BF_{15}N$ [M+NH_4^+] 651.1089, found 651.1088.



Synthesis of 1h: A solution of 3-phenyl-2,6-lutidine (144mg, 0.78mmol) and HBcat (4.8mg, 0.040mmol) in CH_2Cl_2 (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. Then the volatile was removed under vacuum. The resulting solid was washed with toluene/hexane (1ml/3ml) and again pumped to dryness to give compound **1h** (130mg, 48%).

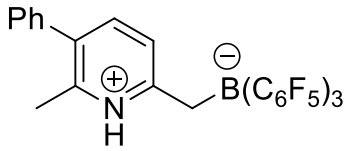
^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 11.00 (br s, 1H, N*H*), 7.91 (d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.44-7.45 (br m, 3H, *meta*-C_6H_5 and *para*-C_6H_5), 7.30 (d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*5(py)), 7.12 (br m, 2H, *ortho*-C_6H_5), 3.44 (q, 2H, $^2J_{B\text{-}H}$ = 6.2 Hz, CH_2) , 2.55 (s, 3H, CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 164.81 (*C2*(py)), 149.44 *(C*6(py)), 148.26 (dm, $^1J_{C\text{-}F}$ = 237 Hz, *C*F), 146.59 (*C*4(py)), 139.79 (*ipso*-C_6H_5), 139.39 (dm, $^1J_{C\text{-}F}$ = 246 Hz, *C*F), 137.24 (dm, $^1J_{C\text{-}F}$ = 240 Hz, *C*F), 135.14 (*C*3(py)), 129.47 (*para*-C_6H_5), 129.27 (*meta*-C_6H_5), 129.24 (*ortho*-C_6H_5), 122.26(*C*5(py)), 28.50 (q, $^1J_{C\text{-}B}$ = 37 Hz, *C*H_2), 20.05 (*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.46 (d, 6F, $^3J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -160.85 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.06 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -13.9 (s).

HRMS (ESI, m/z): calcd for $C_{31}H_{13}BF_{15}N$ [M+Na^+] 718.0799, found 718.0799.



Synthesis of 1h': A solution of 3-phenyl-2,6-lutidine (144mg, 0.78mmol) and HBcat (4.8mg, 0.040mmol) in toluene (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in toluene (2mL). The reaction mixture was stirred at 70 ℃ for 24h. After removal of the volatile under vacuum, the resulting solid was dissolved in CH_2Cl_2. The dichloromethane solution was concentrated to ~2mL and hexane was added drop by drop until precipitation appeared. Then the resulting solution was stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1h'** (169mg, 62%).

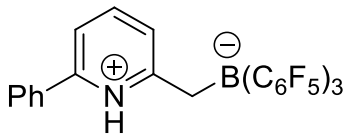
^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 10.88 (br s, 1H, N*H*), 7.85 (d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.51 (br m, 3H, *meta*-C_6H_5 and *para*-C_6H_5), 7.23 (br m, 2H, *ortho*-C_6H_5), 7.07 (d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*3(py)), 3.35 (q, 2H, $^2J_{B\text{-}H}$ = 6.2 Hz, CH_2), 2.51 (s, 3H, CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 165.42 (*C2*(py)), 148.35 (dm, $^1J_{C\text{-}F}$ = 243 Hz, *C*F), 147.69 *(C*6(py)), 146.06 (*C*4(py)), 136.25 (*ipso*-C_6H_5), 139.01 (dm, $^1J_{C\text{-}F}$ = 252 Hz, *C*F), 137.26 (dm, $^1J_{C\text{-}F}$ = 248 Hz, *C*F), 134.61 (*C*5(py)), 129.85 (*para*-C_6H_5), 129.64 (*meta*-C_6H_5), 129.10 (*ortho*-C_6H_5), 125.20(*C*3(py)), 32.26 (q, $^1J_{C\text{-}B}$ = 37 Hz, CH_2), 19.61 (CH_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.31 (d, 6F, $^3J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -161.01 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.32 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -13.1 (s).

HRMS (ESI, m/z): calcd for $C_{31}H_{13}BF_{15}N$ [M+Na^+] 718.0799, found 718.0799.



Synthesis of 1i: A solution of 2-methyl-6-phenylpyridine (86mg, 0.51mmol) and HBcat (6.0mg, 0.050mmol) in CH_2Cl_2 (1mL) was added to the solution of $B(C_6F_5)_3$ (256mg, 0.50mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. Then the volatile was removed under vacuum, and the resulting solid was dissolved in toluene. The resulting toluene solution was concentrated to 2~3mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1i** (272mg, 80%).

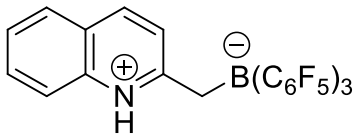
^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 11.23 (br s, 1H, N*H*), 8.02 (t, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.70 (d, 1H, $^3J_{H\text{-}H}$ = 7.4 Hz, *H*5(py)), 7.71-7.63 (m, 3H, C_6H_5), 7.50 (d, 2H, $^3J_{H\text{-}H}$ = 7.4 Hz, *ortho*-C_6H_5), 7.05(d, 1H, $^3J_{H\text{-}H}$ = 7.4 Hz, *H*3(py)), 3.41 (q, 2H, $^2J_{B\text{-}H}$ = 8.0 Hz, CH_2).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 167.33 (*C2*(py)), 150.53 *(C*6(py)), 148.33 (dm, $^1J_{C\text{-}F}$ = 235 Hz, *C*F), 145.60 (*C*4(py)), 140.16 (*ipso*-C_6H_5), 139.07 (dm, $^1J_{C\text{-}F}$ = 249 Hz, *C*F), 137.35 (dm, $^1J_{C\text{-}F}$ = 240 Hz, *C*F), 133.37 (*C*5(py)), 130.94 (*meta*-C_6H_5), 126.69 (*ortho*-C_6H_5), 125.79(*C*3(py)), 119.96 (*para*-C_6H_5), 32.60 (q, $^1J_{C\text{-}B}$ = 36 Hz, CH_2).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.27 (d, 6F, $^3J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -160.86 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.18 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -13.1 (s).

HRMS (ESI, m/z): calcd for $C_{30}H_{11}BF_{15}N$ [M+Na^+] 704.0643, found 704.0642.



Synthesis of 1j: A solution of quinaldine (56mg, 0.39mmol) and HBcat (4.8mg, 0.040mmol) in CH_2Cl_2 (1mL) was added to the solution of $B(C_6F_5)_3$ (200mg, 0.39mmol) in CH_2Cl_2 (1mL). The reaction mixture was stirred at 25 ℃ for 24h. Then the volatile was removed under vacuum, and the resulting solid was dissolved in toluene. The resulting toluene solution was concentrated to 5mL and stored at -40 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **1j** (177mg, 70%).

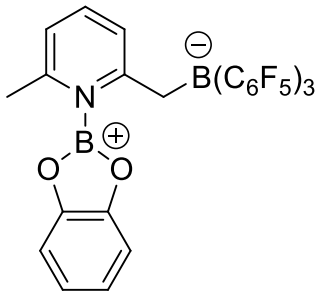
^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 11.24 (br s, 1H, N*H*), 8.41 (d, 1H, $^3J_{H\text{-}H}$ = 8.8 Hz, *H*4(qu)), 8.03 (d, 1H, $^3J_{H\text{-}H}$ = 8.2 Hz, *H*5(qu)), 7.98 (dt, 1H, $^3J_{H\text{-}H}$ = 7.9 Hz, $^4J_{H\text{-}H}$ = 1.3 Hz, *H*7(qu)), 7.79(dt, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, $^4J_{H\text{-}H}$ = 1.1 Hz, *H*6(qu)), 7.72 (d, 1H, $^3J_{H\text{-}H}$ = 8.4 Hz, *H*8(qu)), 7.24 (d, 1H, $^3J_{H\text{-}H}$ = 8.8 Hz, *H*3(qu)),3.60 (q, 2H, $^2J_{B\text{-}H}$ = 5.9 Hz, CH_2).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 171.16 (*C*2(qu)), 148.39 (dm, $^1J_{C\text{-}F}$ = 241 Hz, *C*F), 144.78 (*C*4(qu)), 139.10 (dm, $^1J_{C\text{-}F}$ = 250 Hz, *C*F), 137.33 (dm, $^1J_{C\text{-}F}$ = 240 Hz, *C*F), 136.64 (*C*8a(qu)), 135.18 (*C*7(qu)), 129.57 (*C*5(qu)), 129.47 (*C*6(qu)), 125.99 (*C*4a(qu)), 123.87 (*C*3(qu)), 118.70 (*C*8(qu)), 35.08 (q, $^1J_{C\text{-}B}$ = 36 Hz, *C*H_2).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.28 (d, 6F, $^3J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -160.83 (t, 3F, $^3J_{F\text{-}F}$= 20 Hz, *para*-C_6F_5), -165.26 (t, 6F, $^3J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -12.8 (s).

HRMS (ESI, m/z): calcd for $C_{28}H_9BF_{15}N$ [M+Na^+] 678.0486, found 678.0486.



Synthesis of 2: A solution of $B(C_6F_5)_3$ (410 mg, 0.8 mmol) in toluene (2mL) was added to the solution of ((6-methyl-2-pyridyl)methyl)lithium (90 mg, 0.8 mmol) in toluene at room temperature. Then the reaction mixture was stirred at room temperature for 3 h. Afterwards, hexane (5 mL) was added and the resulting slurry was filtered and washed with hexane (2x2 mL). The resulting solid was pumped to dryness to give compound lithium (6-methyl-2-pyridyl)methyltris(pentafluorophenyl)borate (430mg, 95%) and it was used without further purification. A solution of ClBcat (99 mg, 0.64 mmol) in toluene (2 mL) was added to the solution of lithium (6-methyl-2-pyridyl)methyltris(pentafluorophenyl)borate (400 mg, 0.64 mmol) in toluene (5 mL) at room temperature. The reaction mixture was stirred at room temperature for 5 minutes. Then the resulting slurry was filtered and hexane was added into the filtrate until white precipitation appeared. The solution was stored at -20 ℃ overnight, affording a white solid which was filtered and dried under vacuum to give compound **2** with 1/2 toluene (276 mg, 55%).

X-ray quality crystals were grown from CH_2Cl_2 solution at -20 ℃.

^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 8.05 (t, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)), 7.53(d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*5(py)), 7.40 (d, 1H, $^3J_{H\text{-}H}$ = 8.0 Hz, *H*3(py)), 7.40 (dd, 2H, $^3J_{H\text{-}H}$ = 6.0 Hz, $^4J_{H\text{-}H}$ = 3.4 Hz, C(2)*H*(cat)), 7.33 (dd, 2H, $^3J_{H\text{-}H}$ = 6.0 Hz, $^4J_{H\text{-}H}$ =

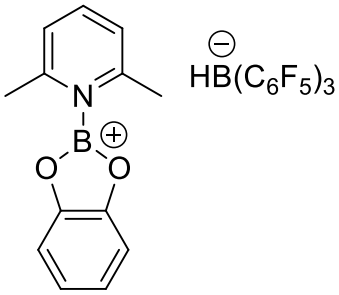
3.4 Hz, C(3)*H*(cat)), 3.30 (q, 2H, $^{2}J_{B\text{-}H}$ = 6.1 Hz, CH_2), 2.52 (s, 3H, CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 171.06 (*C*2(py)), 153.23 *(C*6(py)), 148.54 (dm, $^{1}J_{C\text{-}F}$ = 244 Hz, *C*F), 147.09 (*C*1(cat)), 146.16 (*C*4(py)), 139.08 (dm, $^{1}J_{C\text{-}F}$ = 246 Hz, *C*F), 137.26 (dm, $^{1}J_{C\text{-}F}$ = 240Hz, *C*F), 126.25 (*C*5(py)), 125.55 (*C*3(cat)), 123.51 (*C*3(py)), 114.23 (*C*2(cat)), 35.75 (q, $^{1}J_{C\text{-}B}$ = 38 Hz, *C*H_2), 21.68 (*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -132.41 (d, 6F, $^{3}J_{F\text{-}F}$= 22 Hz, *ortho*-C_6F_5), -161.51 (t, 3F, $^{3}J_{F\text{-}F}$= 20 Hz, *para*- C_6F_5), -165.83 (t, 6F, $^{3}J_{F\text{-}F}$= 20 Hz, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 26.9 (br s, cat*B*), -13.2 (s, *B*$(C_6F_5)_3$).

Element analysis: calcd for $C_{31}H_{12}B_2F_{15}NO_2$+1/2toluene C 52.91, H 2.06, N 1.79%; found C 53.76, H 2.05, N 1.94%.



Synthesis of [LutBcat][HB(C_6F_5)$_3$]: A solution of 2,6-lutidine (42mg, 0.39mmol) and HBcat (48mg, 0.40mmol) in hexane (3mL) was added to the solution of B(C_6F_5)$_3$ (200mg, 0.39mmol) in hexane (10mL). A white precipitation appeared immediately and the reaction mixture was stirred at room temperature for 10 minutes. Then the resulting slurry was filtered and washed with hexane (2x2mL), and the resulting solid was dried under vacuum to give compound [LutBcat][HB(C_6F_5)$_3$] (211mg, 73%).

^{1}H NMR (400 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 8.45 (t, 1H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*4(py)),

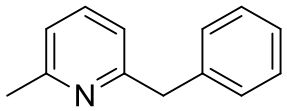
7.81(d, 2H, $^{3}J_{H\text{-}H}$ = 8.0 Hz, *H*3(py)), 7.53 (dd, 2H, $^{3}J_{H\text{-}H}$ = 6.0 Hz, $^{4}J_{H\text{-}H}$ = 3.4 Hz, C(2)*H*(cat)), 7.42 (dd, 2H, $^{3}J_{H\text{-}H}$ = 6.0 Hz, $^{4}J_{H\text{-}H}$ = 3.4 Hz, C(3)*H*(cat)), 3.58 (q, 1H, $^{1}J_{B\text{-}H}$ = 87 Hz, B*H*), 2.83 (s, 6H, CH_3).

^{13}C NMR (100 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 157.12 (*C*2(py)) 149.12*(C*4(py)), 148.61 (dm, $^{1}J_{C\text{-}F}$ = 240 Hz, *C*F), 147.11 (*C*2(py)), 138.30 (dm, $^{1}J_{C\text{-}F}$ = 240 Hz, *C*F), 136.79 (dm, $^{1}J_{C\text{-}F}$ = 240 Hz, *C*F), 126.84 (*C*3(py)), 126.04 (*C*3(cat)), 114.57 (*C*2(cat)), 22.01 (*C*H_3).

^{19}F NMR (376 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = -133.98 (s, 6F, *ortho*- C_6F_5), -164.34 (s, 3F, *para*- C_6F_5), -167.37 (s, 6F, *meta*-C_6F_5).

^{11}B NMR (160 MHz, CD_2Cl_2, 25 ℃): δ [ppm] = 26.8 (s, 1B, *B*cat) -25.4 (d, 1B, $^{1}J_{B\text{-}H}$ = 91 Hz, *B*H).

Element analysis: calcd for $C_{31}H_{14}B_2F_{15}NO_2$ C 50.38, H 1.91, N 1.90%; found C 50.48, H 1.86, N 2.10%.

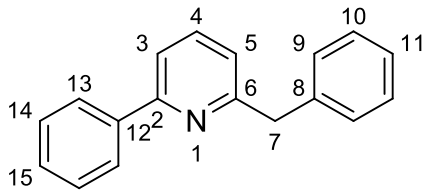


Synthesis of 2-benzyl-6-methylpyridine: A vigorously magnetically stirred mixture of PhI (594mg, 2.9mmol), **1a** (450mg, 0.73mmol), $Pd(PPh_3)_4$ (84mg, 0.073 mmol), and *t*-BuOK (326mg, 2.9mmol) in xylene (6mL) was heated at 140 ℃ (oil bath) under N_2 atmosphere for 24 h. After removal of the volatile under vacuum, the resulting oil was extracted with CH_2Cl_2 (3x10mL). Then the volatile was removed under vacuum, and the resulting oil was purified by column chromatography (petroleum ether--EtOAc, 10:1) to give compound **4a** (110mg, 82%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃): δ [ppm] = 7.44 (t, 1H), 7.19-7.32 (m, 5H), 6.97 (d, 1H), 6.85 (d, 1H), 4.14 (s, 2H), 2.55 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 25 ℃): δ [ppm] = 160.51, 157.97, 139.77, 136.82, 129.31, 128.64, 126.42, 120.83, 120.09, 44.86, 24.69.

HRMS (ESI, m/z): calcd for $C_{13}H_{13}N$ [M+H^+] 184.1126, found 184.1121.



Synthesis of 2-benzyl-6-phenylpyridine: A vigorously magnetically stirred mixture of PhI (539mg, 2.6mmol), **1i** (450mg, 0.66mmol), $Pd(PPh_3)_4$ (76mg, 0.066mol), and *t*-BuOK(296mg, 2.6mmol) in xylene (6mL) was heated at 140 ℃ (oil bath) under N_2 atmosphere for 24 h. After removal of the volatile under vacuum, the resulting oil was extracted with CH_2Cl_2 (3x10mL). Then the volatile was removed under vacuum, and the resulting oil was purified by column chromatography (petroleum ether--EtOAc, 20:1) to give **4i** (89mg, 55%).

^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃): δ [ppm] = 8.03 (d, 2H, $^3J_{H-H}$= 7.2 Hz, *H*13), 7.64 (t, 1H, $^3J_{H-H}$= 7.7 Hz, *H*4), 7.56 (d, 1H, $^3J_{H-H}$= 7.7 Hz, *H*3), 7.49 (t, 2H, $^3J_{H-H}$= 7.6 Hz, *H*14), 7.44 (t, 2H, $^3J_{H-H}$= 7.2 Hz, *H*15), 7.37 (d, 2H, $^3J_{H-H}$= 7.6 Hz, *H*9), 7.35 (t, 2H, $^3J_{H-H}$= 7.6 Hz, *H*10), 7.26 (t, 1H, $^3J_{H-H}$= 7.6 Hz, *H*11), 7.03 (d, 2H, $^3J_{H-H}$= 7.5 Hz, *H*5), 4.27 (s, 2H, *H*7).

^{13}C NMR (100 MHz, $CDCl_3$, 25 ℃): δ [ppm] = 161.03 (*C*6), 156.98 (*C*2), 139.84 (*C*8), 139.77 (*C*12), 137.27 (*C*4), 129.39 (*C*9), 128.92 (*C*15), 128.82 (*C*10), 128.65 (*C*14), 127.14 (*C*13), 126.44 (*C*11), 121.47 (*C*5), 118.11 (*C*3), 45.06 (*C*7).

HRMS (ESI, m/z): calcd for $C_{18}H_{15}N$ [M+H^+] 246.1287, found 246.1277.

II. Mechanism study

Kinetic isotope effect experiments

A solution of 2,6-lutidine (8.4mg, 0.078mmol) or 2,6-lutidine-d_6 (8.8mg, 0.078mmol), and HBcat (1.0mg, 0.0083mmol) in CD_2Cl_2 (0.2mL) was added to the solution of $B(C_6F_5)_3$ (40mg, 0.078mmol) in CD_2Cl_2 (0.3mL). The resulting solution was transferred to a J. Young NMR tube, and analyzed by ^{11}B NMR spectroscopy. From the ^{11}B NMR spectra, the initial rates for the formation of **1a** were determined. KIE k_H/k_D = 5.8.

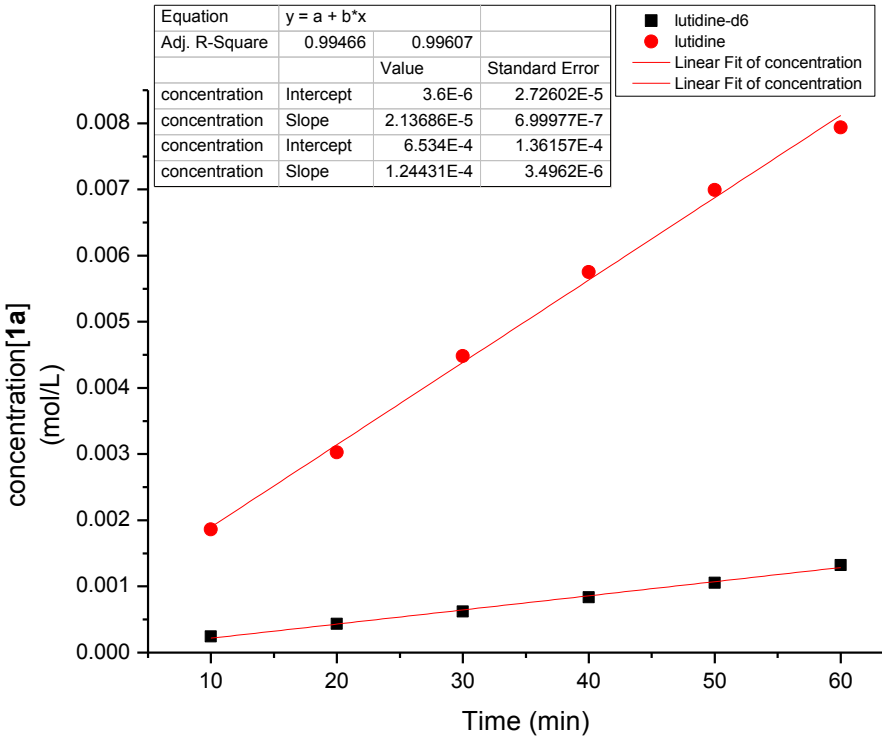
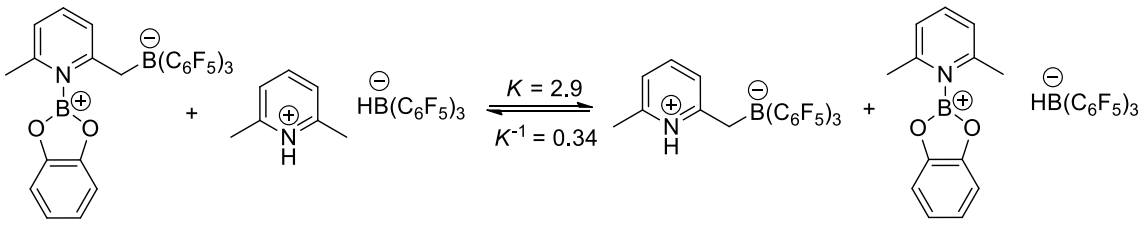


Figure **S1** Formation of **1a** when 2,6-lutidine or 2,6-lutidine-d_6 was used

Equilibrium reaction experiments

A solution of $[2,6\text{-}Me_2C_5H_3NH][HB(C_6F_5)_3]$ (12.6mg, 0.020mmol) in CD_2Cl_2 (0.2mL) was added to the solution of **2** (15.0mg, 0.020mmol) in CD_2Cl_2 (0.3mL). The resulting solution was transferred to a J. Young NMR tube, and ^1H NMR spectra was carried out to calculate the equilibrium constant of this reaction.

A solution of **1a** (12.5mg, 0.020mmol) in CD_2Cl_2 (0.2mL) was added to the solution of [2,6-lutidine/Bcat][$HB(C_6F_5)_3$] (15.0mg, 0.020mmol) in CD_2Cl_2 (0.3mL). The resulting solution was transferred to a J. Young NMR tube, and ^1H NMR spectra was carried out to calculate the equilibrium constant of this reaction.



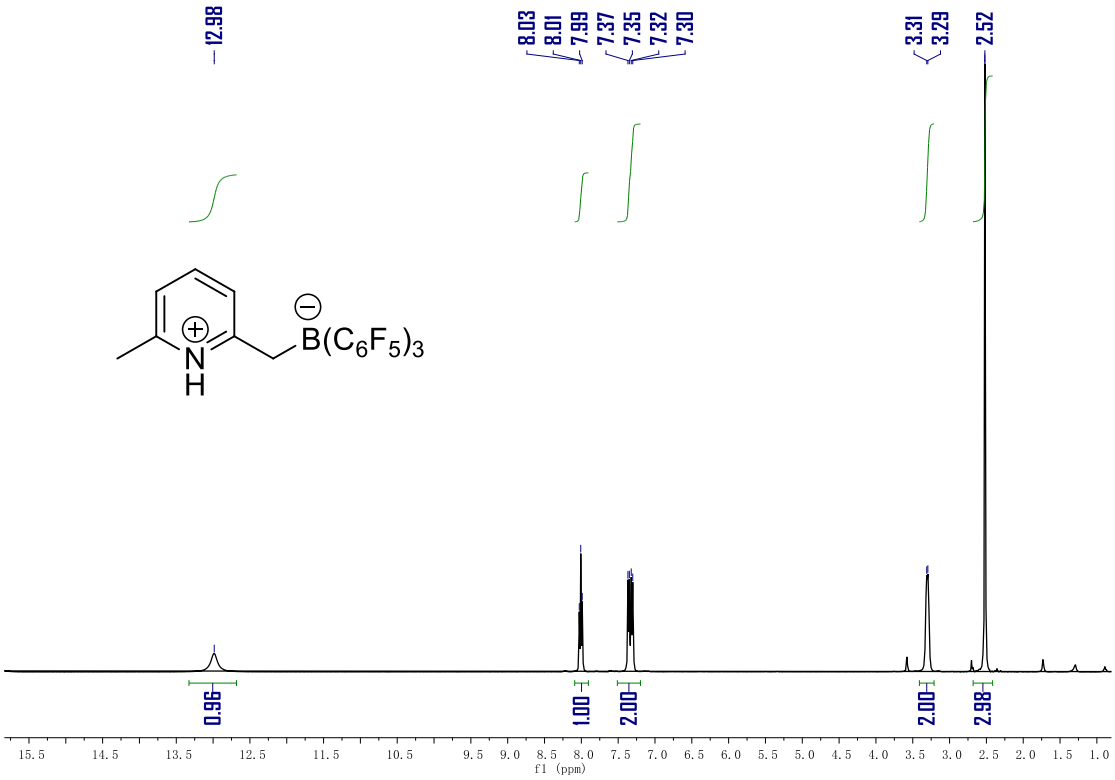


Figure S2: ^{1}H NMR spectrum of **1a** in THF-d_8

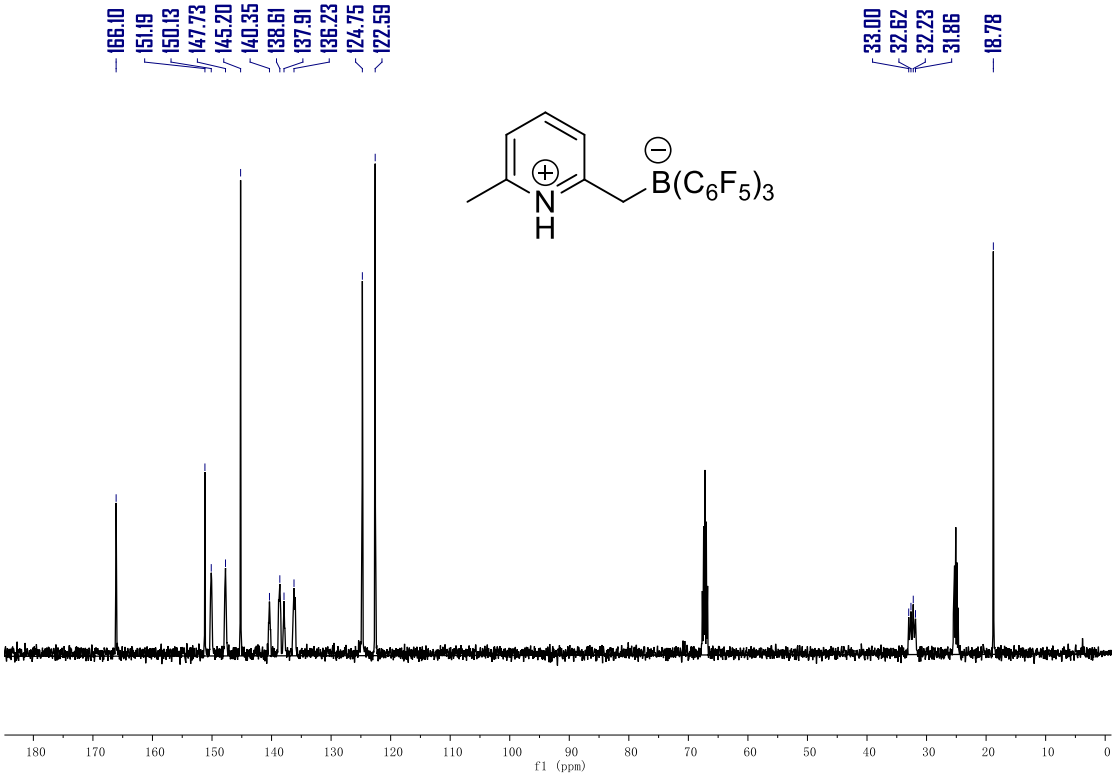


Figure S3: ^{13}C NMR spectrum of **1a** in THF-d_8

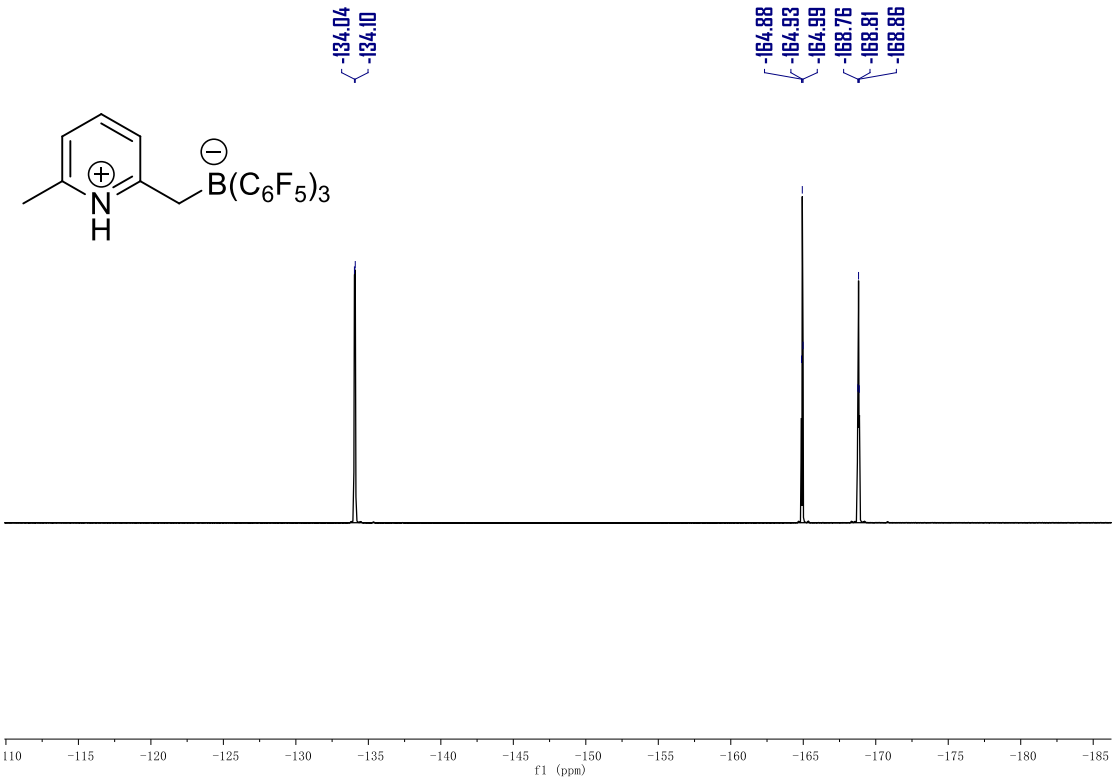


Figure S4: ^{19}F NMR spectrum of **1a** in THF-d_8

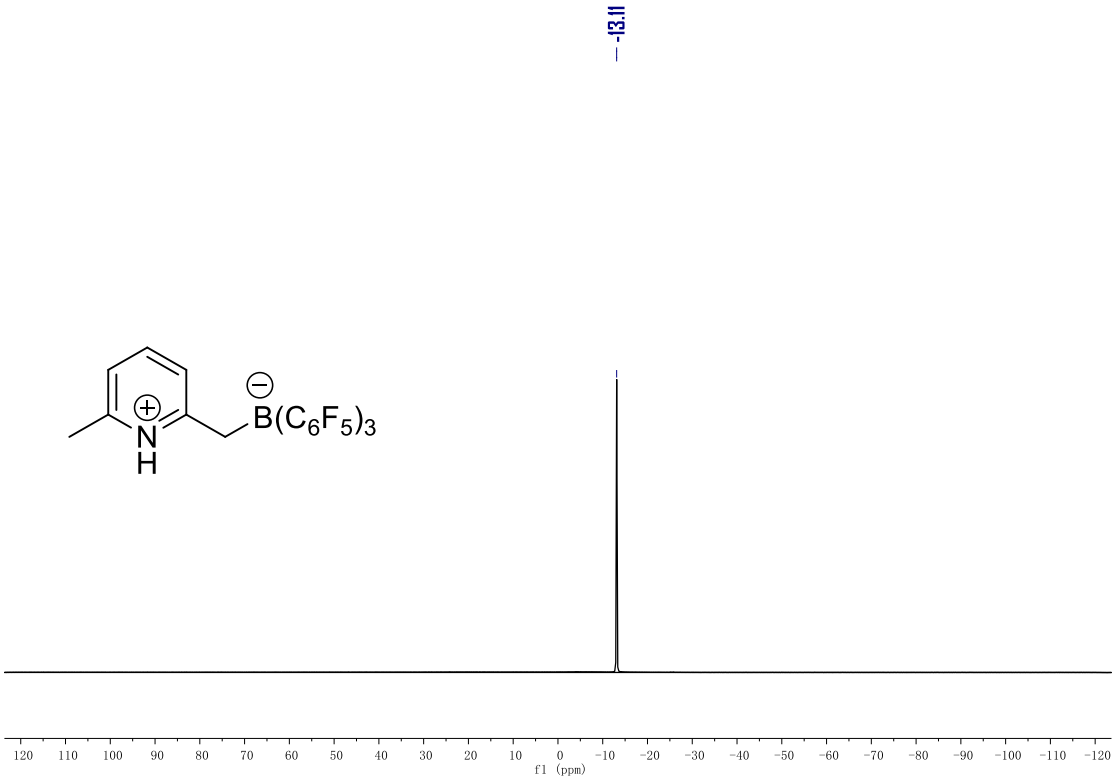


Figure S5: ^{11}B NMR spectrum of **1a** in THF-d_8

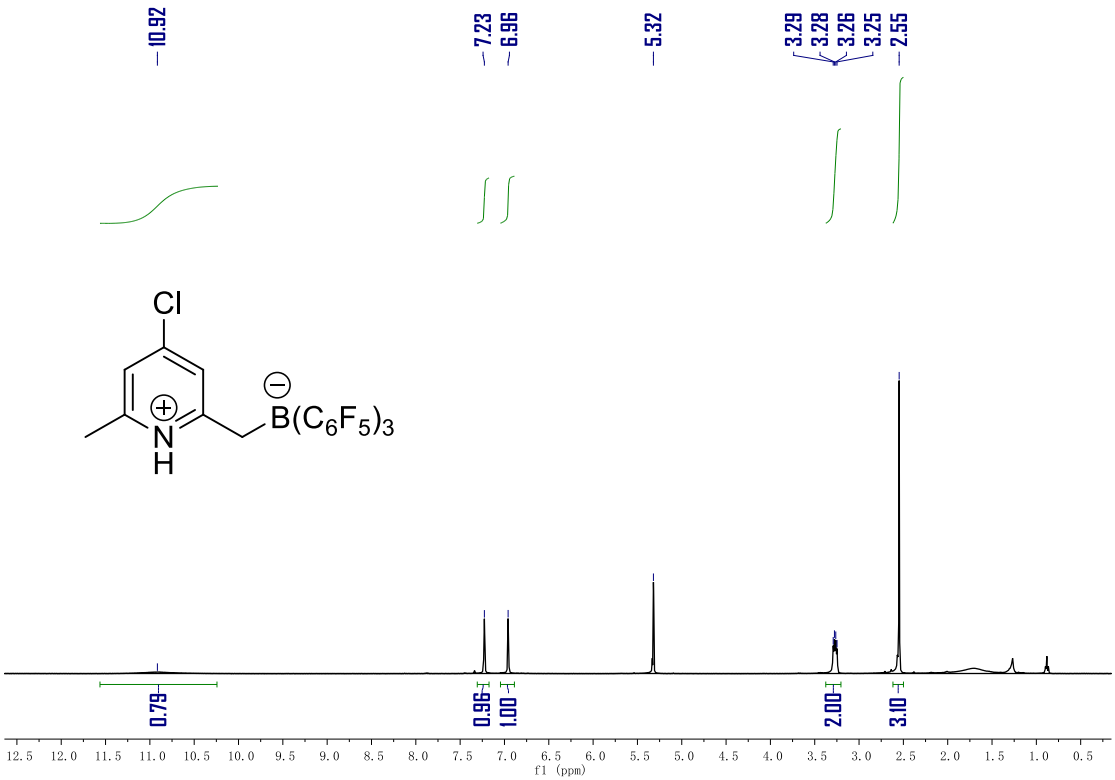


Figure S6: ^{1}H NMR spectrum of **1d** in CD_2Cl_2

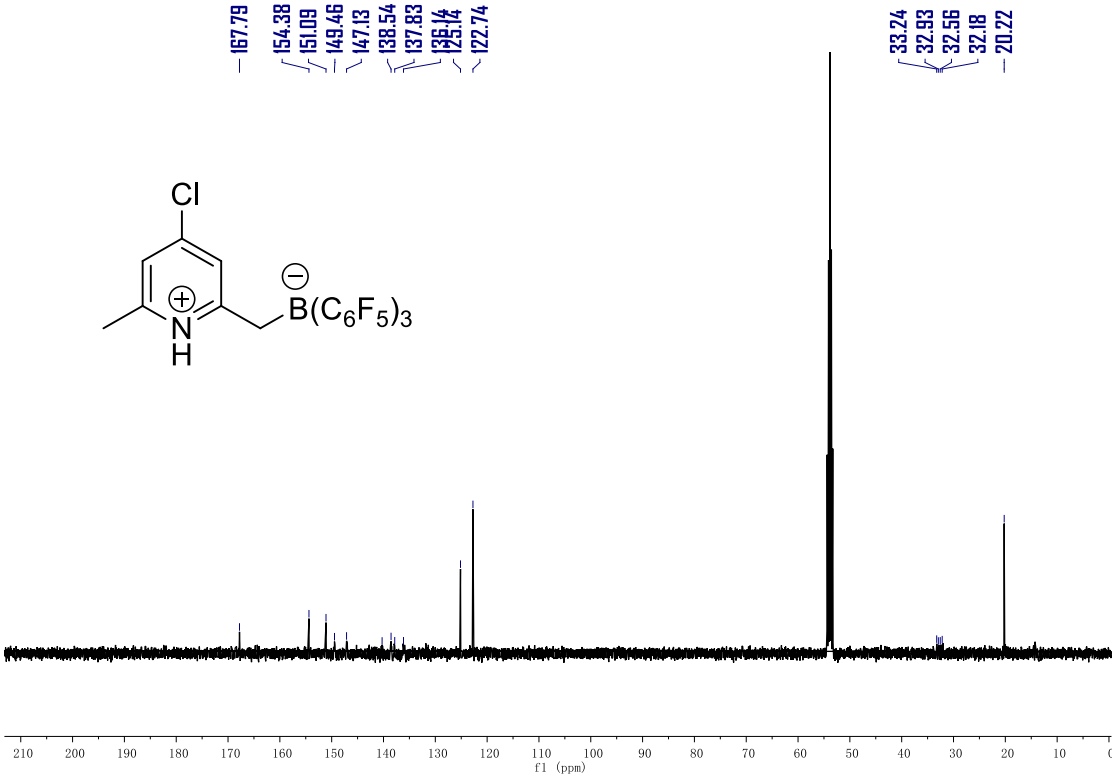


Figure S7: ^{13}C NMR spectrum of **1d** in CD_2Cl_2

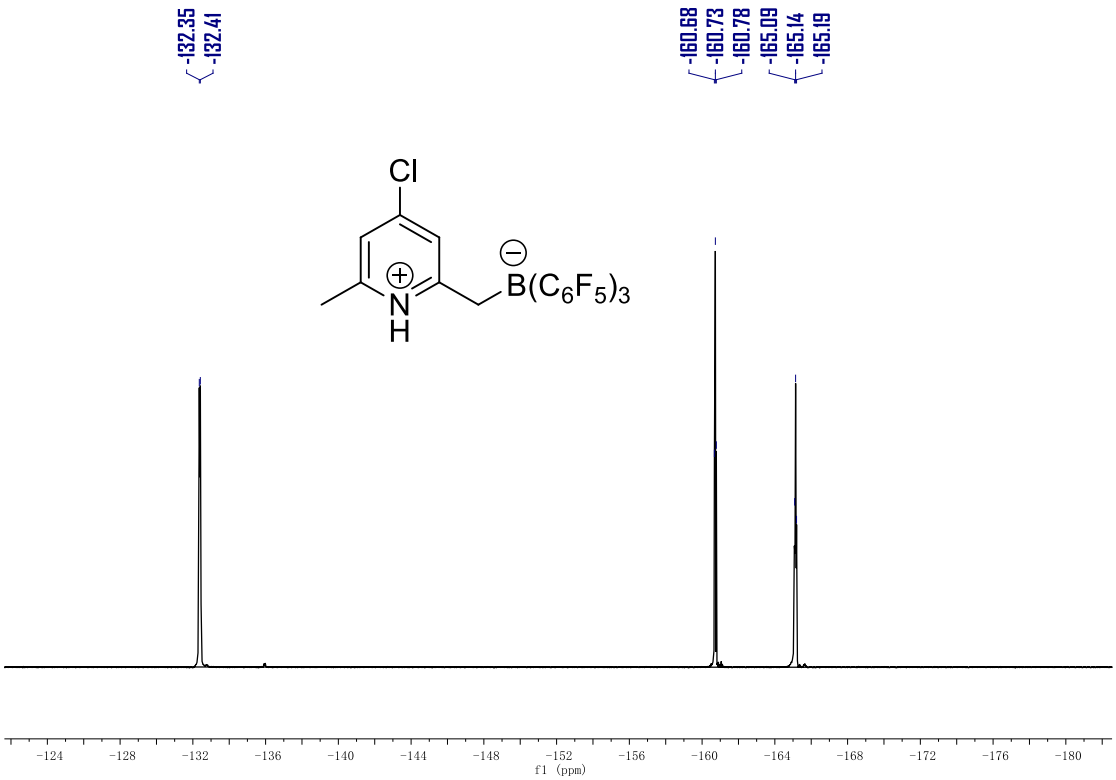


Figure S8: ^{19}F NMR spectrum of **1d** in CD_2Cl_2

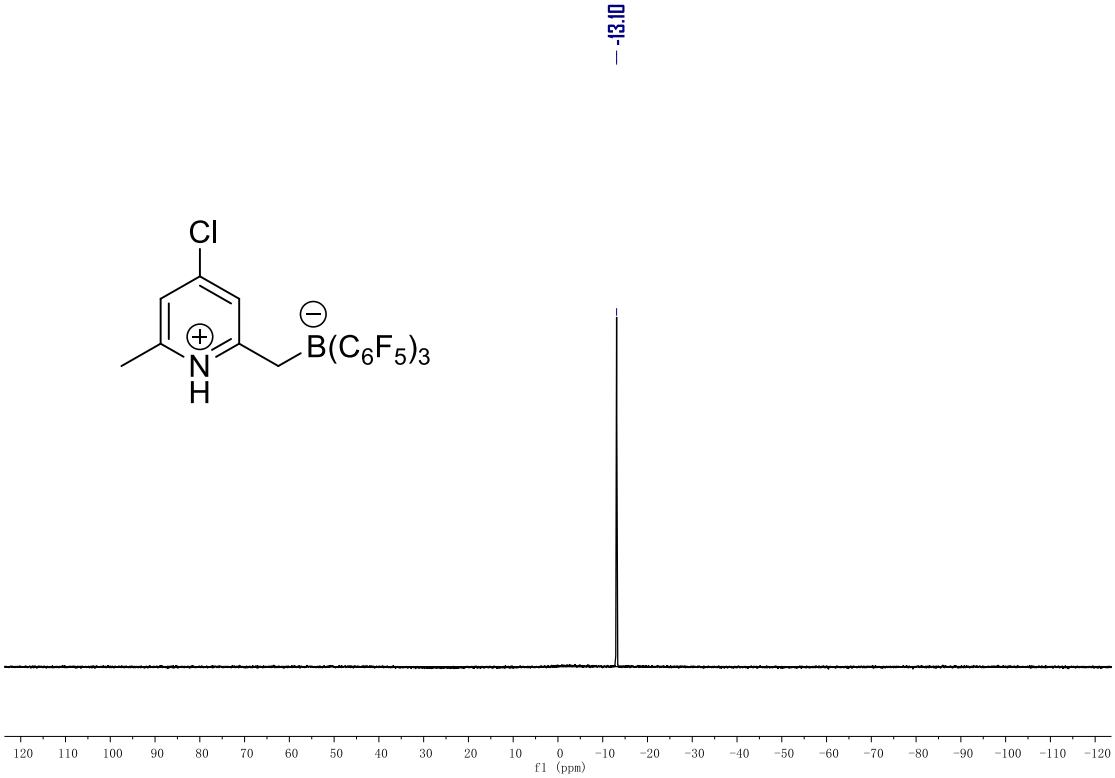


Figure S9: ^{11}B NMR spectrum of **1d** in CD_2Cl_2

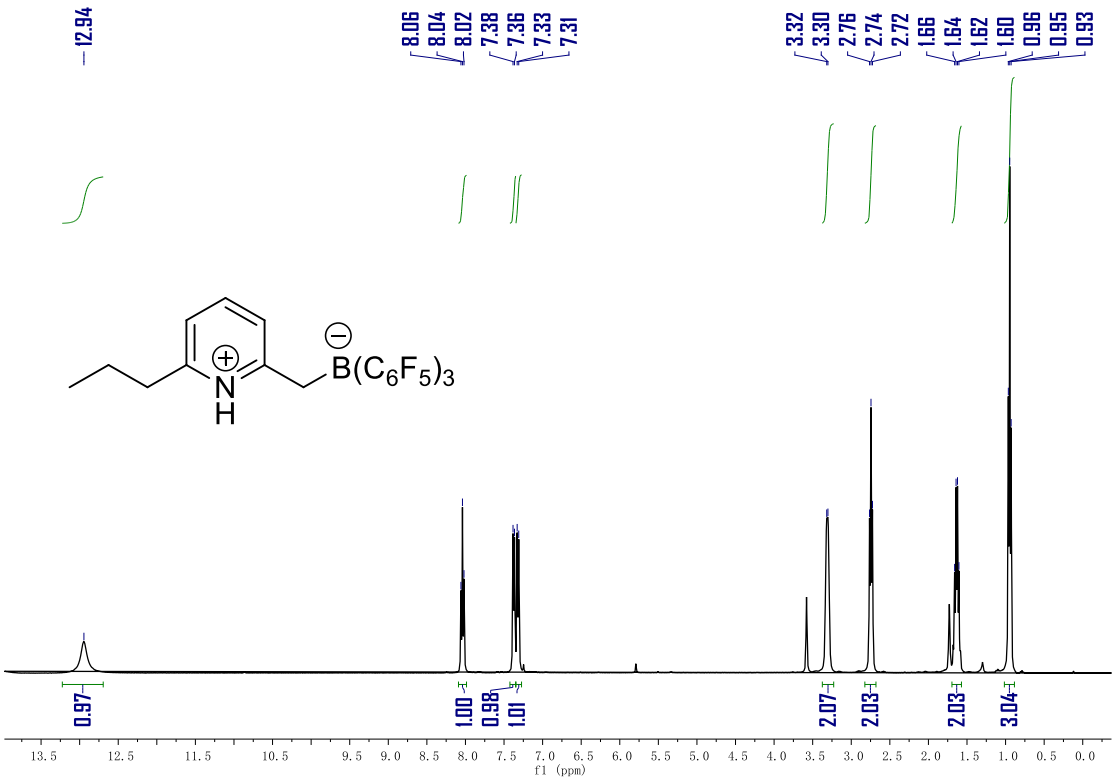


Figure S10: ^{1}H NMR spectrum of **1e** in THF-d_8

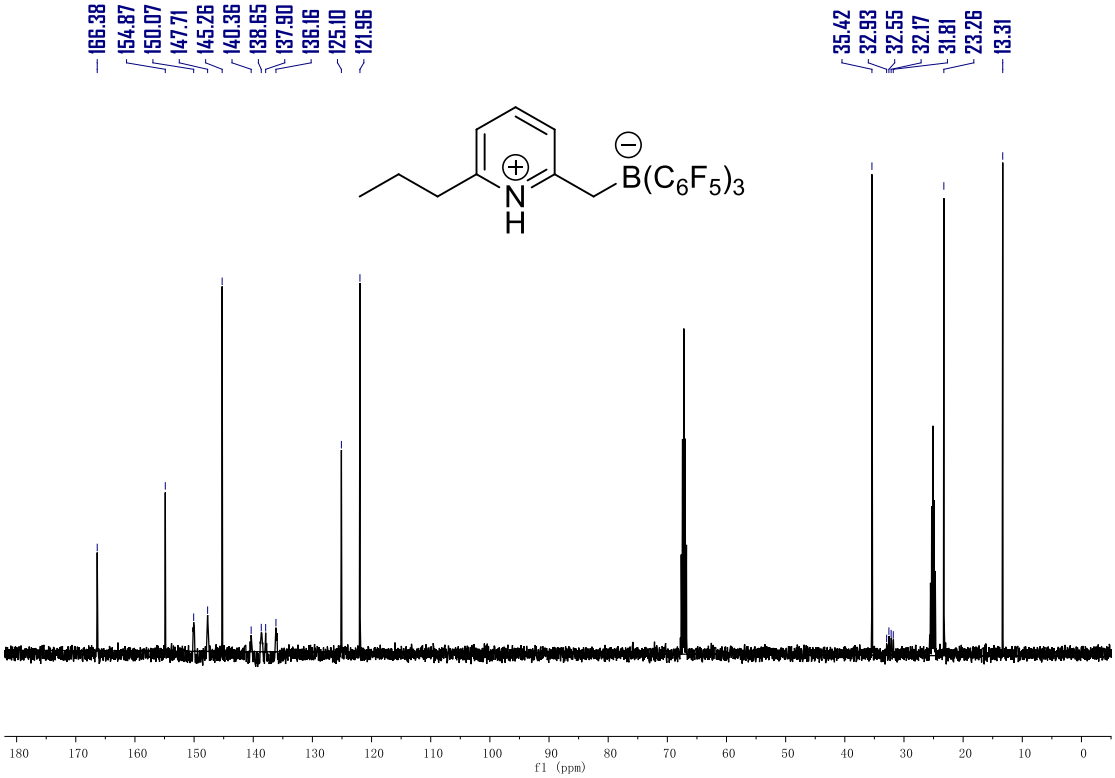


Figure S11: ^{13}C NMR spectrum of **1e** in THF- d_8

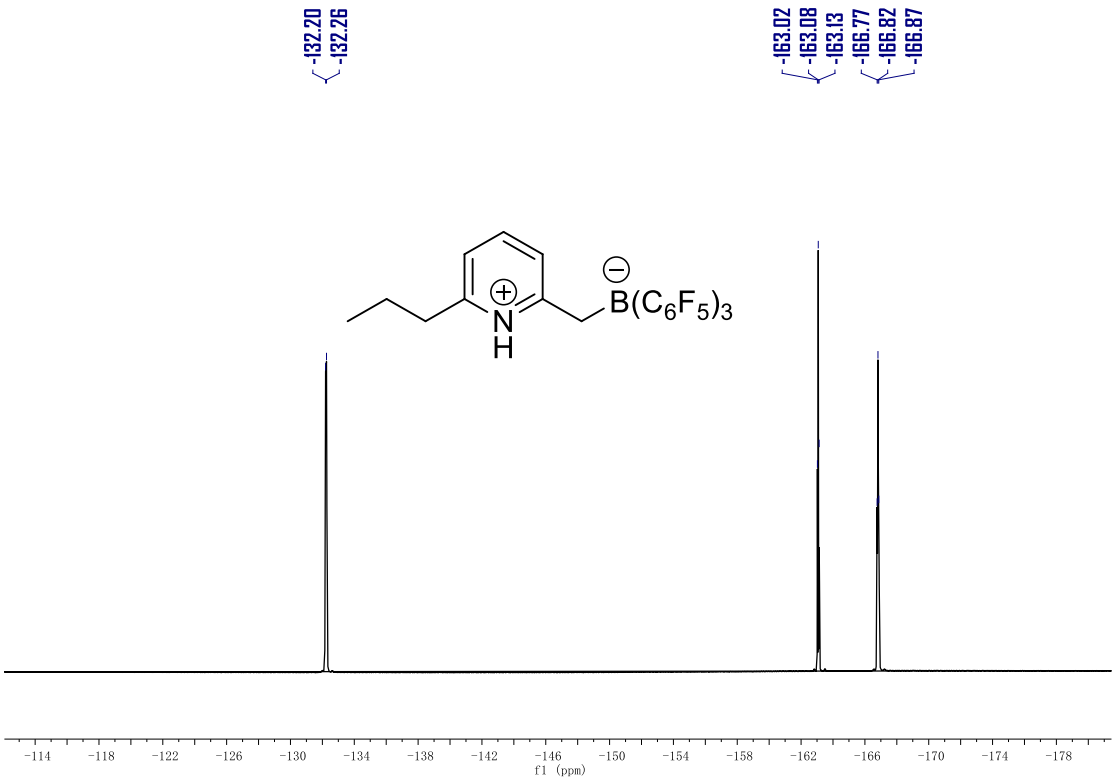


Figure S12: ^{19}F NMR spectrum of **1e** in THF- d_8

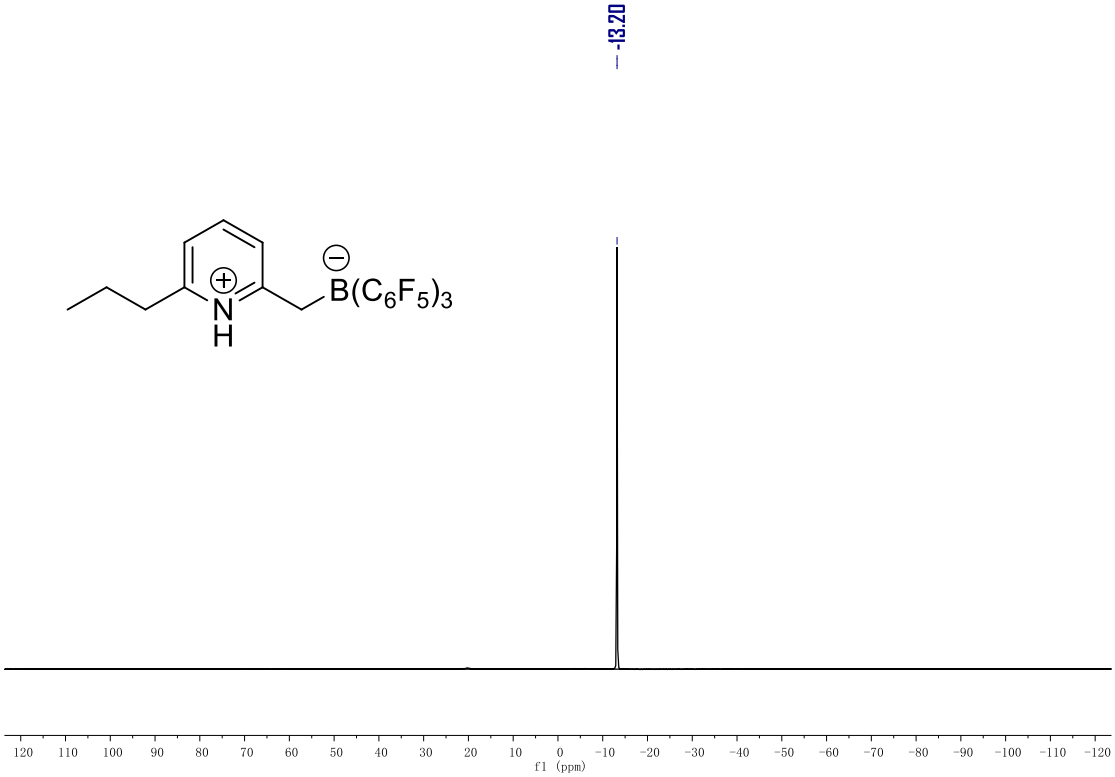


Figure S13: ^{11}B NMR spectrum of **1e** in THF- d_8

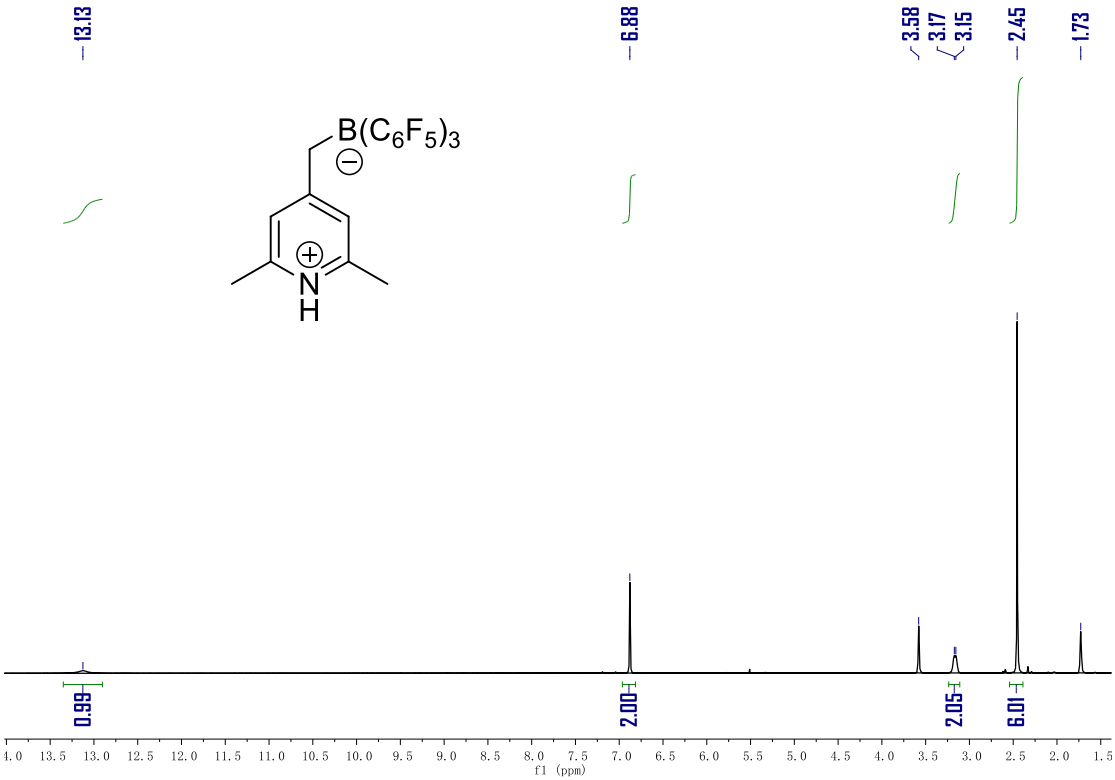


Figure S14: ^{1}H NMR spectrum of **1f** in THF- d_8

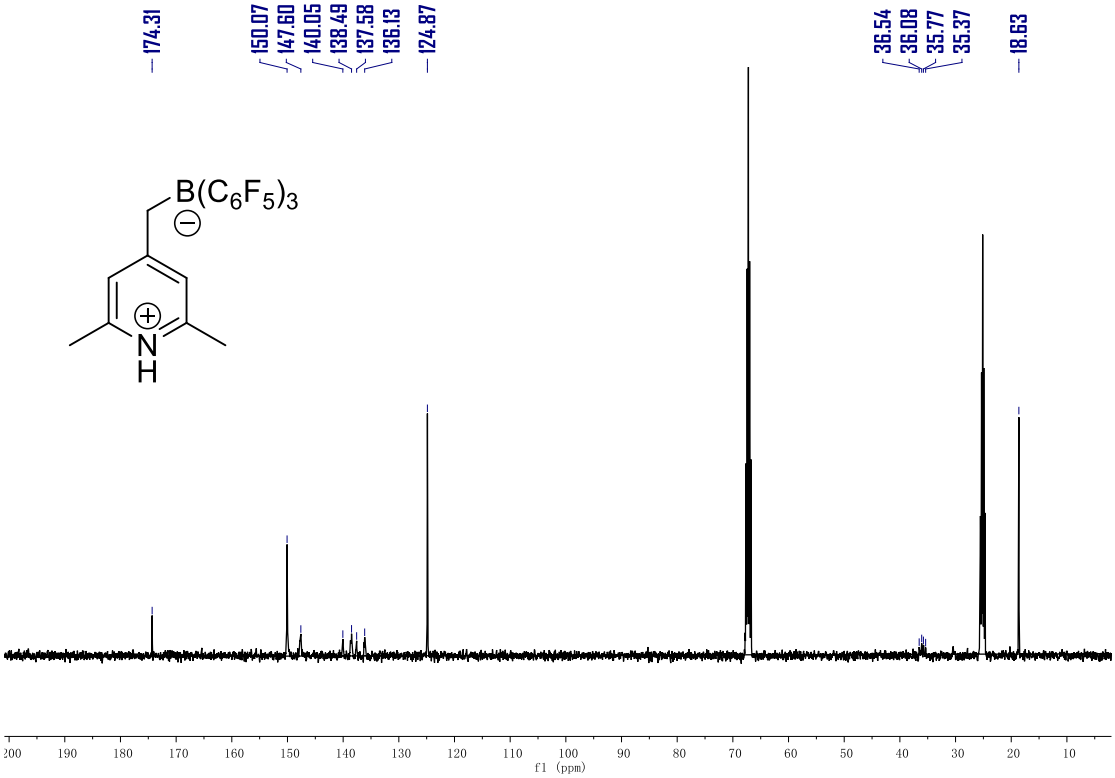


Figure S15: ^{13}C NMR spectrum of **1f** in THF- d_8

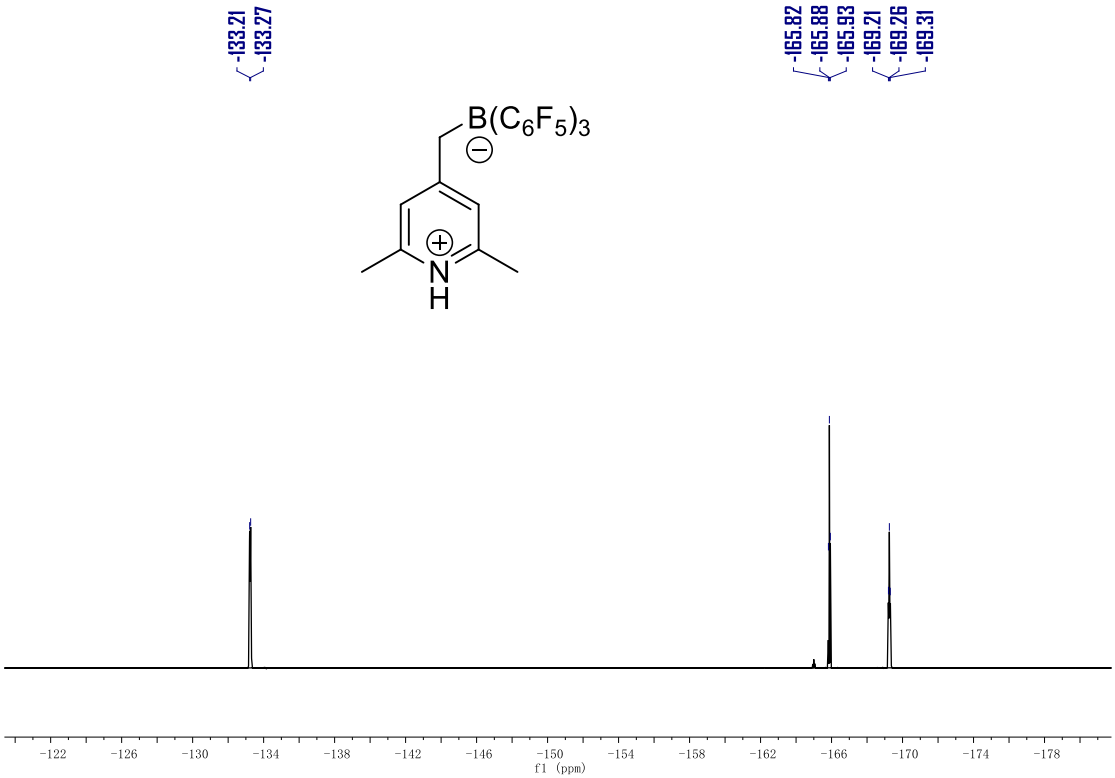


Figure S16: ^{19}F NMR spectrum of **1f** in THF- d_8

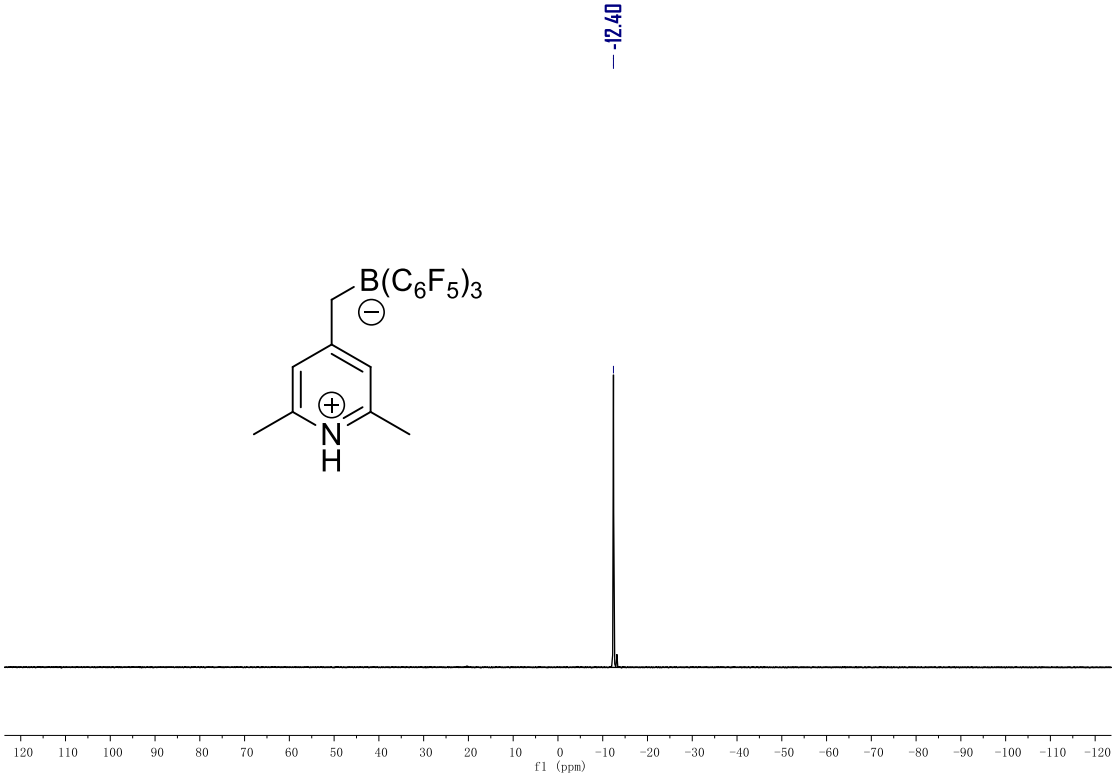


Figure S17: ^{11}B NMR spectrum of **1f** in THF- d_8

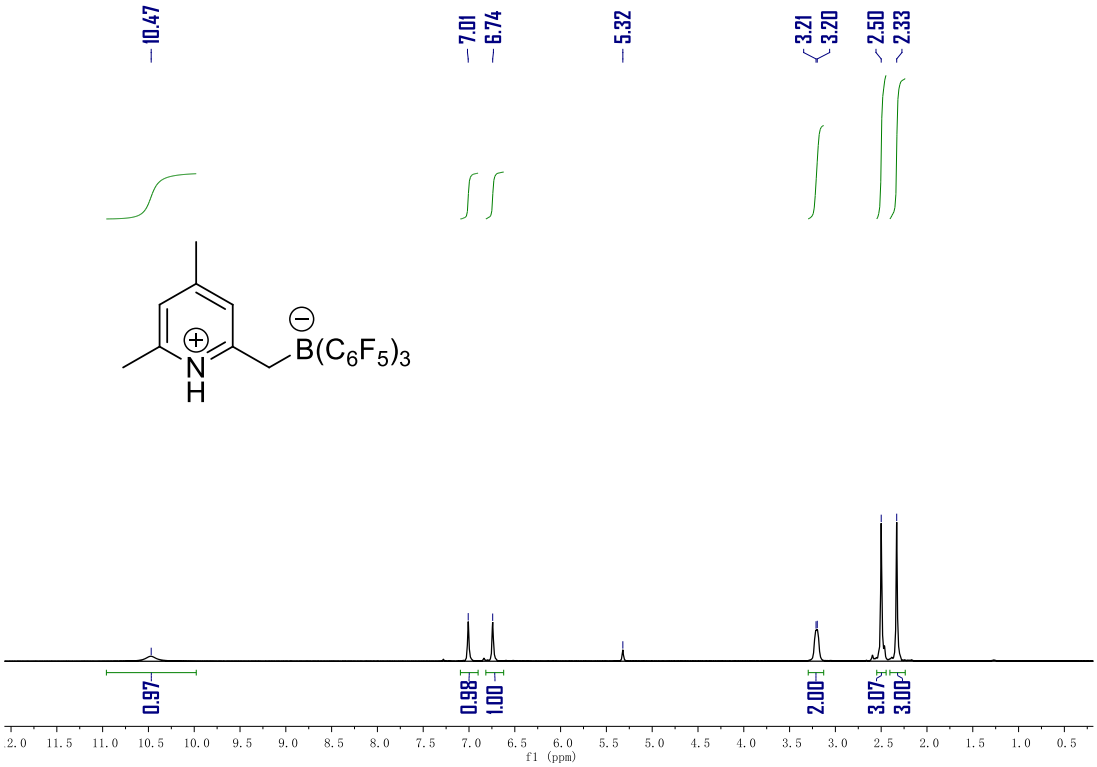


Figure S18: ^{1}H NMR spectrum of **1f'** in CD_2Cl_2

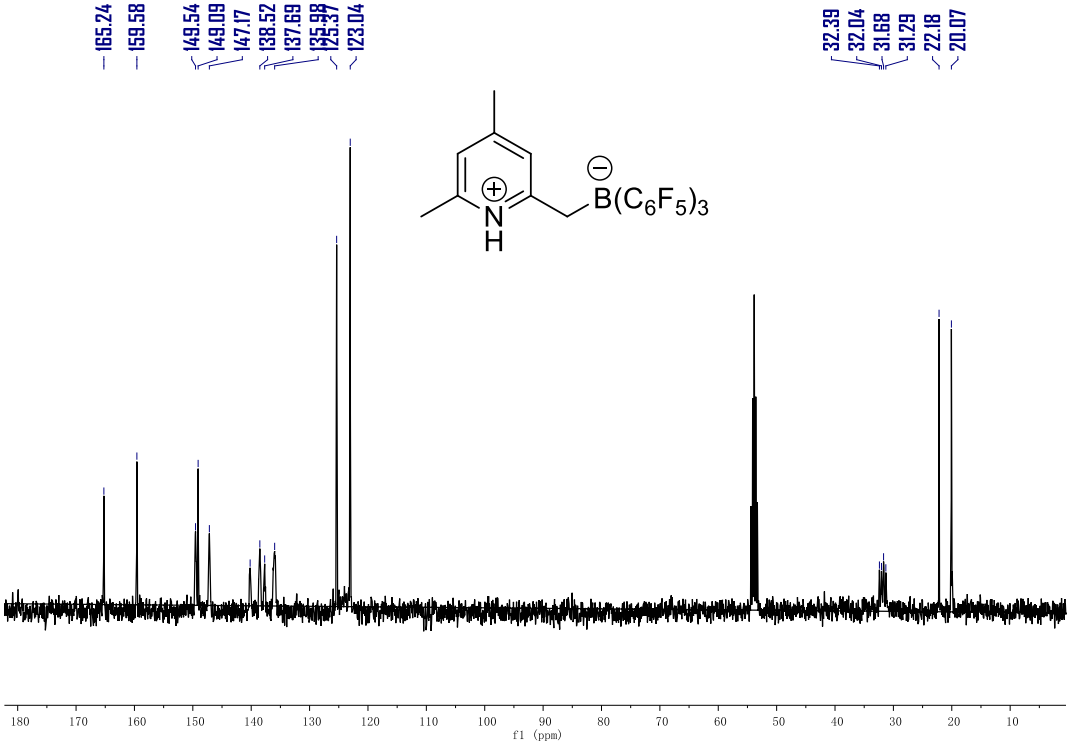


Figure S19: ^{13}C NMR spectrum of **1f'** in CD_2Cl_2

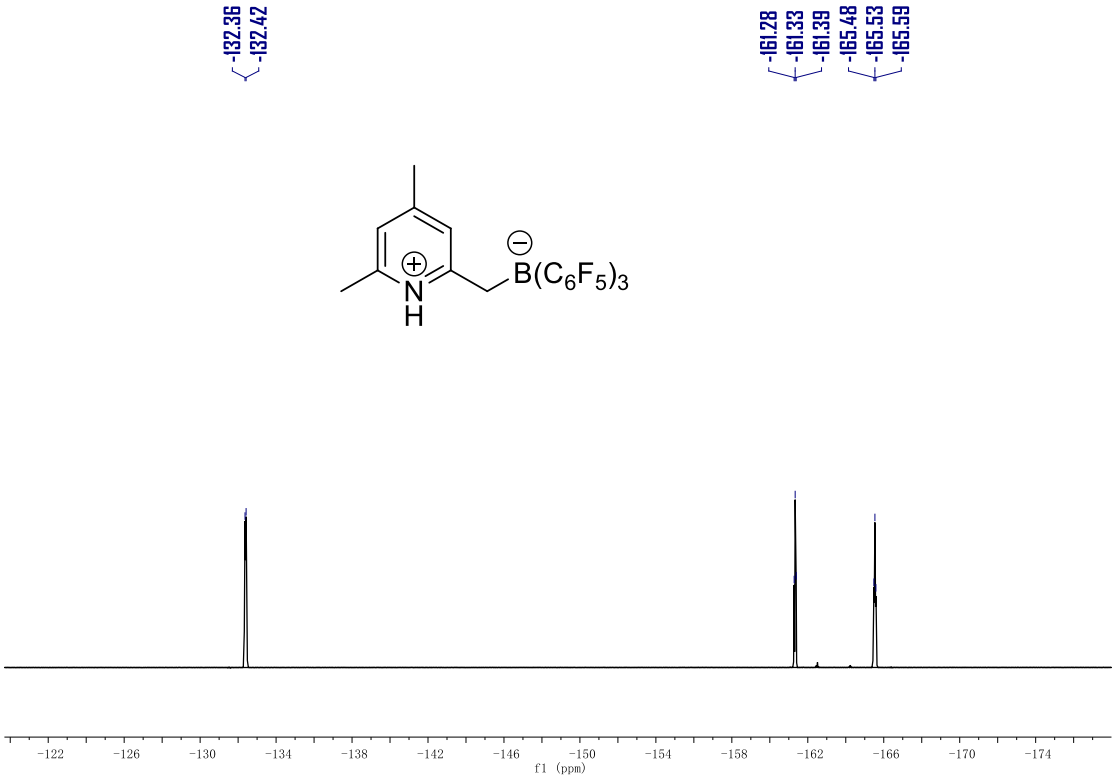


Figure S20: ^{19}F NMR spectrum of **1f'** in CD_2Cl_2

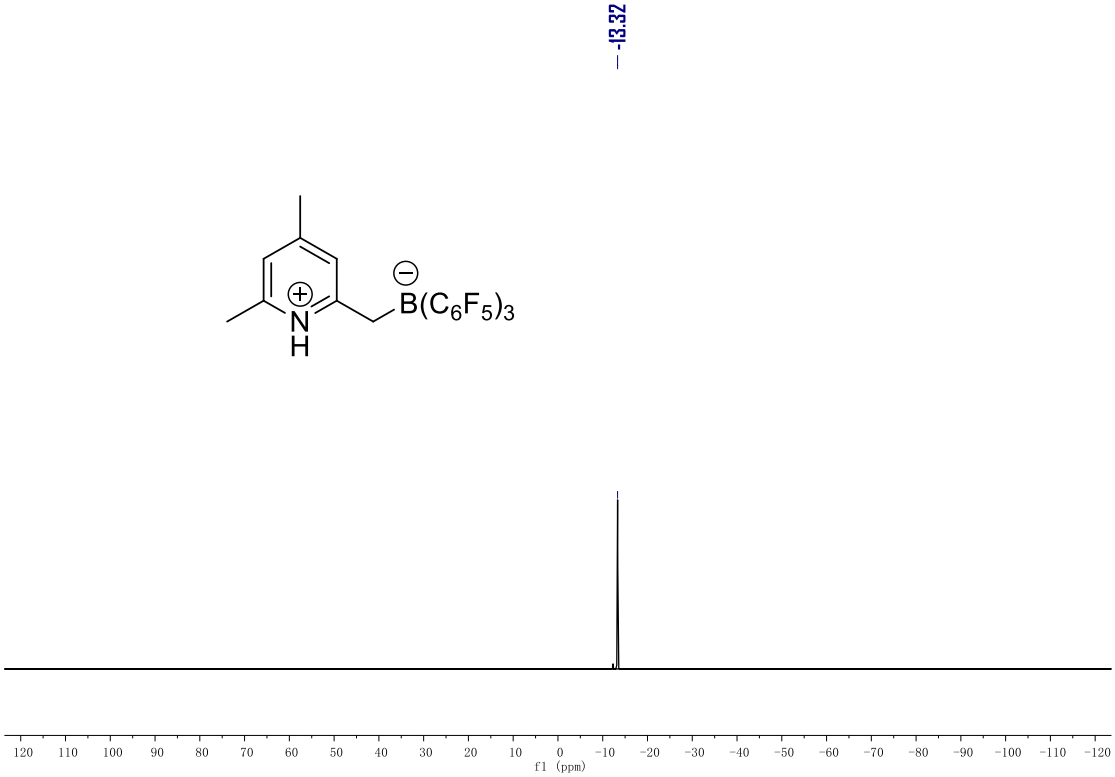


Figure S21: ^{11}B NMR spectrum of **1f'** in CD_2Cl_2

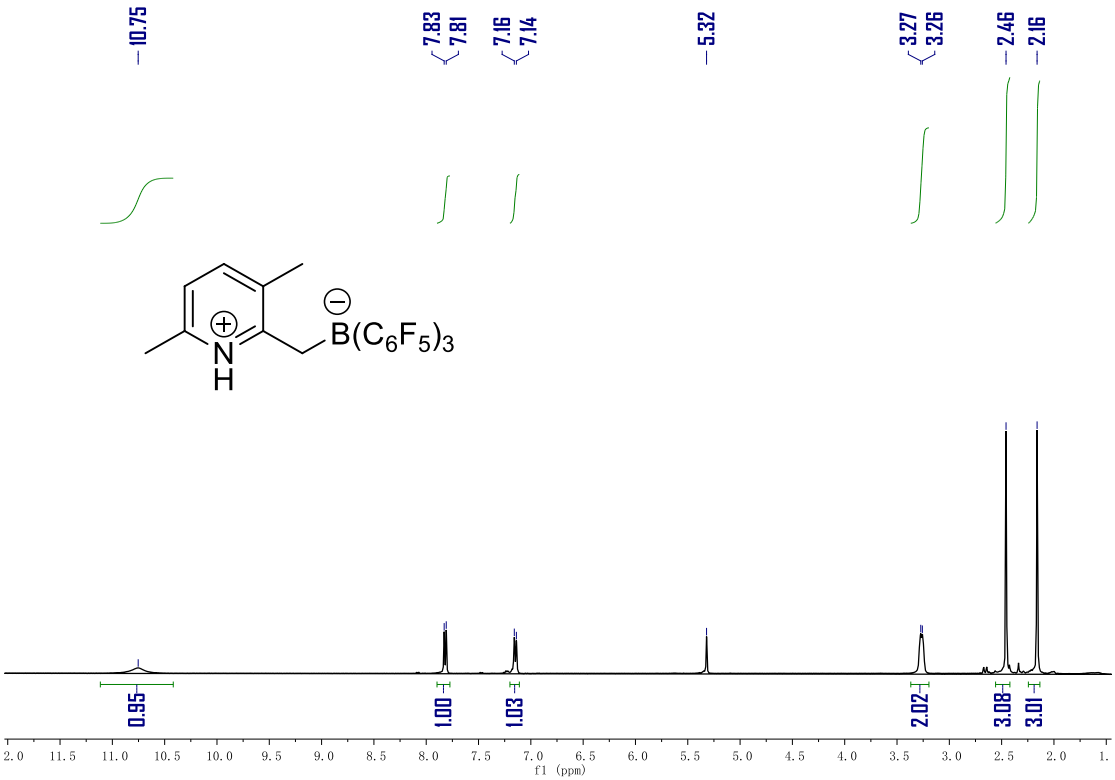


Figure S22: ^{1}H NMR spectrum of **1g** in CD_2Cl_2

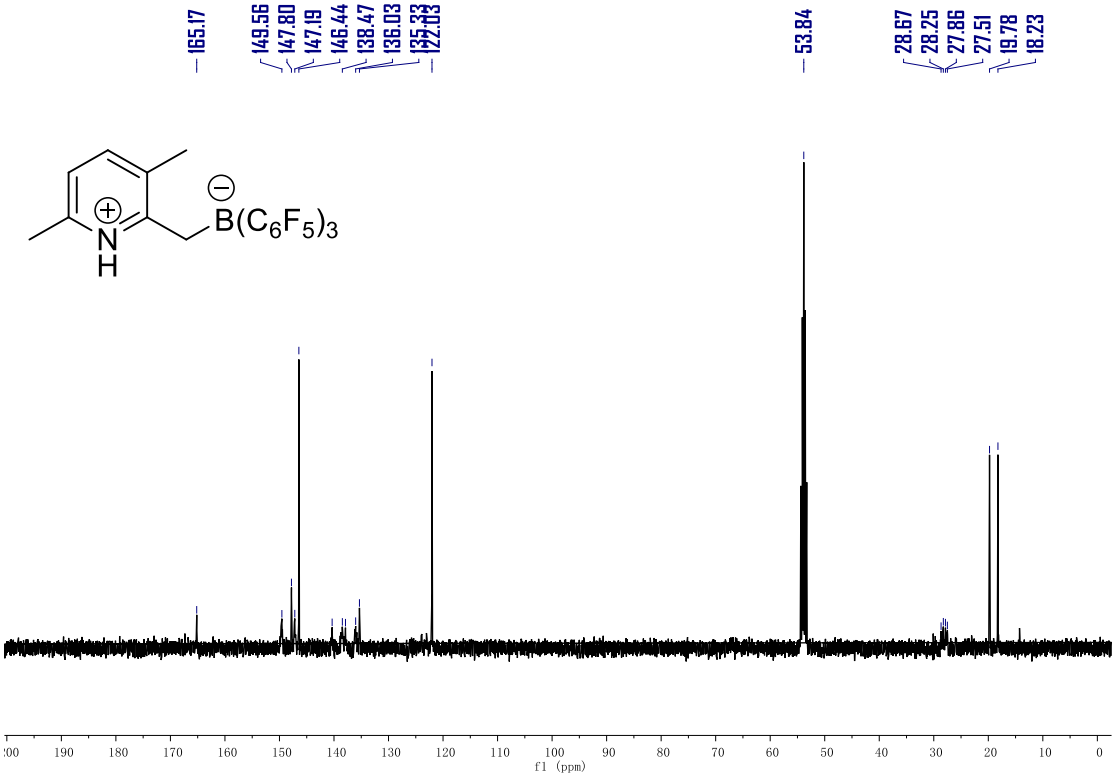


Figure S23: ^{13}C NMR spectrum of **1g** in CD_2Cl_2

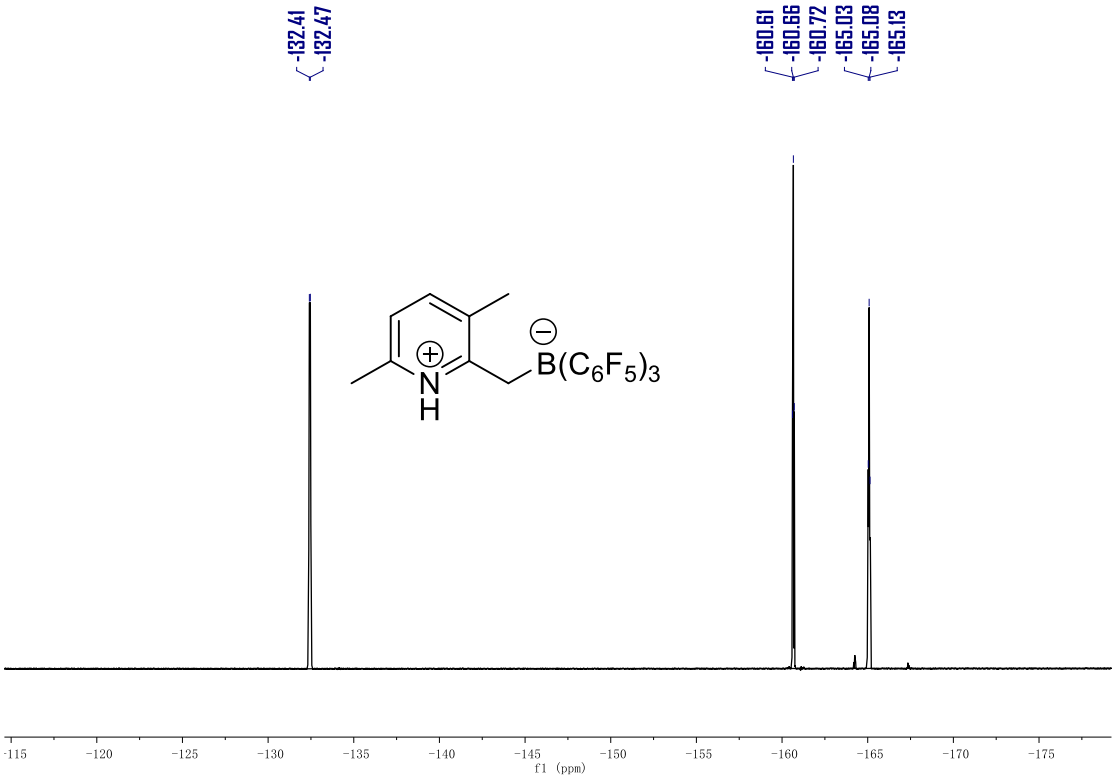


Figure S24: ^{19}F NMR spectrum of **1g** in CD_2Cl_2

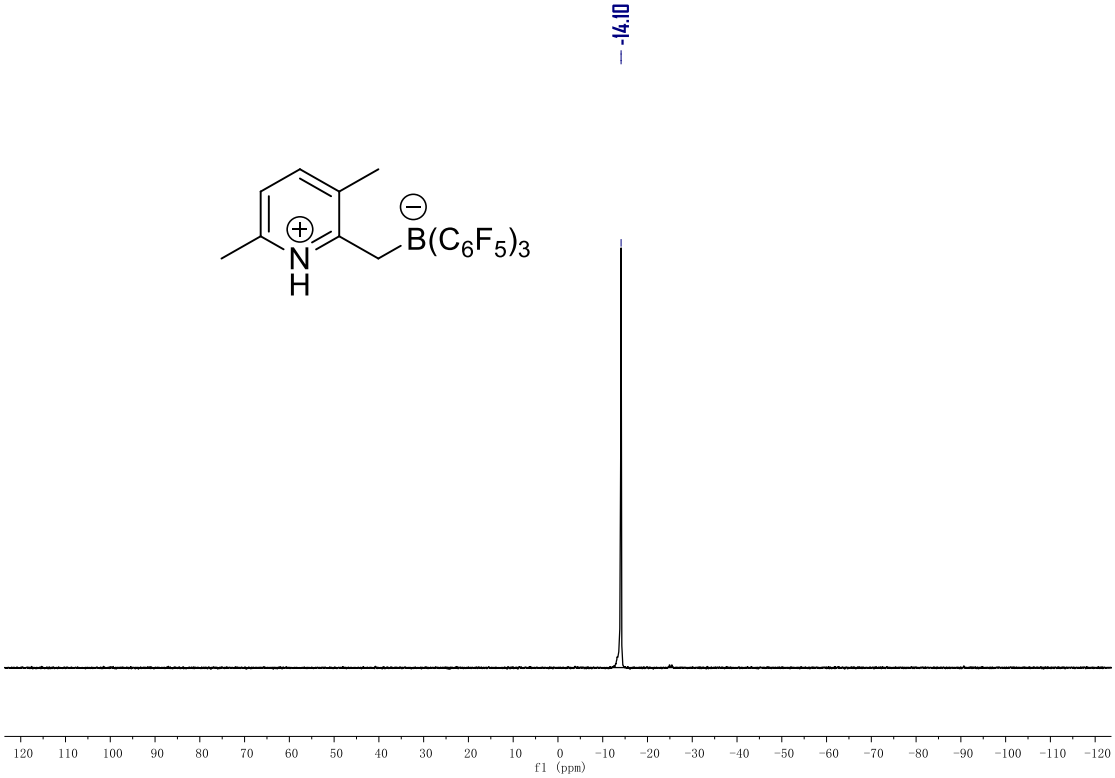


Figure S25: ^{11}B NMR spectrum of **1g** in CD_2Cl_2

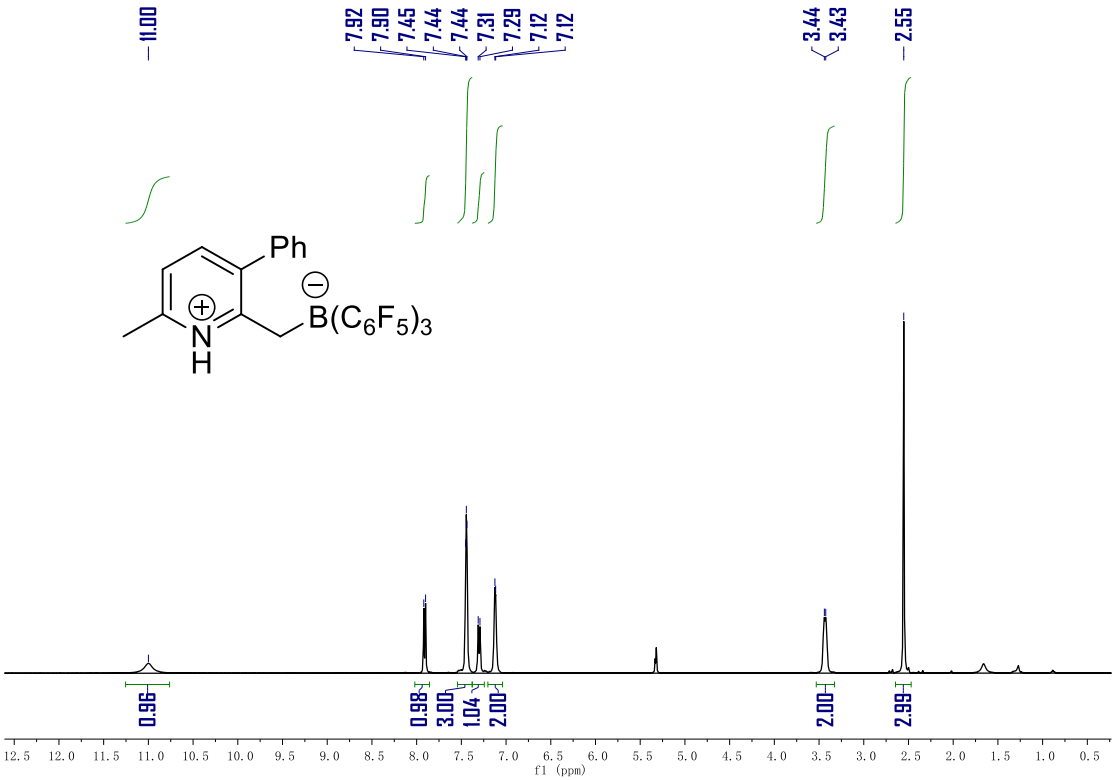


Figure S26: ^{1}H NMR spectrum of **1h** in CD_2Cl_2

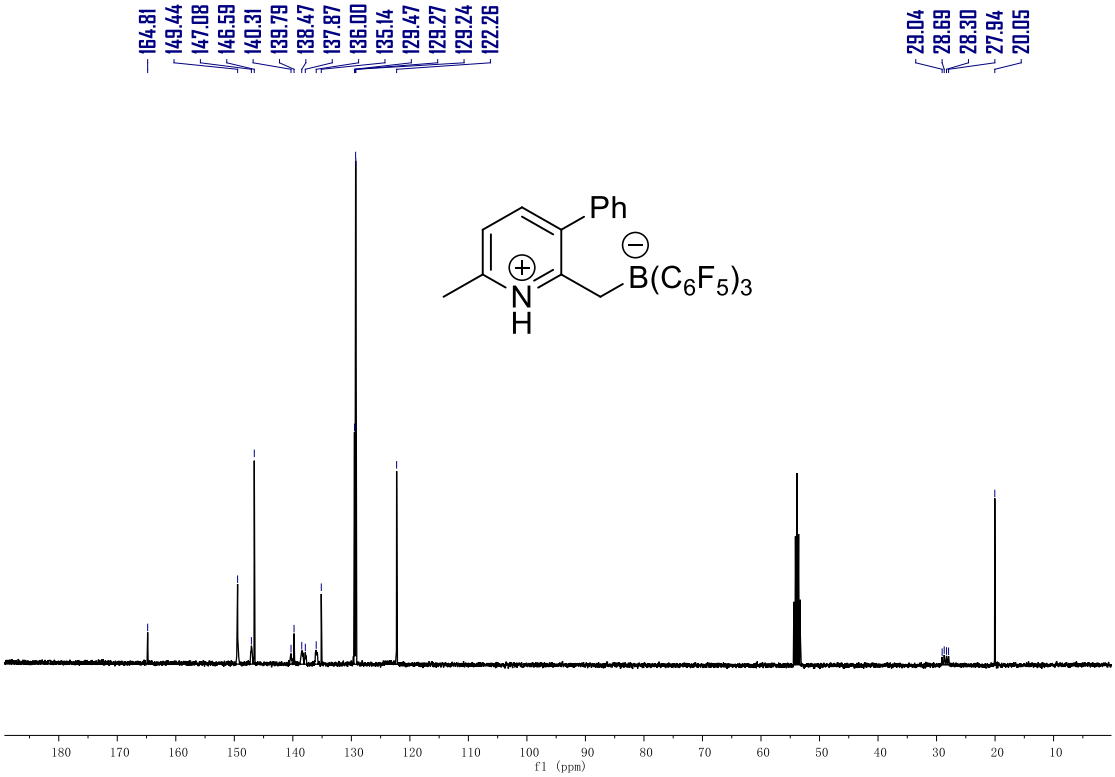


Figure S27: ^{13}C NMR spectrum of **1h** in CD_2Cl_2

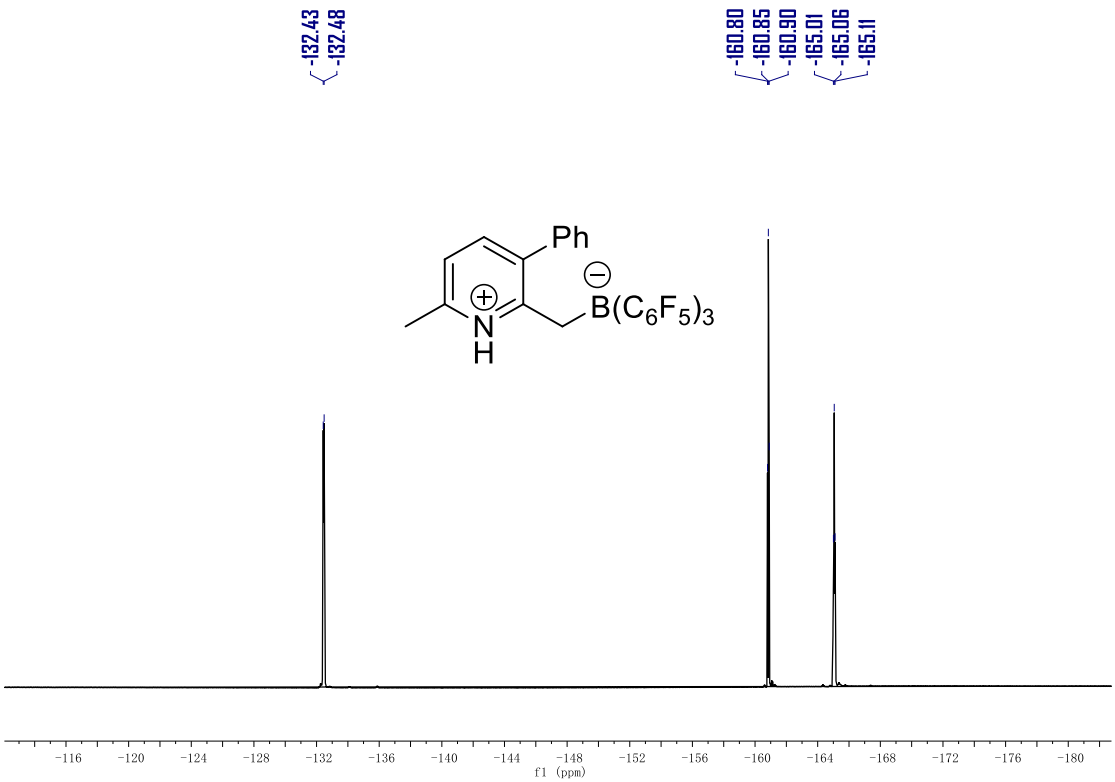


Figure S28: ^{19}F NMR spectrum of **1h** in CD_2Cl_2

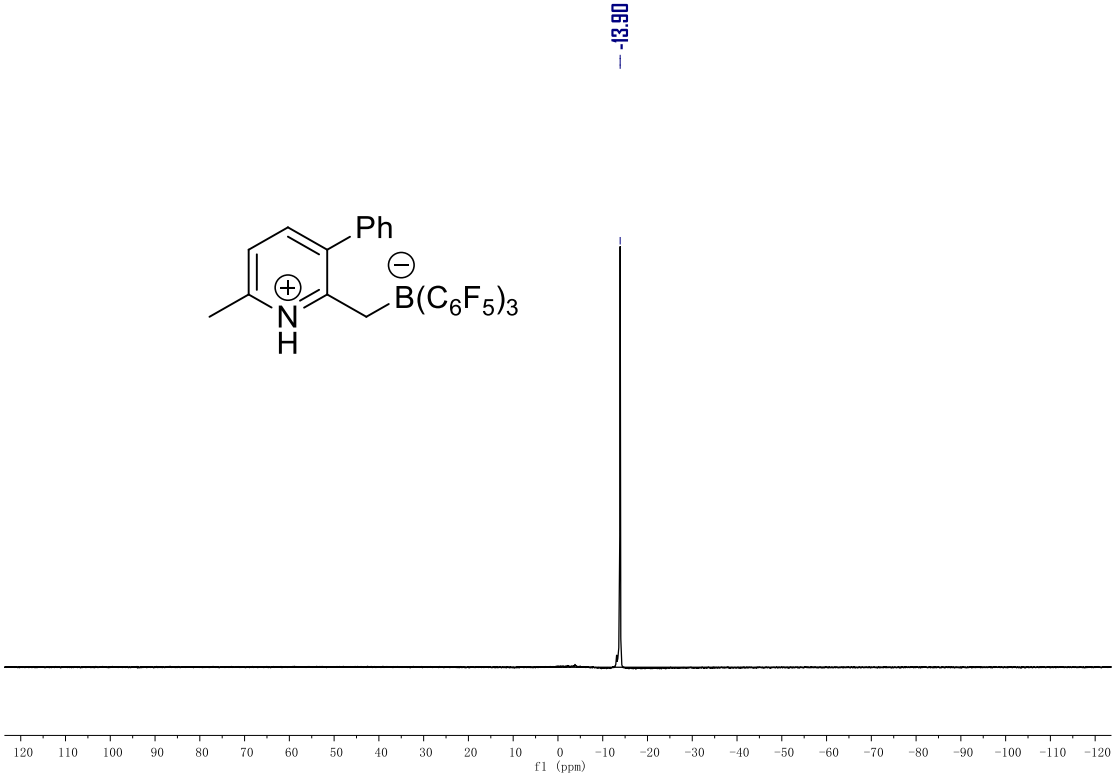


Figure S29: ^{11}B NMR spectrum of **1h** in CD_2Cl_2

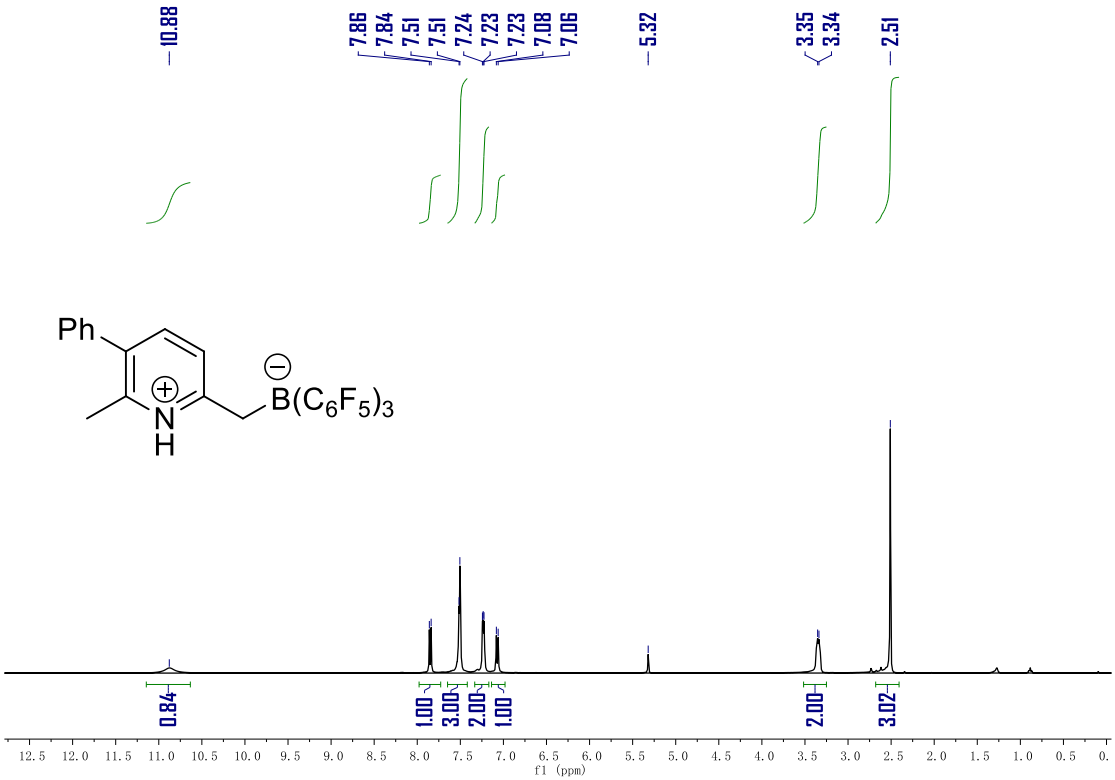


Figure S30: ^{1}H NMR spectrum of **1h'** in CD_2Cl_2

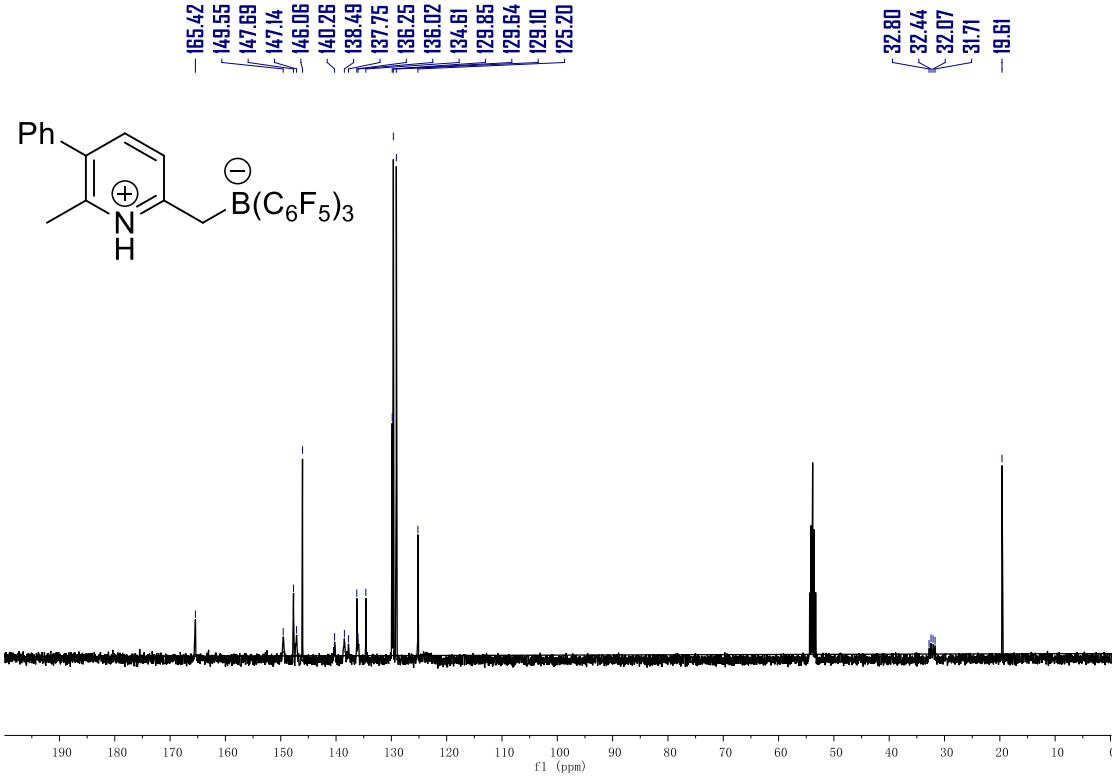


Figure S31: ^{13}C NMR spectrum of **1h'** in CD_2Cl_2

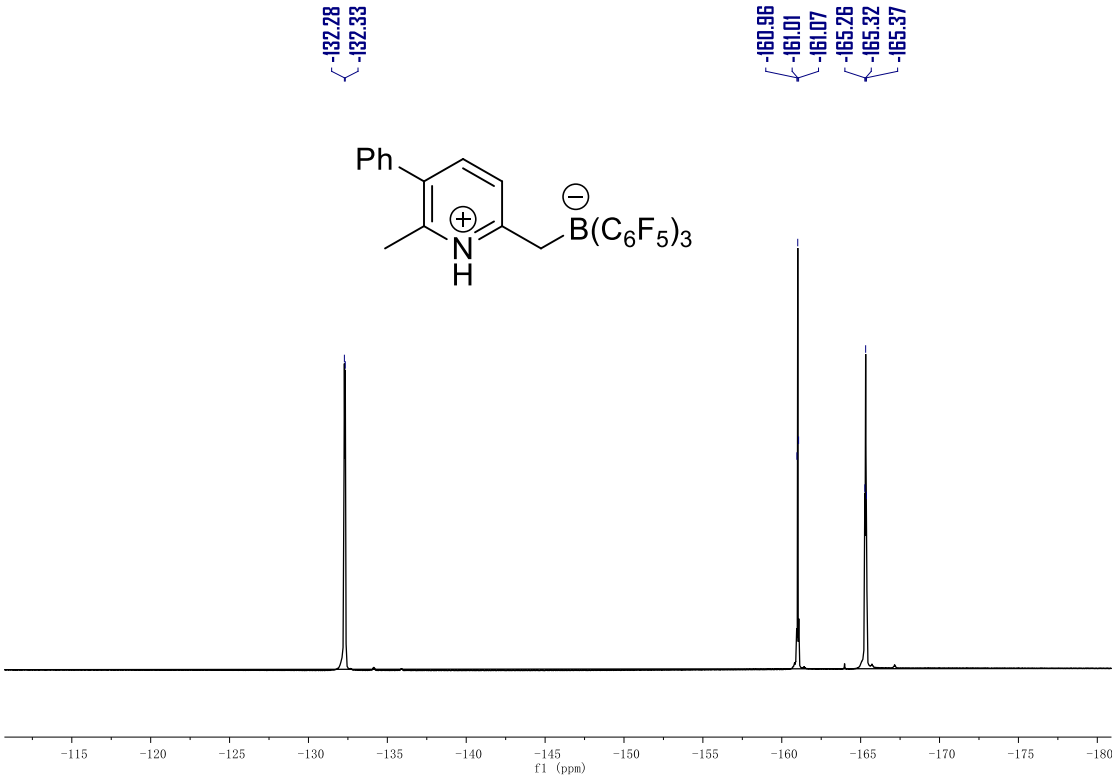


Figure S32: ^{19}F NMR spectrum of **1h'** in CD_2Cl_2

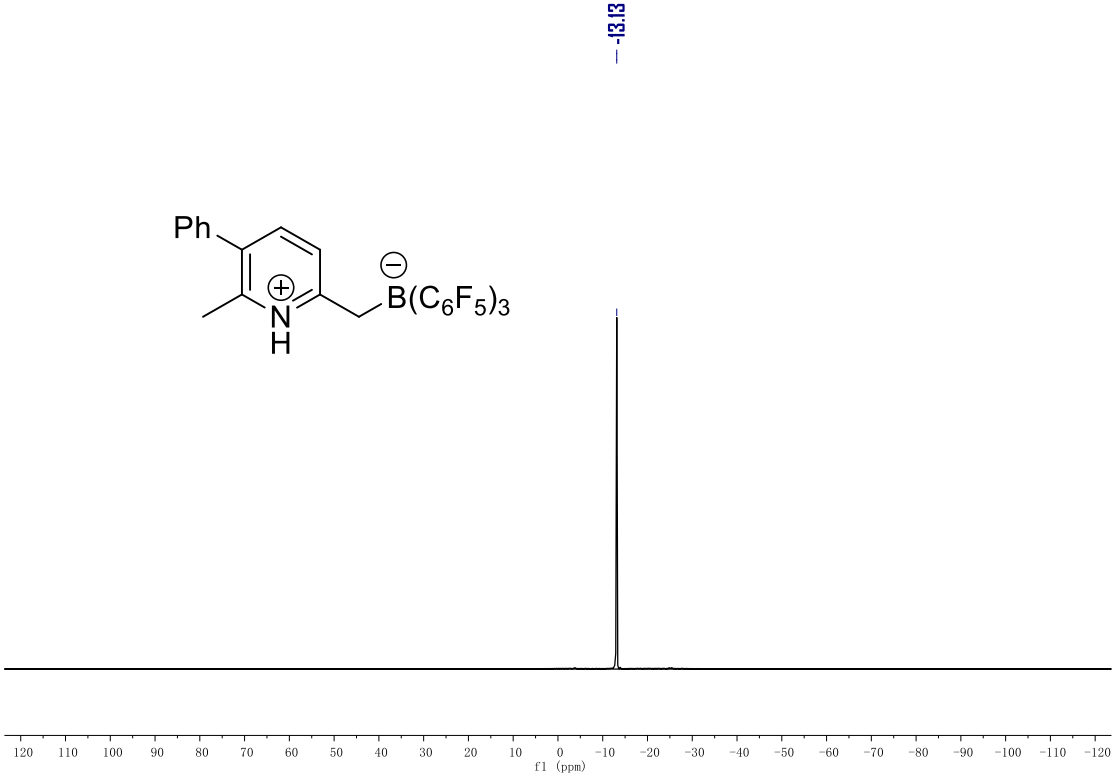


Figure S33: ^{11}B NMR spectrum of **1h'** in CD_2Cl_2

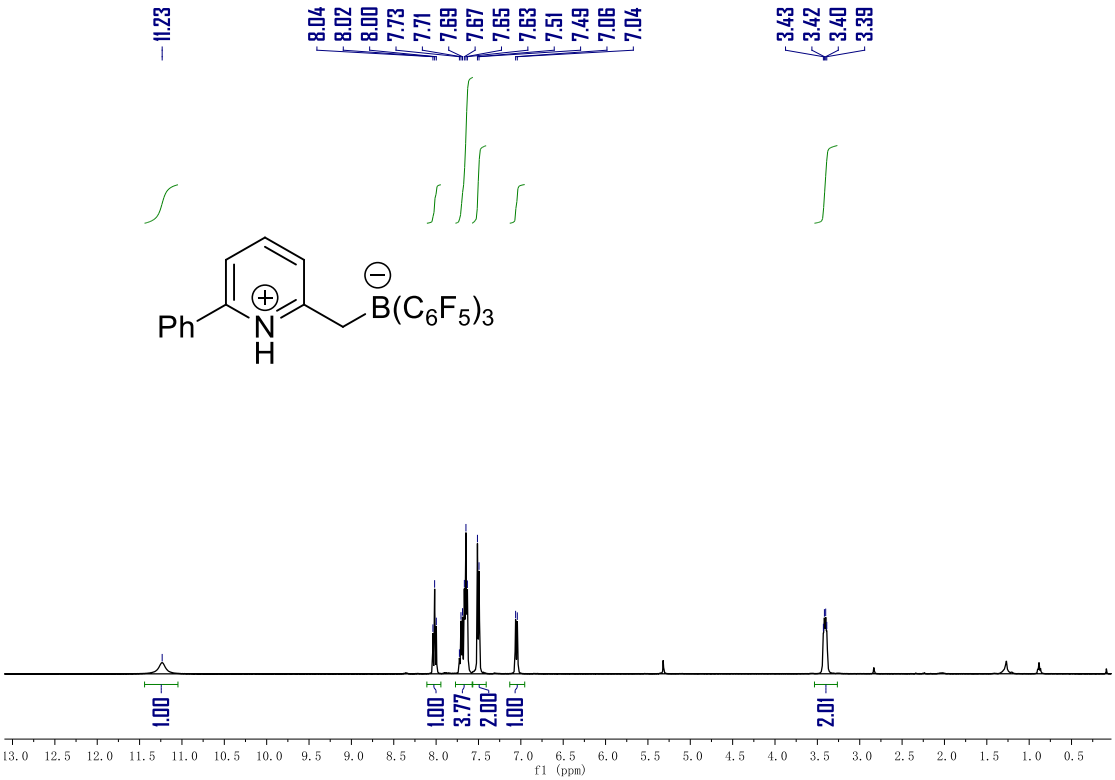


Figure S34: ^{1}H NMR spectrum of **1i** in CD_2Cl_2

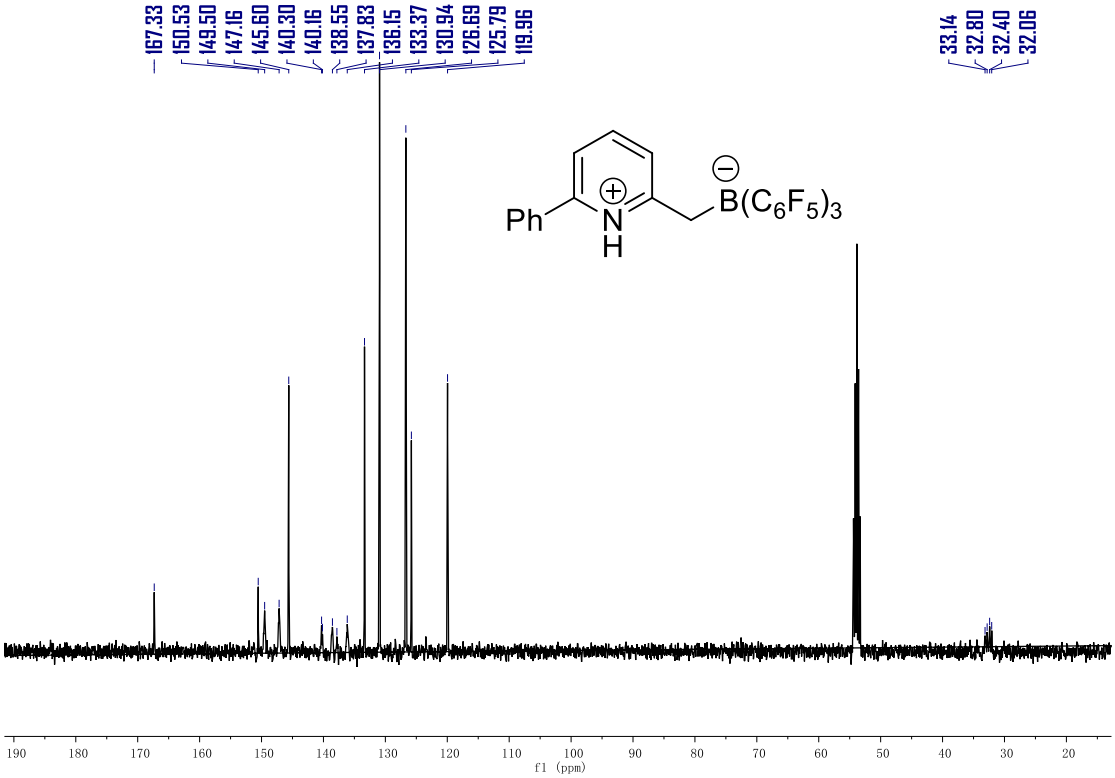


Figure S35: ^{13}C NMR spectrum of **1i** in CD_2Cl_2

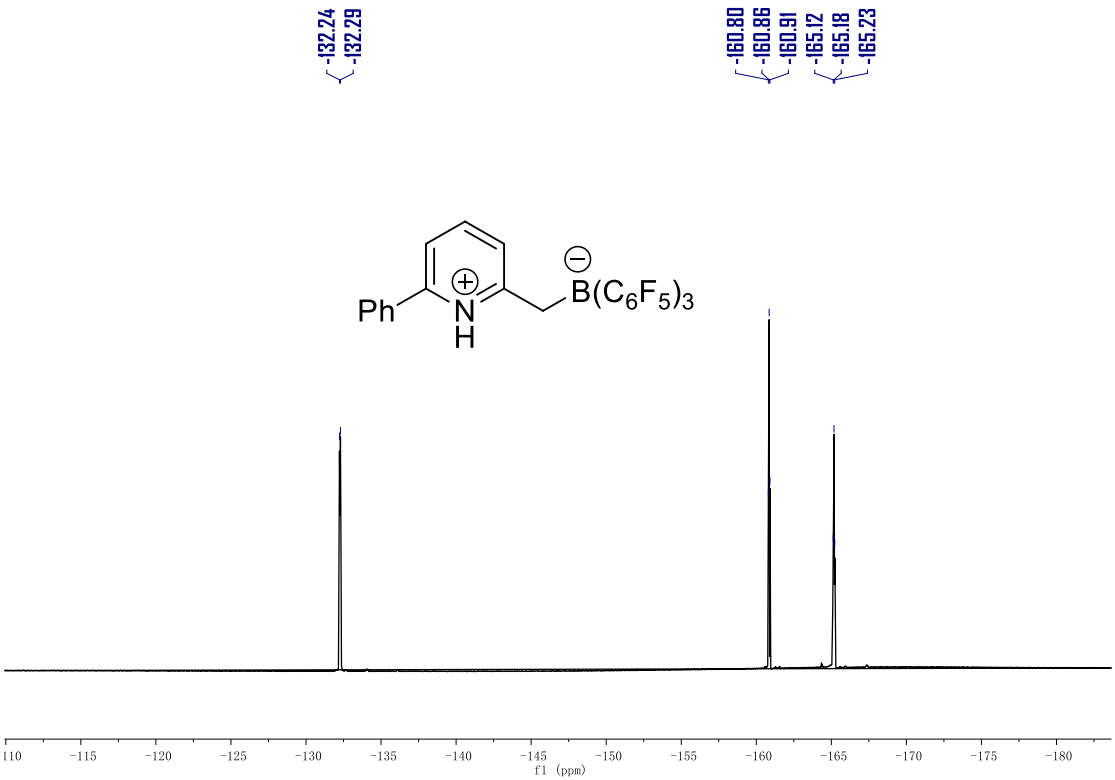


Figure S36: ^{19}F NMR spectrum of **1i** in CD_2Cl_2

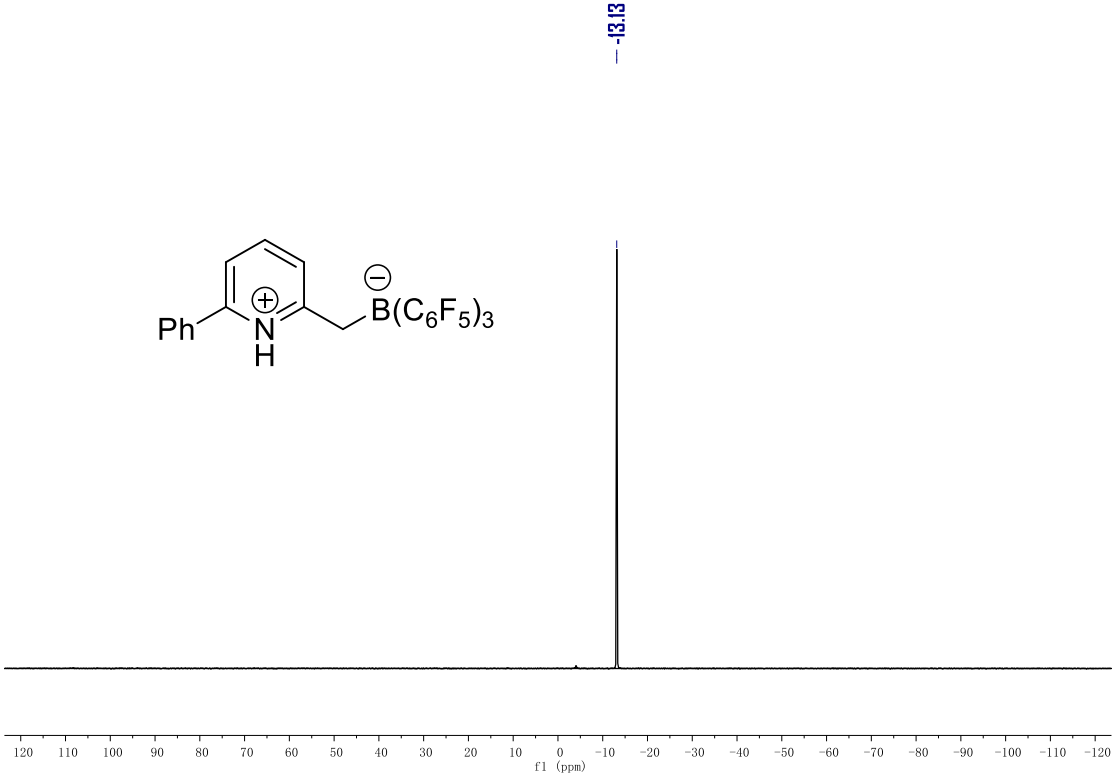


Figure S37: ^{11}B NMR spectrum of **1i** in CD_2Cl_2

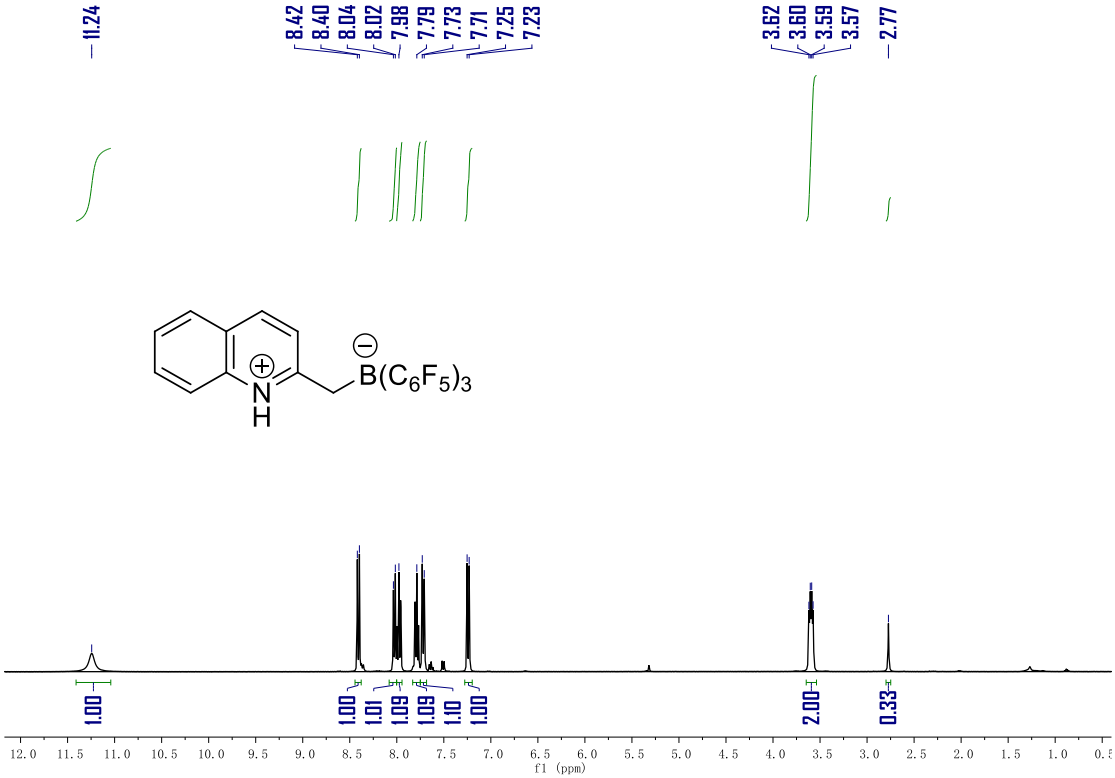


Figure S38: ^{1}H NMR spectrum of **1j** in CD_2Cl_2

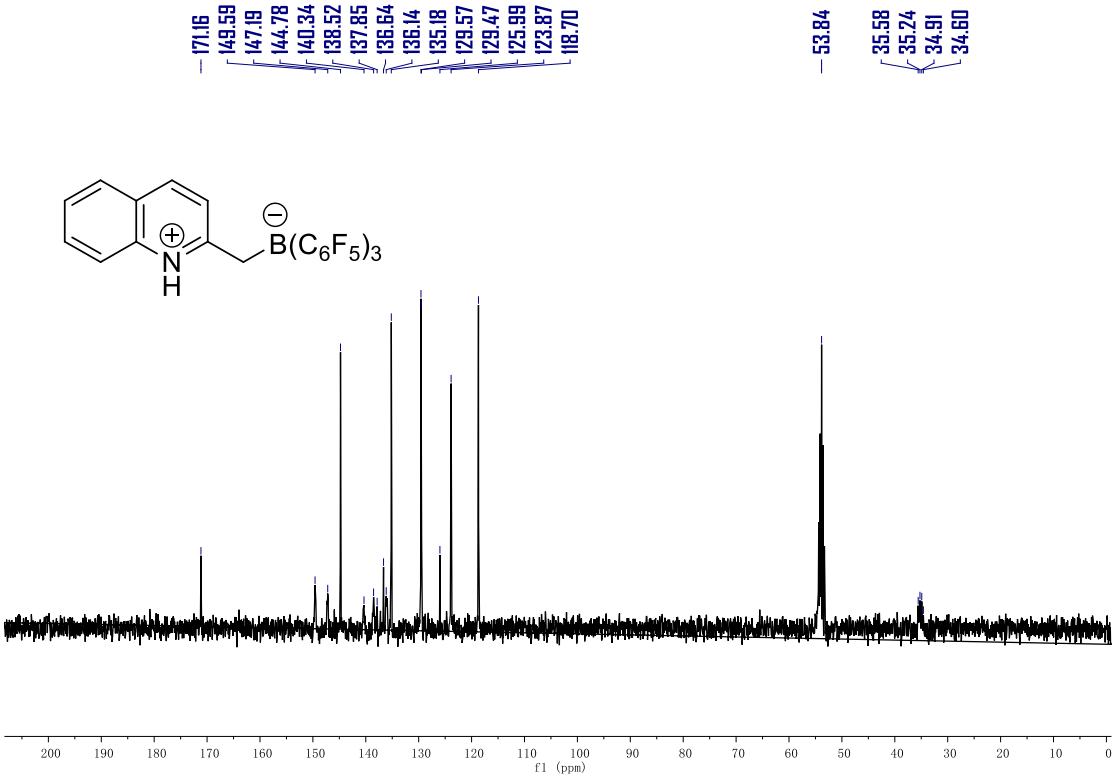


Figure S39: ^{13}C NMR spectrum of **1j** in CD_2Cl_2

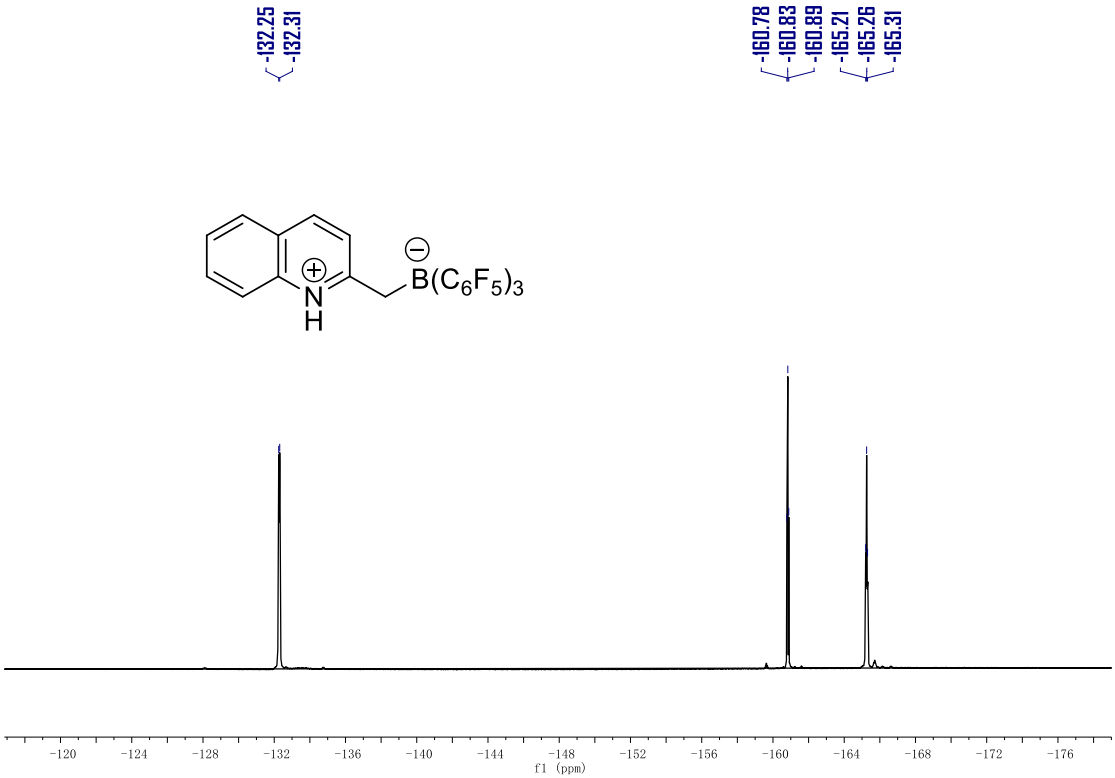


Figure S40: ^{19}F NMR spectrum of **1j** in CD_2Cl_2

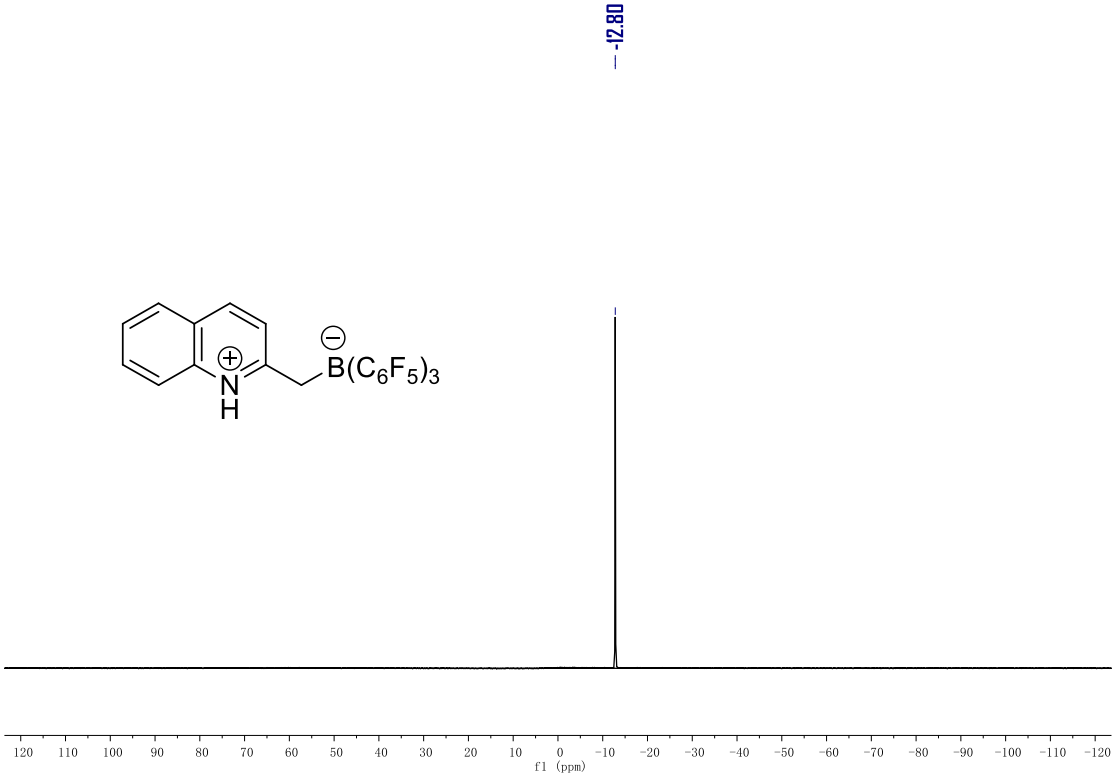


Figure S41: ^{11}B NMR spectrum of **1j** in CD_2Cl_2

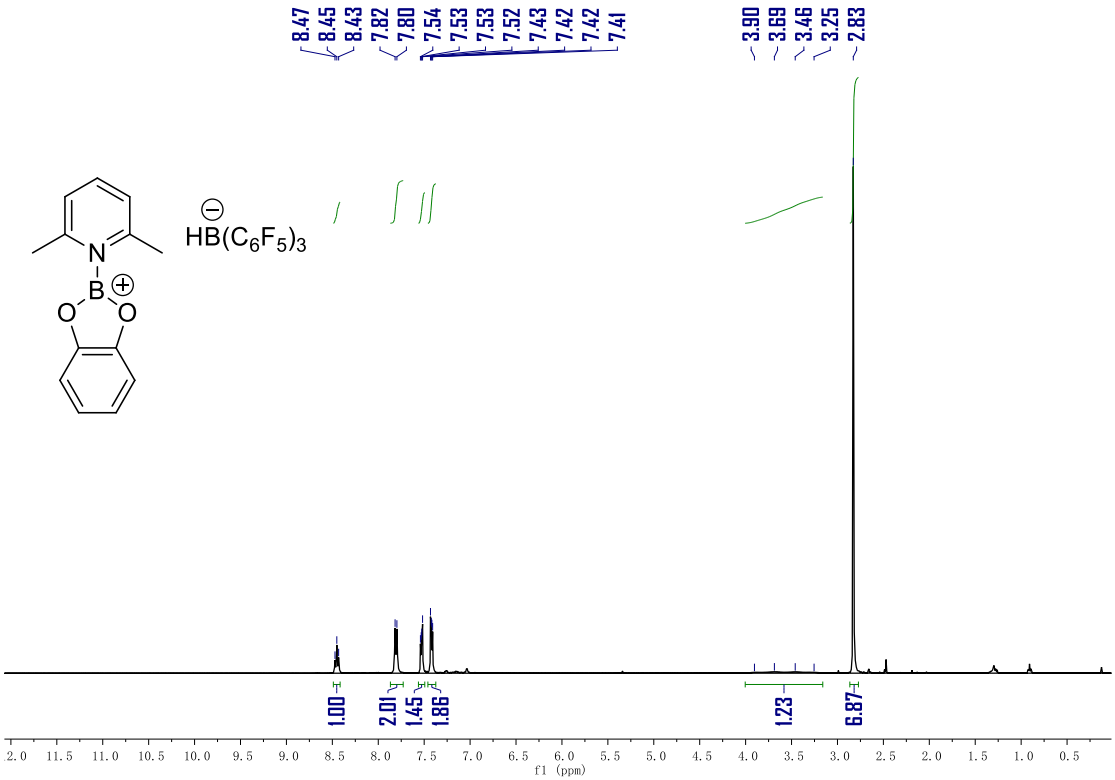


Figure S42: ^{1}H NMR spectrum of [[2,6-lutidine/Bcat]/HB(C_6F_5)$_3$] in CD_2Cl_2

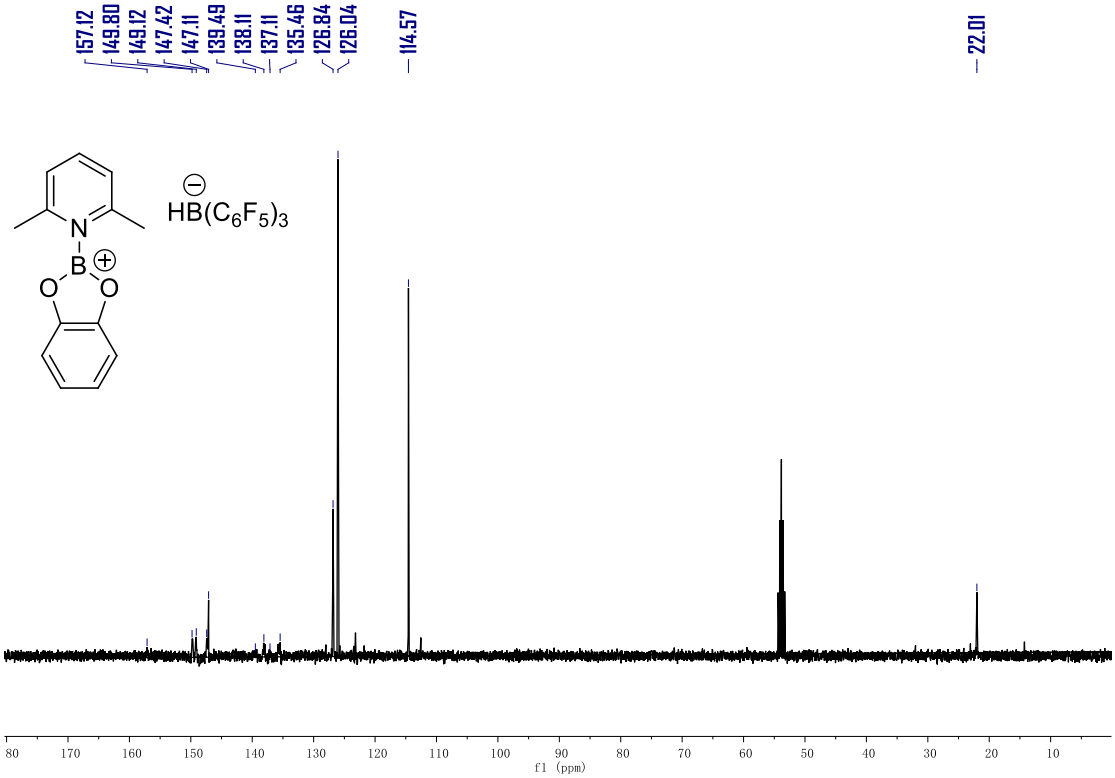


Figure S43: ^{13}C NMR spectrum of [[2,6-lutidine/Bcat]/HB(C_6F_5)$_3$] in CD_2Cl_2

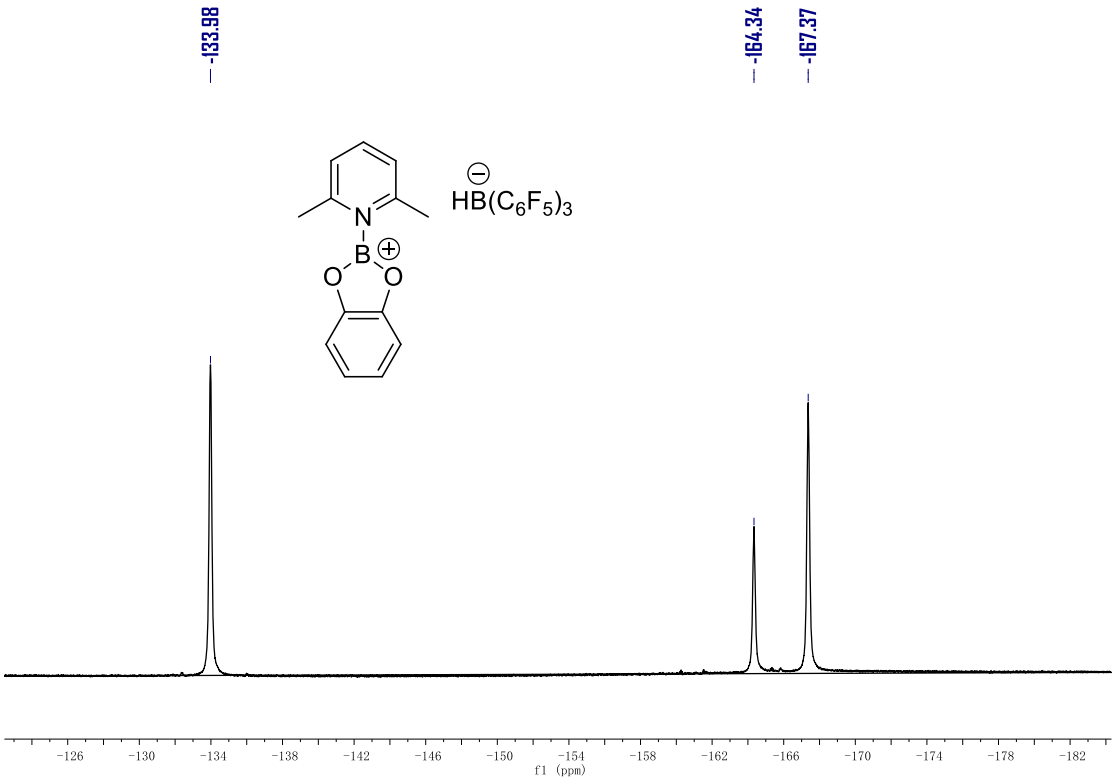


Figure S44: ^{19}F NMR spectrum of [[2,6-lutidine/Bcat]/$HB(C_6F_5)_3$] in CD_2Cl_2

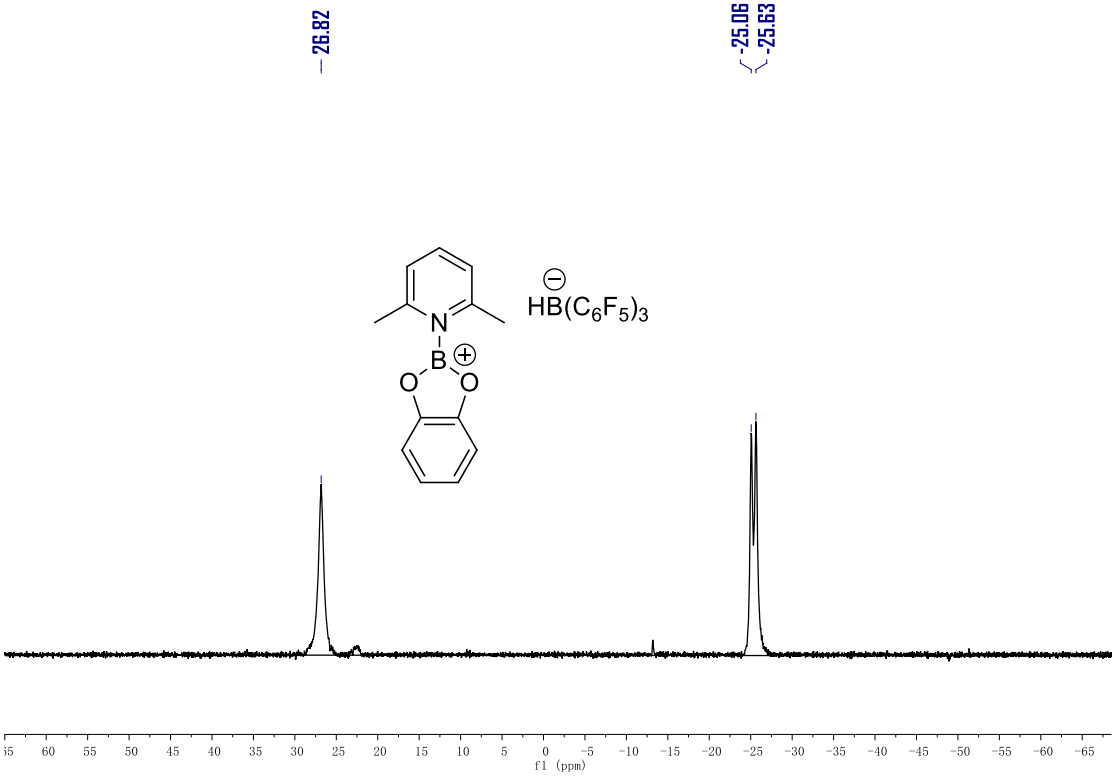


Figure S45: ^{11}B NMR spectrum of [[2,6-lutidine/Bcat]/$HB(C_6F_5)_3$] in CD_2Cl_2

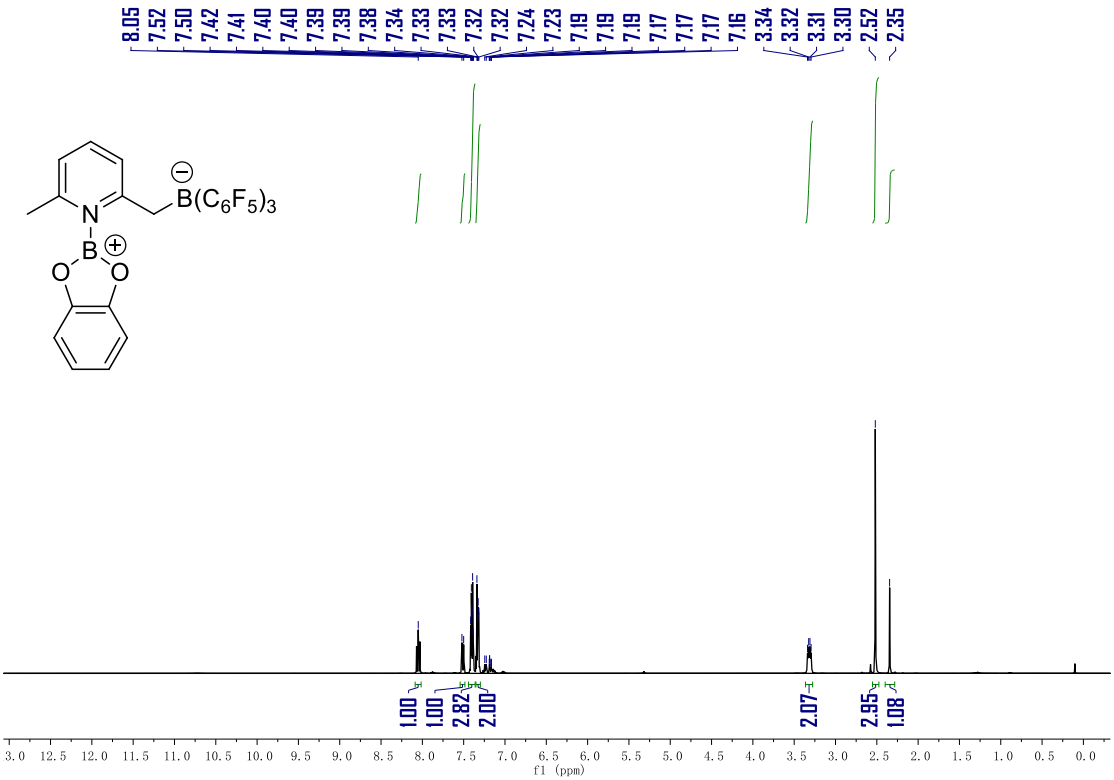


Figure S46: ^{1}H NMR spectrum of **2** in CD_2Cl_2

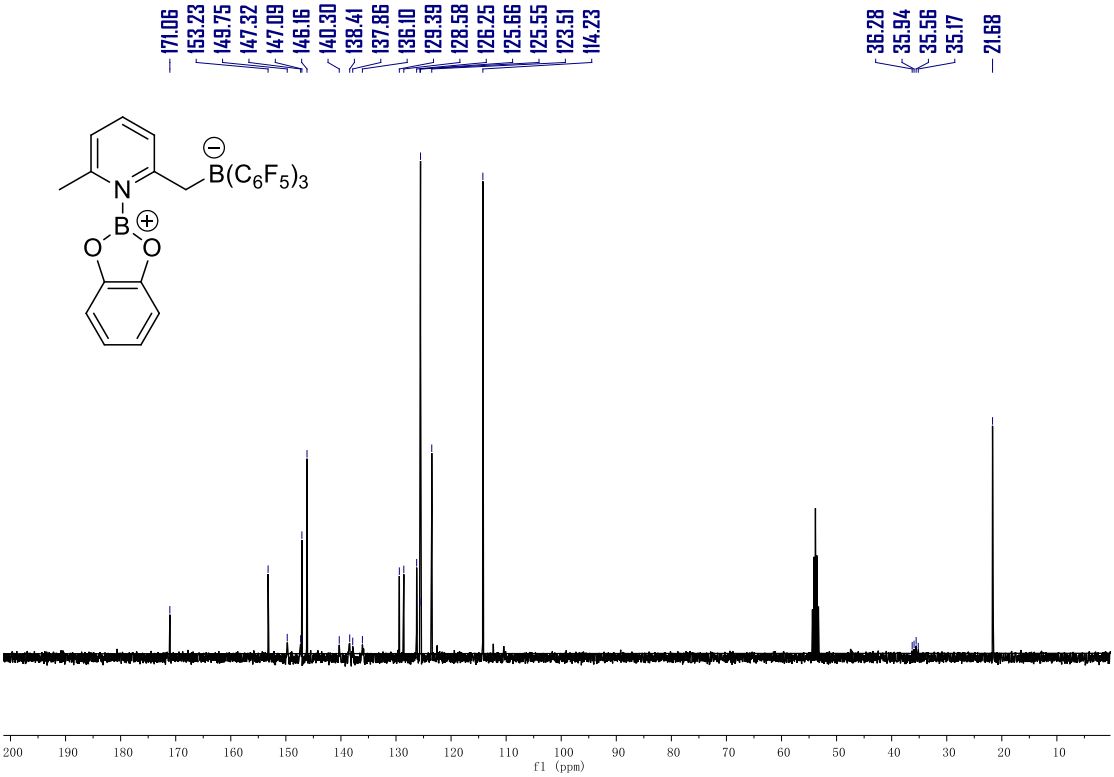


Figure S47: ^{13}C NMR spectrum of **2** in CD_2Cl_2

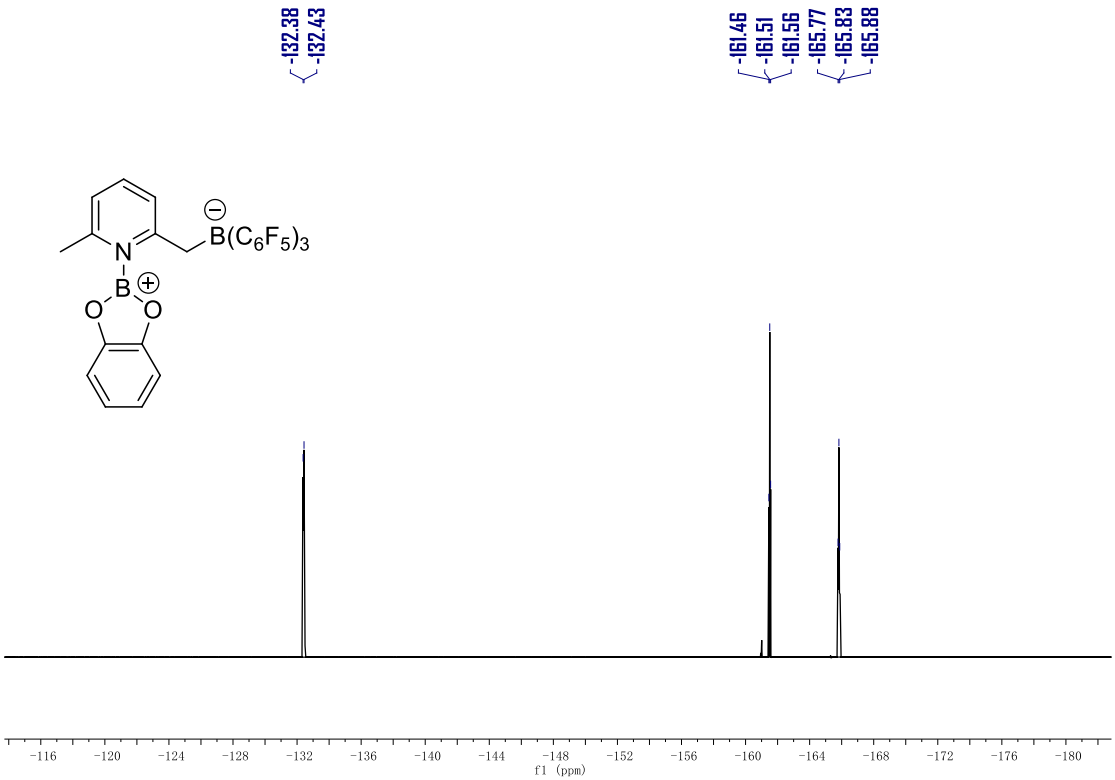


Figure S48: ^{19}F NMR spectrum of **2** in CD_2Cl_2

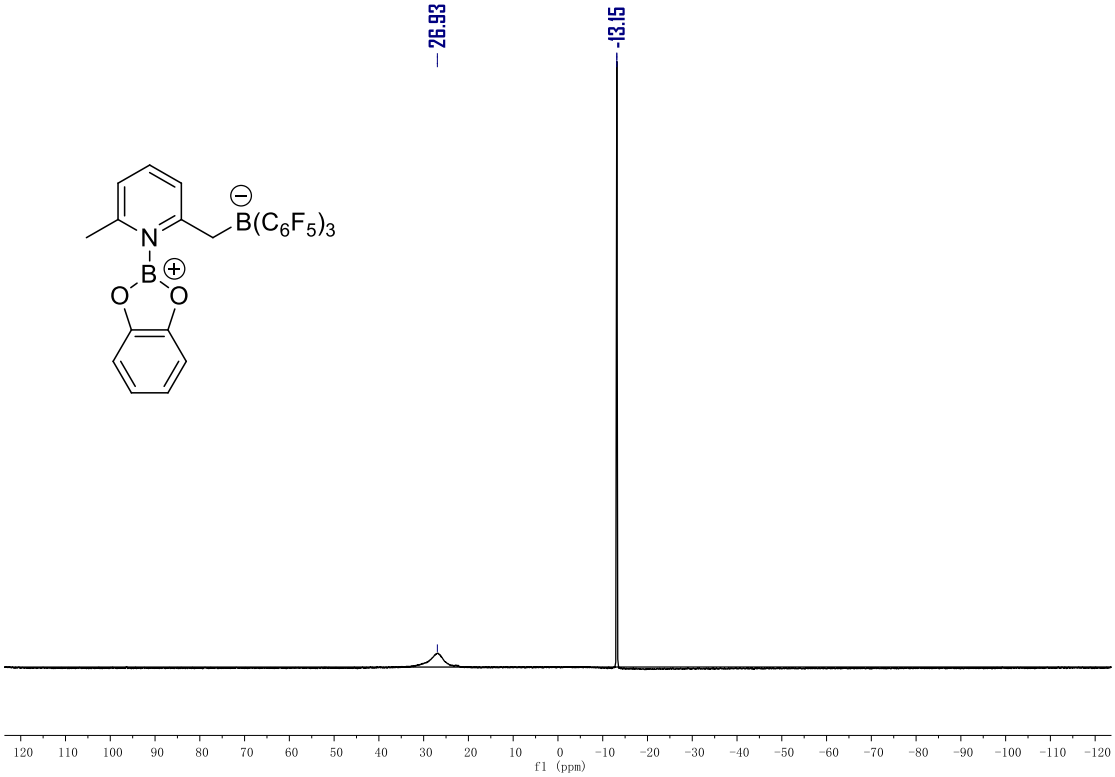


Figure S49: ^{11}B NMR spectrum of **2** in CD_2Cl_2

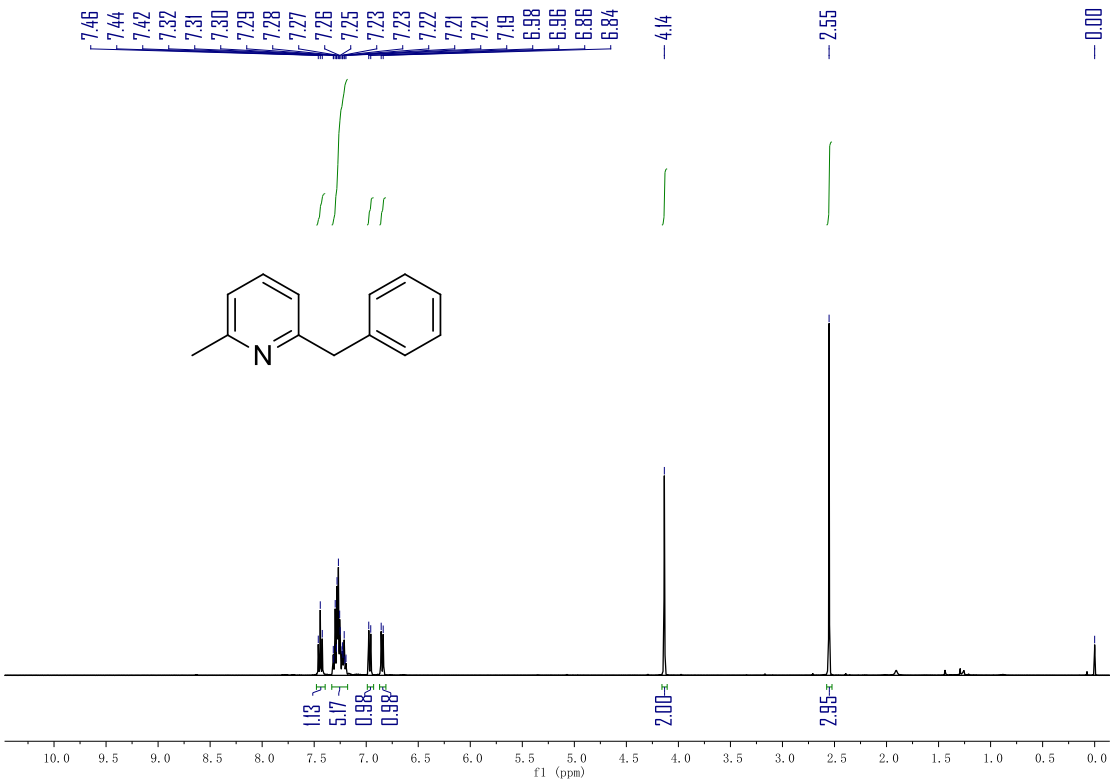


Figure S50: ^{1}H NMR spectrum of **4a** in $CDCl_3$

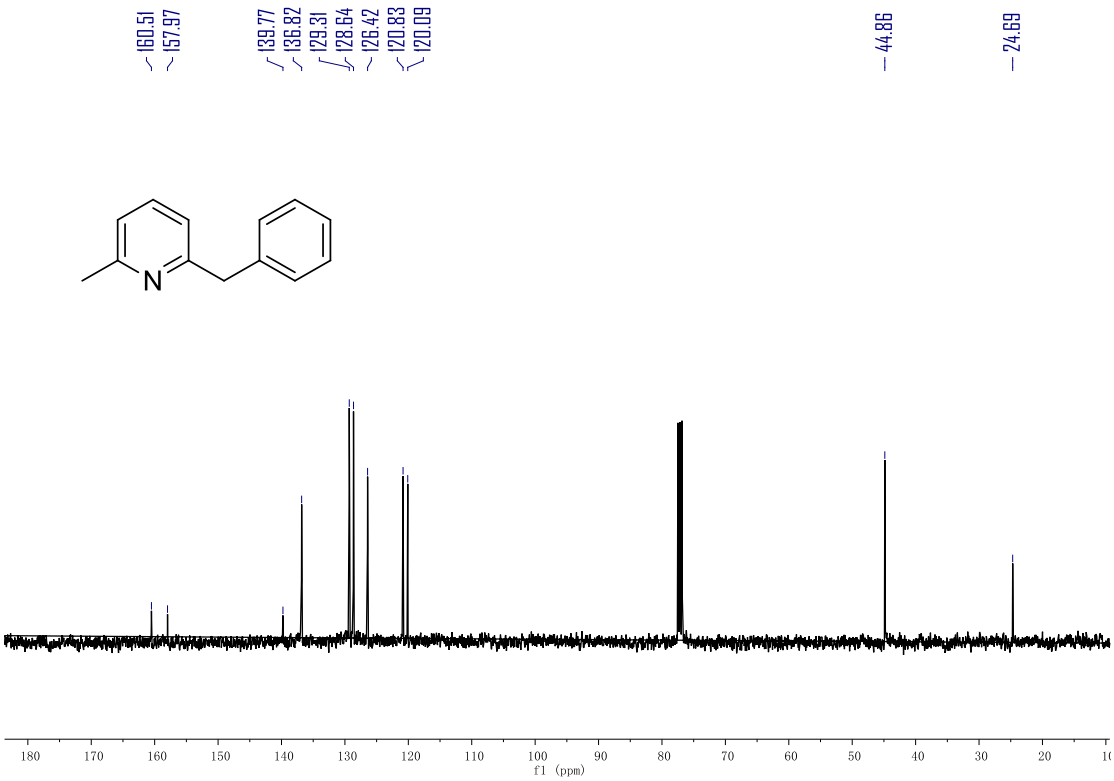


Figure S51: ^{13}C NMR spectrum of **4a** in $CDCl_3$

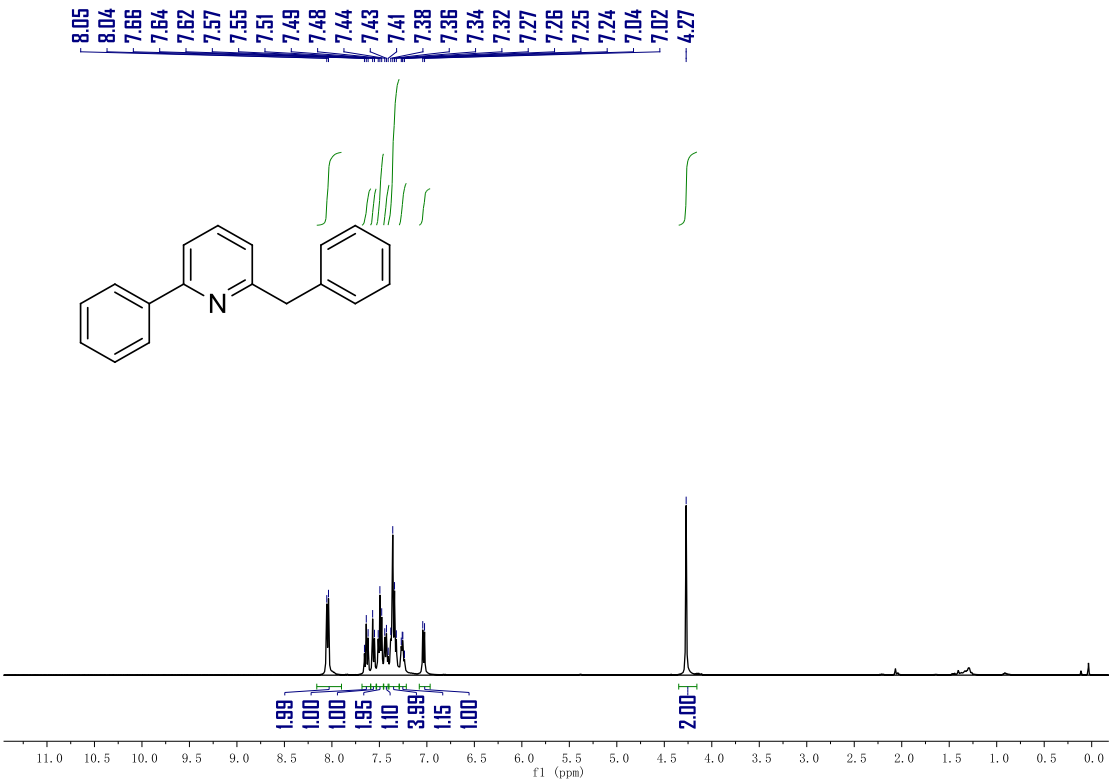


Figure S52: ^{1}H NMR spectrum of **4i** in $CDCl_3$

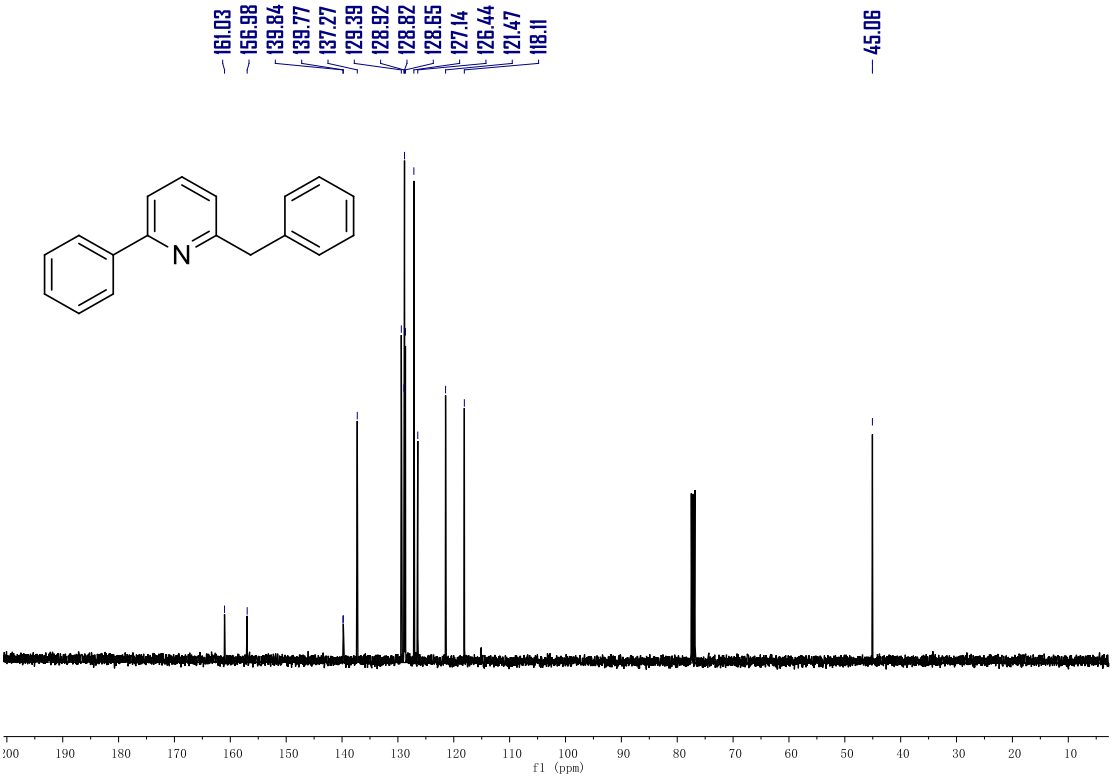


Figure S53: ^{13}C NMR spectrum of **4i** in $CDCl_3$

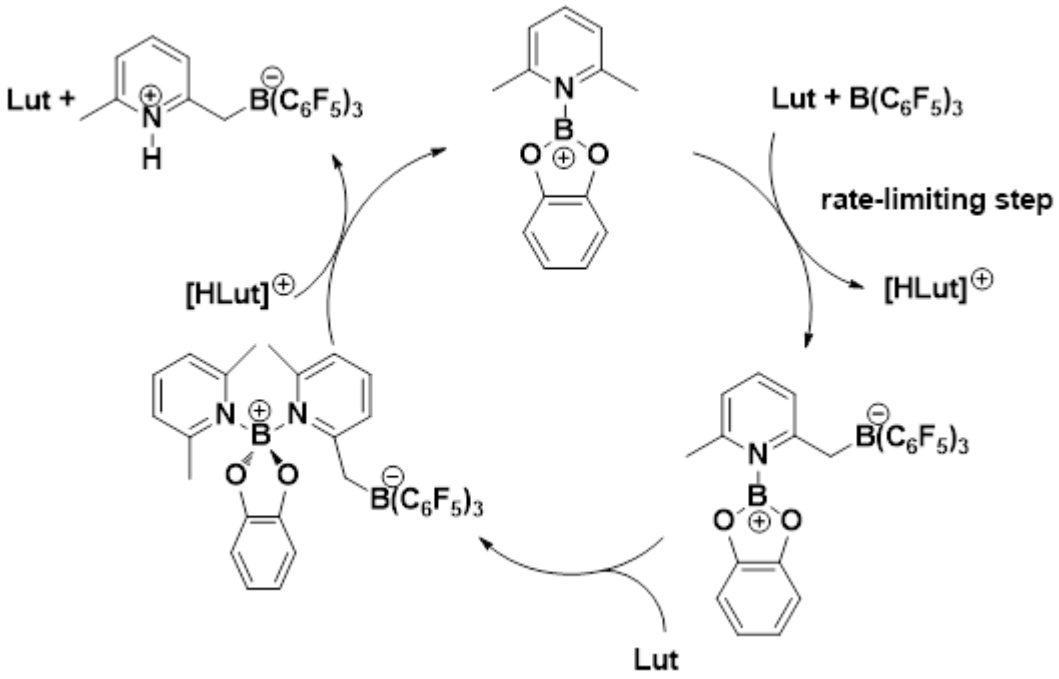


Figure S54: Proposed mechanism of formation of **1a**

III. Computation details

Quantum chemical calculations were all performed at the density functional theory (DFT) level using the hybrid meta-GGA M06-2x functional,[1] which has been proven to give reliable results to the structural and energetic properties of non-covalent systems and reaction energy barriers.[2] The M06-2x functional has a mean absolute error in energy barriers of about 1.3 kcal/mol. To reduce computational costs, a combined basis set was used: The 6-31+G(d,p) basis set[3] was employed for the atoms involved directly in the reaction which are O, B, the H atoms bonded to B, the C and H atoms of 2,6-lutidine; The 6-31G(d) basis set was used for the rest atoms. Single-point energy calculations were then performed with the full 6-31+G(d,p) basis set for all the atoms and the empirical long-range correction of Grimme et al.[4] All the DFT calculations were performed with a pruned (99,590) integration grid.

Full geometry optimization were carried out in the dichlromethane solution which

was modeled by the polarizable continuum solvation model (IEFPCM)[5] with radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.[6] 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.[7] All the calculations were performed by using the Gaussian 09 program.[8]

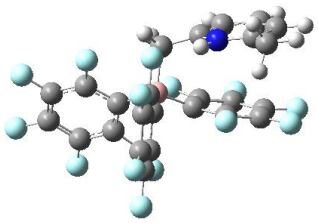
References:

1. (a) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* 2006, *125*, 194101; (b) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* 2006, *110*, 5121.
2. Zhao, Y.; Truhlar, D. G. *Theo. Chem. Acc.* 2008, *120*, 215.
3. (a) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* 1980, *72*, 5639-5648. (b) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* 1980, *72*, 650-654.
4. Grimme, S.; Antony, J.; Ehrlich S.; Krieg, H. *J. Chem. Phys*., 2010, *132*, 154104.
5. Scalmani, G.; Frisch, M. J.; Map, V. *J. Chem. Phys.* 2010, *132*, 114110.
6. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* 2009, *113*, 6378.
7. Hratchian, H. P.; Schlegel, H. B. *J. Chem. Phys.* 2004, *120*, 9918-24. (b) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Theory and Comput.* 2005, *1*, 61-69.
8. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N.

Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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

1a:

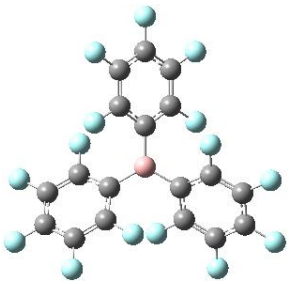


Charge = 0 Multiplicity = 1

C,0,-1.4324561999,-1.3761659964,0.2739640309
C,0,1.1291609109,-1.0224121951,0.1173541505
C,0,-0.4697306326,1.1052509912,-0.4783464239
C,0,-1.5540807816,-2.3866717428,1.2209728573
C,0,-2.291218897,-1.5093957456,-0.8118678304
C,0,2.173249077,-1.3463691454,0.9688217357
C,0,1.2893691671,-1.5243835687,-1.1730032144
C,0,-1.696729742,1.7581693872,-0.5358543556
C,0,0.5968329344,1.8728361312,-0.9312145127
C,0,-2.4659270894,-3.4279078523,1.1444022309
C,0,-3.2197698597,-2.534290895,-0.9356925108
C,0,3.2877606912,-2.0900779668,0.6011502057
C,0,2.3747594097,-2.2721435496,-1.5948145181
C,0,-1.8692016208,3.0558184131,-0.988827236
C,0,0.4796384477,3.1836176531,-1.3743848934
C,0,-3.312040826,-3.5009949049,0.050990996
C,0,3.388829182,-2.5623780792,-0.6938700982
C,0,-0.7653485853,3.7844774083,-1.4015757313
F,0,-0.7307554889,-2.3993621404,2.2971442486
F,0,-2.2669012129,-0.6256078186,-1.828685025
F,0,2.1870093089,-0.9028155111,2.2596149979
F,0,0.3445914352,-1.2616940549,-2.1010245695
F,0,-2.7952465066,1.1672852273,-0.012969234
F,0,1.8677135467,1.40211017,-0.8620842711
F,0,-2.5278835411,-4.3596051753,2.1052341338
F,0,-4.0258952839,-2.5974447987,-2.0040566821
F,0,4.2595213958,-2.3447763227,1.4861349225
F,0,2.4575332578,-2.7158842203,-2.8548181367
F,0,-3.0713987801,3.6455347205,-0.9347593829
F,0,1.5712357862,3.8922137112,-1.6990504608
F,0,-4.2019697542,-4.4932169354,-0.0527834782

F,0,4.4493691301,-3.2797492835,-1.0752029156
F,0,-0.8928934287,5.0677437041,-1.7557110089
C,0,0.1939829883,1.7574439619,2.1155510352
C,0,-0.5686227342,2.927798894,2.1006425907
C,0,0.0556724106,4.1557383578,1.9391802025
C,0,1.4480151853,4.2372663772,1.8270854455
C,0,2.1981424815,3.0793061234,1.9037805622
N,0,1.5366201562,1.9044723592,2.0485547384
H,0,-0.5413447593,5.0618905421,1.8891175295
H,0,-1.6475934544,2.849042738,2.1778361683
H,0,1.9505162535,5.1869937197,1.6866321143
C,0,-0.3767818158,0.3894591984,2.0384003155
H,0,0.1001411176,-0.2716273969,2.7616327625
H,0,-1.4365855944,0.4608435492,2.3003437024
C,0,3.6880020698,3.0110888874,1.8310683713
H,0,3.9965584277,2.3975450589,0.9782037114
H,0,4.1041293885,4.0116004946,1.7139391191
H,0,4.0945127893,2.561070981,2.7419455596
H,0,2.099445901,1.0547564828,2.099599349
B,0,-0.2745012611,-0.2276119432,0.467937702

$B(C_6F_5)_3$:

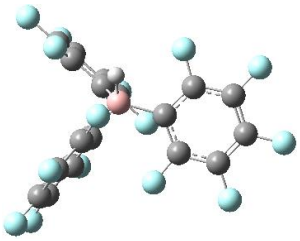


Charge = 0 Multiplicity = 1

5	0	0.000000	0.000000	0.001103
6	0	0.000296	1.568753	0.000918
6	0	-1.358727	-0.784120	0.000918
6	0	1.358432	-0.784632	0.000918
6	0	0.982625	2.312949	-0.653646
6	0	0.994445	3.697118	-0.672743
6	0	0.000000	4.391442	-0.000535
6	0	-0.994439	3.697551	0.672273
6	0	-0.982372	2.313427	0.654601
6	0	-2.494385	-0.305496	-0.653646
6	0	-3.699021	-0.987344	-0.672743
6	0	-3.803100	-2.195721	-0.000535
6	0	-2.704954	-2.709985	0.672273
6	0	-1.512301	-2.007473	0.654601

6	0	1.511760	-2.007453	-0.653646
6	0	2.704576	-2.709774	-0.672743
6	0	3.803100	-2.195721	-0.000535
6	0	3.699393	-0.987567	0.672273
6	0	2.494673	-0.305955	0.654601
9	0	1.967910	1.693199	-1.319681
9	0	1.948763	4.365429	-1.324349
9	0	-0.000164	5.720831	-0.001116
9	0	-1.948755	4.366456	1.323271
9	0	-1.967579	1.694074	1.321092
9	0	-2.450309	0.857661	-1.319681
9	0	-4.754954	-0.495037	-1.324349
9	0	-4.954303	-2.860558	-0.001116
9	0	-2.807084	-3.870899	1.323271
9	0	-0.483321	-2.551011	1.321092
9	0	0.482398	-2.550860	-1.319681
9	0	2.806191	-3.870392	-1.324349
9	0	4.954467	-2.860273	-0.001116
9	0	4.755839	-0.495557	1.323271
9	0	2.450901	0.856937	1.321092

$[HB(C_6F_5)_3]^-$:



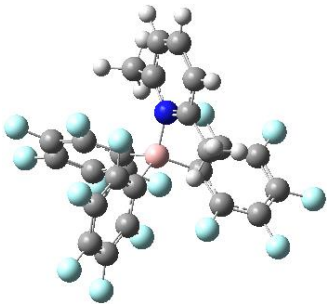
Charge = -1 Multiplicity = 1

H	0.019406000000	-0.009625000000	2.078702000000
B	0.029625000000	-0.005359000000	0.871573000000
C	-0.932135000000	-1.236731000000	0.388261000000
C	-0.583972000000	1.437467000000	0.406891000000
C	1.586629000000	-0.208983000000	0.415722000000
C	-1.125051000000	-2.348940000000	1.197638000000
C	-1.957233000000	-3.410386000000	0.866407000000
C	-2.641168000000		

-3.384380000000	-0.336473000000	
C		-2.475201000000
-2.303185000000	-1.186879000000	
C		-1.631727000000
-1.267978000000	-0.811847000000	
C		-1.605154000000
2.021074000000	1.146822000000	
C		-2.182778000000
3.245164000000	0.839923000000	
C		-1.733911000000
3.944526000000	-0.267410000000	
C		-0.725856000000
3.402326000000	-1.046876000000	
C		-0.183709000000
2.172412000000	-0.701027000000	
C		2.617527000000
0.270598000000	1.214740000000	
C		3.964907000000
0.113543000000	0.918148000000	
C		4.329385000000
-0.554372000000	-0.238161000000	
C		3.341194000000
-1.041505000000	-1.077523000000	
C		2.008719000000
-0.855512000000	-0.739229000000	
F		-0.480827000000
-2.450005000000	2.379049000000	
F		-2.105595000000
-4.456177000000	1.694065000000	
F		-3.450850000000
-4.395210000000	-0.677582000000	
F		-3.126316000000
-2.275364000000	-2.359906000000	
F		-1.498903000000
-0.260720000000	-1.699432000000	
F		-2.101101000000
1.384303000000	2.228890000000	
F		-3.165151000000
3.756752000000	1.597268000000	
F		-2.272797000000
5.128802000000	-0.585291000000	
F		-0.294675000000
4.066946000000	-2.129906000000	
F		0.767744000000

1.693709000000 -1.529232000000
F 2.337193000000
0.944676000000 2.350153000000
F 4.913615000000
0.596936000000 1.734740000000
F 5.622027000000
-0.721877000000 -0.545916000000
F 3.684599000000
-1.677532000000 -2.208066000000
F 1.105445000000
-1.327951000000 -1.623425000000

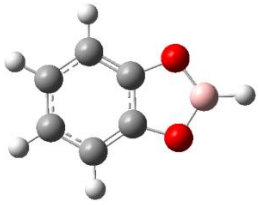
Lutidine. $B(C_6F_5)_3$:



Charge = 0 Multiplicity = 1
C,0,3.6609157244,0.2153832526,-0.5170215461
C,0,3.8309540831,-1.1364472541,-0.2788317195
C,0,2.7413173827,-1.889234647,0.1315782861
C,0,1.5145978375,-1.2690303149,0.2887872337
C,0,1.276994976,0.0800470423,0.0353286864
C,0,2.4074743471,0.7895511636,-0.347880758
C,0,-1.4762752122,-0.0985292392,-0.3028347688
C,0,-1.4209085125,-1.1011908605,-1.2637841869
C,0,-2.77130282,0.3004627061,0.0109499435
C,0,-2.54170003,-1.6637851687,-1.8613407931
C,0,-3.9207367124,-0.2251957576,-0.5527884375
C,0,-3.8039882623,-1.2255647433,-1.5042884863
C,0,-0.1646410765,0.4674881492,2.047528276
C,0,-0.9180914885,-0.4398826191,2.7807528825
C,0,0.8482169818,1.0883228981,2.7745103636
C,0,-0.7197638385,-0.679076359,4.1365456725
C,0,1.0763001645,0.8945189948,4.12368989
C,0,0.2796663711,-0.0062108943,4.8155075743
F,0,5.0272783081,-1.7075478517,-0.436804208
F,0,2.3416868987,2.117544071,-0.5959722672
F,0,4.7024660021,0.9627094755,-0.9020592526
F,0,2.8857964336,-3.1961851742,0.3786092673

F,0,0.499150669,-2.0475691425,0.7221894806
F,0,-0.2394382528,-1.5616689953,-1.7280831488
F,0,-2.9558730186,1.2595463817,0.9465973591
F,0,-5.1289938891,0.2128926528,-0.1821363261
F,0,-2.4036503761,-2.6108217382,-2.7967320227
F,0,-4.8904158948,-1.7527662391,-2.071738509
F,0,1.641901015,1.9918578043,2.1520718161
F,0,2.0419864747,1.5648062924,4.7621547994
F,0,-1.4826341181,-1.5667640185,4.7842036266
F,0,-1.9061864549,-1.1541512191,2.209351424
F,0,0.4797205073,-0.2216412084,6.1172182171
B,0,-0.2173796533,0.675032726,0.4189191327
C,0,-0.7062055264,3.2844349085,0.7762837824
C,0,-0.6567042408,4.5978413732,0.3114882459
N,0,-0.3813182709,2.2434751856,-0.0537654454
C,0,-0.3392942979,4.8828628555,-1.0028359388
H,0,-0.8967886583,5.3918279966,1.009563339
C,0,-0.1575933653,2.5120638798,-1.3819908857
C,0,-0.1235997162,3.8164401541,-1.857731268
H,0,0.0768557414,3.9725840426,-2.9111179944
C,0,-1.1744243874,3.1529880569,2.2052601985
H,0,-1.9002393555,3.9514990139,2.3729662789
H,0,-1.6566673857,2.2136211564,2.4404968736
C,0,-0.0021022562,1.436794552,-2.4230183662
H,0,0.5008079889,0.5331190848,-2.0980500251
H,0,-0.9943811041,1.1574388845,-2.7960049042
H,0,0.5605920324,1.8507721505,-3.2614191529
H,0,-0.2926057617,5.9069533687,-1.3590197502
H,0,-0.3488525425,3.3234987908,2.902501282

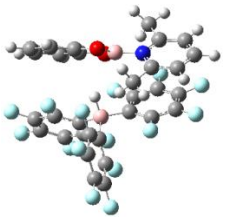
catBH:



Charge = 0 Multiplicity = 1
C,0,-0.6986832142,0.,2.0849996218
C,0,-1.4309124101,0.,0.8927311254
C,0,-0.6953692333,0.,-0.275809656
C,0,0.6953692333,0.,-0.275809656
C,0,1.4309124101,0.,0.8927311254
C,0,0.6986832142,0.,2.0849996218
H,0,-1.2312211945,0.,3.0304616624

H,0,-2.5155868577,0.,0.8803116673
H,0,2.5155868577,0.,0.8803116673
H,0,1.2312211945,0.,3.0304616624
O,0,-1.1424486603,0.,-1.5789243183
O,0,1.1424486603,0.,-1.5789243183
B,0,0.,0.,-2.3585110964
H,0,0.,0.,-3.5373571991

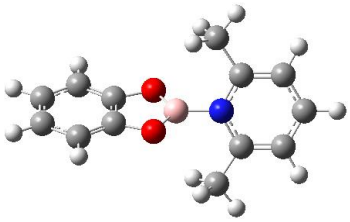
[LutBCat][$HB(C_6F_5)_3$]:



Charge = 0 Multiplicity = 1
C,0,1.4002298563,-1.1081368053,1.1745038
C,0,0.9069382246,-1.469127356,-1.3916686487
C,0,-1.094245402,-0.4548648542,0.1972666709
C,0,2.7249983076,-0.7010814372,1.2811847205
C,0,0.9702567683,-1.9510495601,2.1900157457
C,0,1.6278059055,-0.9778133542,-2.4699775921
C,0,0.5804006165,-2.8160031443,-1.4736113356
C,0,-1.5903156164,0.0277105664,1.4092251632
C,0,-2.0692042978,-0.6071485121,-0.7819084266
C,0,3.5591587296,-1.0495856653,2.3327467301
C,0,1.7687129574,-2.3353179279,3.2581458499
C,0,1.9782740084,-1.7493367243,-3.5707300969
C,0,0.9078481702,-3.6277746719,-2.5466035304
C,0,-2.9166563278,0.3652242281,1.6299377129
C,0,-3.409814476,-0.281734491,-0.6085789314
C,0,3.0741945178,-1.8769381174,3.3321483848
C,0,1.6163303251,-3.0847432468,-3.6087159513
C,0,-3.8385682946,0.2203909159,0.6055095755
F,0,3.262090273,0.0877883379,0.3275824845
F,0,-0.2964430485,-2.4173351325,2.1982674308
F,0,2.0189801082,0.3182991942,-2.512647808
F,0,-0.123403003,-3.3787956032,-0.467190005
F,0,-0.759172934,0.2290157849,2.4528829718
F,0,-1.7428978274,-1.0282328977,-2.0270350062
F,0,4.8187342763,-0.5917213489,2.3948072061
F,0,1.2904495296,-3.1376031652,4.2209512564
F,0,2.6581109681,-1.2133121852,-4.5956845787
F,0,0.5528882607,-4.91989196,-2.5760000754

F,0,-3.3090033194,0.8897844287,2.8018202041
F,0,-4.2759353196,-0.3829008898,-1.6297800421
F,0,3.859199138,-2.2322855737,4.3568527812
F,0,1.9470488047,-3.8453912122,-4.6585346114
F,0,-5.1082229082,0.6145333339,0.771136226
C,0,1.3670725871,2.6427497551,1.286865605
C,0,1.8664346009,3.1101397717,0.0763860202
C,0,2.1837569118,2.3621195373,2.3639640954
C,0,3.2100127225,3.3444672434,-0.1302111351
C,0,3.5512800905,2.5874569274,2.1671445993
H,0,1.7849728809,1.9767002809,3.2965724656
C,0,4.0500357622,3.0707886003,0.9539214529
H,0,3.5856132805,3.7042167161,-1.0818924399
H,0,4.2412936153,2.3729248061,2.9767169994
H,0,5.1177140792,3.2284680441,0.8434244757
C,0,-2.7043577023,3.3587201881,0.0506127723
C,0,-3.9826405901,3.3563579461,-0.4848056763
C,0,-4.2042599022,2.8507441075,-1.7607243497
C,0,-3.1352529835,2.3578886581,-2.498060449
C,0,-1.8583714493,2.3554067564,-1.9587716589
N,0,-1.6672350689,2.8493634485,-0.691597262
H,0,-5.2073766871,2.8339259786,-2.1755301584
H,0,-4.7962579521,3.7481663365,0.1139924864
H,0,-3.2772998999,1.9463182347,-3.4903349651
C,0,-2.44438146,3.9168700028,1.4162547397
H,0,-1.6556810058,4.6754033416,1.395478168
H,0,-3.3604787728,4.3775738702,1.7856012847
C,0,-0.7036060371,1.7945444856,-2.7266847672
H,0,-0.0983237169,1.1266838133,-2.1113138139
H,0,-1.0873751171,1.2398568021,-3.5832478027
H,0,-0.053003301,2.5951881894,-3.090696309
B,0,0.5146480699,-0.5756403555,-0.0863362624
B,0,-0.2824895811,2.8540629543,-0.1094919091
O,0,-0.0049484412,2.5064031492,1.1800346624
O,0,0.8154379969,3.2655732829,-0.8115373332
H,0,-2.1408971633,3.1332142648,2.1148847525
H,0,0.8778952629,0.5579969089,-0.3098025621

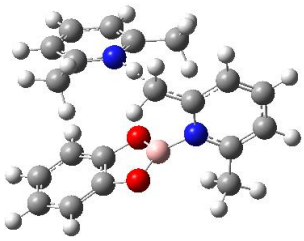
$[LutBcat]^+$:



Charge = 1 Multiplicity = 1

C,0,2.3954914849,2.6777195681,0.3427490476
C,0,2.330304772,3.5765188696,-0.716126942
C,0,3.5899209973,2.3010063325,0.9209824508
C,0,3.4552976562,4.15696697,-1.2642105828
C,0,4.7401607648,2.8808695853,0.3759208538
H,0,3.6279744528,1.5964252934,1.7443499632
C,0,4.6745536337,3.785239376,-0.688349411
H,0,3.3911849183,4.8592645016,-2.087912337
H,0,5.7073733616,2.6206704118,0.7926860632
H,0,5.5920278074,4.2109912432,-1.0806159696
C,0,-1.8868183916,3.284558829,0.8366401274
C,0,-3.2663663597,3.167688838,0.8222099591
C,0,-3.897810891,2.5770413196,-0.2677849436
C,0,-3.1452544111,2.1080759587,-1.3398894272
C,0,-1.7665659135,2.2336914962,-1.3186462368
N,0,-1.1763624418,2.8162817748,-0.2325942867
H,0,-4.979059604,2.4819811893,-0.2817654617
H,0,-3.831721559,3.5423815094,1.6672577914
H,0,-3.6147003802,1.6424268385,-2.1983284092
C,0,-1.1374487104,3.900880167,1.9760490407
H,0,-0.4359854828,4.6683319208,1.62920144
H,0,-1.8443348139,4.3695804308,2.6607269344
C,0,-0.8921369163,1.7601656483,-2.4370362326
H,0,-0.0768255208,1.125877161,-2.0705673034
H,0,-1.4886163446,1.177093302,-3.1387416389
H,0,-0.4570417691,2.6094454644,-2.9726497601
B,0,0.3150854086,2.9472650277,-0.2132838036
O,0,1.109086372,2.2703501354,0.6656382888
O,0,1.0013480191,3.7541775135,-1.0729945316
H,0,-0.5749561389,3.139309324,2.5247563176

TS1:

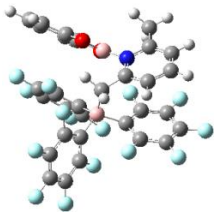


Charge = 0 Multiplicity = 1

C,0,-2.7572184194,-0.7400424489,0.7711285815
C,0,-2.5683661397,-0.4504746249,2.1194283827
C,0,-3.0350034111,-2.015718868,0.323206106
C,0,-2.6477328997,-1.4159191405,3.1026359991
C,0,-3.1119050917,-3.0079403966,1.307998051
H,0,-3.1777571623,-2.2314277495,-0.7299136251
C,0,-2.9237324323,-2.716216431,2.662665156
H,0,-2.4973515273,-1.1749665945,4.1499898691
H,0,-3.3249960551,-4.0287918473,1.00941086
H,0,-2.9961333197,-3.515177501,3.3929617701
C,0,-0.4750843631,2.9375701922,0.5109568609
C,0,-0.0185108514,4.2798833425,0.4350877329
C,0,-0.9093277224,5.3202611453,0.476661406
C,0,-2.2989373836,5.0812564409,0.5991708421
C,0,-2.7470240918,3.7925010914,0.6969767891
N,0,-1.8367124928,2.7576967638,0.6626412725
H,0,-0.5490526484,6.3420570484,0.4049338681
H,0,1.0473186042,4.4477633658,0.3273363602
H,0,-3.0113884814,5.8965814746,0.6190289225
C,0,0.3810840883,1.8053239093,0.5449755203
H,0,1.4061488533,2.0169897888,0.2454290409
H,0,-0.0096094004,0.8939013425,0.0866465553
C,0,-4.1885053121,3.4129230007,0.8361546686
H,0,-4.3564111456,2.8179636926,1.7413206857
H,0,-4.8046007821,4.3102859237,0.9002044928
H,0,-4.5193031228,2.8263554291,-0.0277872008
B,0,-2.2623291323,1.3712221313,0.9653130324
O,0,-2.5862402347,0.4195512855,0.0346824952
O,0,-2.2711281555,0.8925622848,2.2510446104
C,0,0.336228868,1.6401281319,4.14724264
C,0,0.3391539061,1.1016519234,5.4304410607
C,0,0.5670250771,-0.2630794063,5.590127075
C,0,0.7836389228,-1.0658897643,4.473908044
C,0,0.7696589542,-0.4843293231,3.2085585621
N,0,0.553966754,0.8372055645,3.0919195471
H,0,0.5751556518,-0.700124987,6.583907968
H,0,0.1666247054,1.7491778096,6.2829860763

H,0,0.9593824374,-2.1316024436,4.57009546
C,0,0.0821376135,3.0909638208,3.8641590176
H,0,0.067405542,3.6612766307,4.7938667425
H,0,0.8551897082,3.4992812585,3.2065163814
H,0,-0.8872533587,3.2163884947,3.3667578003
C,0,0.968606944,-1.2680863719,1.945532181
H,0,1.2353514434,-2.2994327594,2.1800285304
H,0,0.0473894377,-1.2762936709,1.3515989749
H,0,1.7597857924,-0.8248648716,1.3336699872
H,0,0.4929838335,1.3365889129,1.9455818456

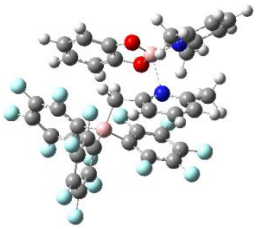
2:



Charge = 0 Multiplicity = 1
C,0,-1.2603744373,-1.155755068,-0.4131148268
C,0,-0.6535813441,1.3251767495,-0.1530506679
C,0,1.2617682189,-0.5079720026,0.5551588221
C,0,-2.2371463713,-1.1199005362,-1.4074919137
C,0,-1.6024838412,-1.961451362,0.6719971521
C,0,-0.9993870386,2.2999046849,-1.0802003001
C,0,-1.0486451531,1.6178759621,1.1494706717
C,0,1.7194028929,-1.8091873215,0.7518999558
C,0,2.1443929185,0.4614075871,1.0176360826
C,0,-3.4184706571,-1.8469656642,-1.3800364796
C,0,-2.7524018518,-2.7378332235,0.7265833029
C,0,-1.6581831256,3.4795230477,-0.7525525287
C,0,-1.702011482,2.7783365063,1.5267825087
C,0,2.9384466398,-2.1370406199,1.3221674885
C,0,3.3747176164,0.1860597938,1.6008089373
C,0,-3.6684255192,-2.6871978208,-0.3105091971
C,0,-2.0113854373,3.7238828436,0.5613085065
C,0,3.7838433319,-1.1273478761,1.7482822356
F,0,-2.08126244,-0.310755702,-2.4821966709
F,0,-0.824772878,-2.0166125686,1.7713027853
F,0,-0.7129100262,2.1534551561,-2.3948297087
F,0,-0.7897269456,0.7299097517,2.1346828405
F,0,1.0136289599,-2.864825368,0.2774308977
F,0,1.8775955073,1.7742606158,0.8300241519
F,0,-4.3042440445,-1.7531247031,-2.3791623316

F,0,-2.9913460739,-3.5231062392,1.785361643
F,0,-1.9578111598,4.376849185,-1.701704044
F,0,-2.0427501428,2.994102989,2.8043331809
F,0,3.3335229595,-3.4172941205,1.3952720017
F,0,4.1926528913,1.1816044778,1.9663693236
F,0,-4.7750090886,-3.4350531086,-0.2802159831
F,0,-2.6492565847,4.8502064233,0.8957559428
F,0,4.9907573361,-1.4148697204,2.2469448471
C,0,-1.3824928865,-4.1237985185,-2.5969951319
C,0,-1.4568833808,-3.2377939896,-3.6669491611
C,0,-2.3837928573,-5.0320118492,-2.3195472923
C,0,-2.5314190102,-3.2088971475,-4.5315947151
C,0,-3.4825995434,-5.0131510185,-3.1864125441
H,0,-2.3229351702,-5.7068817364,-1.4722430646
C,0,-3.5522199218,-4.1278597493,-4.2663986075
H,0,-2.5810545115,-2.5041133208,-5.3544096449
H,0,-4.3011041728,-5.7038701536,-3.012983155
H,0,-4.424454172,-4.1437566276,-4.9113604326
C,0,1.9576025902,-1.0156243648,-2.091885321
C,0,3.2589322737,-0.5582163723,-1.8711490818
C,0,4.3082138647,-1.4527423323,-1.7702088071
C,0,4.0711328591,-2.8196294566,-1.932610351
C,0,2.7963248967,-3.2676305515,-2.2130068474
N,0,1.7673421429,-2.3577470586,-2.2829221539
H,0,5.3126584629,-1.0949835404,-1.5637174349
H,0,3.4137227004,0.5072825277,-1.7433599258
H,0,4.8737413146,-3.5440711008,-1.8594589752
C,0,0.8002845211,-0.0916720904,-1.996577896
H,0,1.2120220694,0.9125293727,-2.1127309256
H,0,0.0947093137,-0.2462634776,-2.81229307
C,0,2.5059826863,-4.7199998146,-2.4363471383
H,0,1.8963621485,-4.8810340594,-3.3310388336
H,0,3.4489497212,-5.2521218001,-2.5627486078
H,0,1.9744866192,-5.1424917817,-1.5786424454
B,0,0.0350920032,-0.133123776,-0.483373398
B,0,0.3948647505,-2.87264438,-2.5852648107
O,0,-0.2104126374,-3.8896602747,-1.9027743243
O,0,-0.3253249741,-2.4409917761,-3.6668664294

TS2:

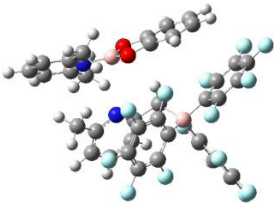


Charge = 0 Multiplicity = 1

C,0,2.0725601719,-1.1943523841,-0.3567836115
C,0,2.6165634405,1.1958069247,0.5302373297
C,0,0.5635404248,0.9190628094,-1.2833807811
C,0,2.4142829848,-2.0737503948,0.665147802
C,0,2.3914909503,-1.6596847018,-1.6283572301
C,0,2.9183160047,1.506978625,1.8488990914
C,0,3.5538204699,1.6680885091,-0.3848611181
C,0,-0.3459258377,0.1426992733,-1.9945898442
C,0,0.3956570766,2.2855381729,-1.4701578915
C,0,2.9654768613,-3.3306785689,0.4667908088
C,0,2.9444387417,-2.9082901198,-1.8789177318
C,0,4.024313319,2.255517876,2.2377315402
C,0,4.6715890509,2.4130610411,-0.0517956012
C,0,-1.3597900842,0.651944935,-2.7872594316
C,0,-0.6082267988,2.8470307978,-2.2502551782
C,0,3.2277174862,-3.7570739729,-0.8227234521
C,0,4.9097959957,2.7142420087,1.2807391819
C,0,-1.4989608799,2.0229156447,-2.9135475922
F,0,2.2141889905,-1.7231489113,1.9579199191
F,0,2.1499476414,-0.907942272,-2.7225551242
F,0,2.1247670067,1.0982010055,2.8701795414
F,0,3.3760429995,1.4116765154,-1.6994456168
F,0,-0.3286448262,-1.2030931391,-1.8654365852
F,0,1.1831018192,3.1766289344,-0.8207463875
F,0,3.2202063474,-4.1420170403,1.5044394293
F,0,3.1986958903,-3.3036824006,-3.1349855168
F,0,4.2313271409,2.5369370912,3.5327559411
F,0,5.5206107082,2.8457777754,-0.9942152323
F,0,-2.2555830709,-0.1642314774,-3.3701335661
F,0,-0.7630062797,4.1791616246,-2.3151192089
F,0,3.7385864436,-4.974099457,-1.0457370787
F,0,5.9813271854,3.4338208442,1.6319985511
F,0,-2.5126234954,2.5409510043,-3.6222180694
C,0,-1.7365847534,-2.7755590334,0.1949045302
C,0,-1.6319372106,-2.610714692,1.5709960578
C,0,-1.0051430975,-3.7248488032,-0.4909774287
C,0,-0.7790976596,-3.3738660429,2.3433729041

C,0,-0.1470215611,-4.5184315821,0.2808734964
H,0,-1.0834685034,-3.8332862194,-1.5672765497
C,0,-0.0334430224,-4.3451189154,1.6636364004
H,0,-0.6835859244,-3.2129675366,3.4121557197
H,0,0.4519080344,-5.2791161037,-0.2108288043
H,0,0.6580889367,-4.9663094545,2.2234239183
C,0,-0.8290509992,1.1542480399,1.1135206609
C,0,-0.4734776907,2.3658965291,1.7193715165
C,0,-1.2903258311,3.4759453305,1.5611653407
C,0,-2.4209993032,3.3689650002,0.7583524458
C,0,-2.7410224666,2.1282271515,0.2058434601
N,0,-1.9994234752,1.0273888497,0.4418077968
H,0,-1.0258648317,4.4248748396,2.0193832178
H,0,0.4514442313,2.4303787134,2.2790396978
H,0,-3.0419698263,4.2313466095,0.5357804391
C,0,0.1271135384,0.0085259175,1.0774833804
H,0,0.4883487974,-0.2369409045,2.0757671966
H,0,-0.3929416695,-0.8572253696,0.6751053589
C,0,-3.9185734897,2.0288520824,-0.7278258792
H,0,-4.870302602,2.0330029211,-0.1841974878
H,0,-3.9287514587,2.901575555,-1.3874303852
H,0,-3.8608533446,1.1316613058,-1.3479431337
B,0,1.3759410775,0.2594421805,-0.0081583742
B,0,-3.0431363608,-1.1151892111,0.7919882537
O,0,-2.6236048685,-1.8451053931,-0.3025268221
O,0,-2.4493313367,-1.5720565984,1.9612242311
C,0,-5.3789058756,-0.7396375595,-0.071119097
C,0,-6.6745574934,-0.2727329681,0.1024188703
C,0,-7.0197787775,0.4512496501,1.2339388129
C,0,-6.0466878627,0.7064080824,2.1880756076
C,0,-4.7547018501,0.2249028188,2.0263092158
N,0,-4.4336456429,-0.4942662175,0.8982297135
H,0,-8.0321424408,0.8196017378,1.3657228886
H,0,-7.4027579735,-0.4778402937,-0.6728804963
H,0,-6.2747148767,1.2767256592,3.0807709793
C,0,-5.0557538698,-1.4932961163,-1.3265994152
H,0,-4.8158042052,-2.5375468012,-1.1127443853
H,0,-5.931808343,-1.461969987,-1.9742845297
H,0,-4.2057249615,-1.0616660258,-1.8573294114
C,0,-3.7569929116,0.4938225196,3.1141638983
H,0,-3.6803485036,-0.3760212126,3.7732315733
H,0,-2.7584842007,0.7151202623,2.7418856537
H,0,-4.1136410945,1.3419212564,3.6999176464

3:

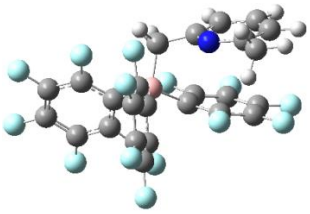


Charge = 0 Multiplicity = 1

C,0,1.8886017074,1.2655754746,0.3586617907
C,0,2.6098734033,-1.0156208335,-0.6210646112
C,0,0.5765762623,-1.0025011948,1.2267782696
C,0,2.2266584434,2.164129891,-0.6477112033
C,0,2.1794452258,1.7205697683,1.6405179399
C,0,2.9192109731,-1.2784842997,-1.948303638
C,0,3.6112621997,-1.3914934615,0.2709476592
C,0,-0.3932804148,-0.3528532069,1.9819999343
C,0,0.5583798455,-2.3844254305,1.368050531
C,0,2.7680552261,3.4208454056,-0.4272255744
C,0,2.7110790535,2.9739424817,1.9135217348
C,0,4.0933454273,-1.897866611,-2.3644407865
C,0,4.7959485029,-2.0087585252,-0.0890900043
C,0,-1.3240623909,-0.992823677,2.7813884574
C,0,-0.3629043366,-3.0761793153,2.1448019814
C,0,3.0042893526,3.835645891,0.8711000601
C,0,5.0406806166,-2.2685108091,-1.4292674668
C,0,-1.3188485645,-2.3745796058,2.8563627029
F,0,2.0353933907,1.8268181571,-1.9456521379
F,0,1.950662216,0.9473918503,2.7225008631
F,0,2.0713415057,-0.9457527441,-2.953339292
F,0,3.4342877292,-1.1631213487,1.5915307546
F,0,-0.5352694593,0.9889992284,1.8843022777
F,0,1.4201214036,-3.1651991182,0.672079433
F,0,3.0222031898,4.251668082,-1.4499017985
F,0,2.9383077014,3.3597982237,3.1777057523
F,0,4.3086284164,-2.1367929591,-3.6668617147
F,0,5.7049933419,-2.3540578567,0.8332151885
F,0,-2.2861143493,-0.2954226336,3.4120766378
F,0,-0.3724617305,-4.4190598528,2.1639589495
F,0,3.4840816918,5.0613318184,1.1160075332
F,0,6.1780641722,-2.8622366754,-1.8080894946
F,0,-2.2557650307,-3.0214848847,3.565116495
C,0,-1.8398640407,2.8366156223,-0.043927343
C,0,-1.7882642158,2.8397090519,-1.4318427515
C,0,-1.0595752246,3.6784352732,0.7257341661
C,0,-0.9440737511,3.6700352956,-2.1420248177

C,0,-0.2170018472,4.543675274,0.0205605462
H,0,-1.1007074643,3.6612000378,1.8091490745
C,0,-0.1559499125,4.5372620165,-1.3778383594
H,0,-0.8988819899,3.6459284204,-3.2254979909
H,0,0.4138140043,5.2318337745,0.5753841051
H,0,0.5288117177,5.2107099152,-1.882617571
C,0,-0.8217525872,-1.2955190408,-1.1498602496
C,0,-0.4001105933,-2.4513600091,-1.8197670004
C,0,-1.1387191085,-3.620525146,-1.6848282935
C,0,-2.2675529389,-3.6207955157,-0.8709068729
C,0,-2.6443431605,-2.424744665,-0.2530944153
N,0,-1.9578285074,-1.2855912314,-0.4216156526
H,0,-0.8215170981,-4.5307900476,-2.1864703636
H,0,0.5065174705,-2.430625466,-2.4122227457
H,0,-2.8400251267,-4.5270525348,-0.6961411489
C,0,0.0194237902,-0.0580571814,-1.1097308904
H,0,0.3594590841,0.2240253295,-2.1063249622
H,0,-0.5998534513,0.751317711,-0.7163818824
C,0,-3.842763857,-2.3859071209,0.6582082677
H,0,-4.7764151528,-2.384037517,0.0839311935
H,0,-3.8645953719,-3.2741244817,1.2970803616
H,0,-3.8179861988,-1.4948837238,1.2918744803
B,0,1.2909640451,-0.2177879647,-0.0355786314
B,0,-3.2590793814,1.3571762713,-0.7917201536
O,0,-2.7650030417,1.8949208407,0.3643501169
O,0,-2.6819346349,1.9023489626,-1.9129354197
C,0,-5.4374412365,0.5463550039,0.1027706528
C,0,-6.6343524479,-0.133270316,-0.0656124158
C,0,-6.8635327769,-0.8854558734,-1.2090536488
C,0,-5.8710198346,-0.9649818484,-2.1755328751
C,0,-4.6811200593,-0.2687299322,-2.0215795288
N,0,-4.4834491198,0.4872165483,-0.8888067703
H,0,-7.8016881415,-1.4157127268,-1.3388937743
H,0,-7.3790903634,-0.0670290217,0.7182962027
H,0,-6.0048937806,-1.560801829,-3.0708375708
C,0,-5.2060237566,1.3235260881,1.3620779202
H,0,-5.0400847316,2.384265678,1.1590774305
H,0,-6.0879452578,1.2228678625,1.9940602711
H,0,-4.3360344314,0.9461817346,1.9043415508
C,0,-3.6490059312,-0.3507320662,-3.104905392
H,0,-3.7081510276,0.5274034998,-3.7546515275
H,0,-2.6332602569,-0.415648,-2.7165702284
H,0,-3.8580473617,-1.2379317247,-3.7038032559

IM4:

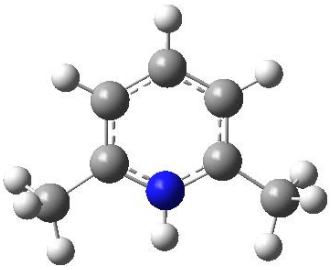


Charge = -1 Multiplicity = 1

C,0,-1.7839859637,-0.9190155381,-0.4171427901
C,0,-0.557069271,1.3397701359,-0.0255103729
C,0,0.8412174204,-0.9776327827,0.4250438061
C,0,-2.7571460768,-0.5763512087,-1.3501361667
C,0,-2.2218575764,-1.8067933247,0.5594469164
C,0,-0.5778650567,2.473181498,-0.8308489062
C,0,-0.8510544194,1.5882836837,1.3118605892
C,0,1.0485897875,-2.3433684557,0.2587521464
C,0,1.8850445406,-0.3328104823,1.0791019939
C,0,-4.045967782,-1.0889024479,-1.3614158895
C,0,-3.5024627841,-2.3447026873,0.593343284
C,0,-0.8004763236,3.7554828332,-0.3384919073
C,0,-1.0856460781,2.8433114248,1.8473325153
C,0,2.1879935323,-3.0203855474,0.6612207594
C,0,3.0565022851,-0.9616975896,1.4827107674
C,0,-4.4226992402,-1.9866154581,-0.3766951335
C,0,-1.0554341779,3.9449217872,1.0072734372
C,0,3.2154408155,-2.3175735961,1.2679833588
F,0,-2.4733566921,0.3230625163,-2.3195788407
F,0,-1.4030520261,-2.2076981075,1.5516976548
F,0,-0.3951940577,2.4108669181,-2.1635074754
F,0,-0.8820207046,0.5526588905,2.1812276395
F,0,0.1440018308,-3.0822728516,-0.4278261057
F,0,1.8563703891,0.9998059693,1.3062158311
F,0,-4.9282595945,-0.7213560689,-2.3029328548
F,0,-3.8593751956,-3.2047709329,1.559008979
F,0,-0.7842019839,4.8149345722,-1.1637887092
F,0,-1.3409957982,3.0062620198,3.1552322833
F,0,2.3431200532,-4.3283999445,0.398224737
F,0,4.05959428,-0.2533055498,2.0273414334
F,0,-5.6614672761,-2.4971774257,-0.359823474
F,0,-1.2827068096,5.1747720089,1.4902621824
F,0,4.3613575865,-2.9319105199,1.5978636962
C,0,1.8130409385,-0.0695923364,-1.9933262512
C,0,2.7620907416,-1.0953059805,-2.1486332967
C,0,4.0942434766,-0.8344522415,-1.8596727907

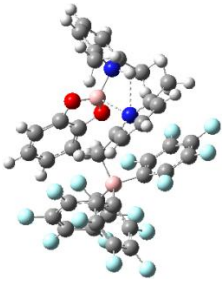
C,0,4.4613139549,0.4469750597,-1.4500217217
C,0,3.470519662,1.4283345229,-1.3774692799
N,0,2.184673589,1.1698296289,-1.6436388849
H,0,4.8395269049,-1.6226726628,-1.9332548848
H,0,2.4387039956,-2.0878713514,-2.4492204375
H,0,5.4878715293,0.6830878059,-1.1876250914
C,0,0.3410888155,-0.3568946867,-2.0343782546
H,0,-0.1621902277,0.314076236,-2.729525993
H,0,0.1862088684,-1.3838959759,-2.3870733302
C,0,3.7760989005,2.8392030448,-0.9540822308
H,0,3.2887316309,3.0454191083,0.0047103035
H,0,4.8504928101,3.0079991087,-0.8447041226
H,0,3.3740620519,3.5464988725,-1.6852538529
B,0,-0.2981012743,-0.2151548909,-0.5003232652

HLutidine+



Charge = 1 Multiplicity = 1
C,0,1.2012667606,0.2620085635,0.
C,0,1.2086693225,-1.1247521552,0.
C,0,0.,-1.8159317823,0.
C,0,-1.2086693225,-1.1247521552,0.
C,0,-1.2012667606,0.2620085635,0.
N,0,0.,0.8819413095,0.
H,0,0.,-2.9014568778,0.
H,0,2.1590350028,-1.6460934899,0.
H,0,-2.1590350028,-1.6460934899,0.
C,0,2.4373575893,1.1010450984,0.
H,0,3.0383058982,0.8703442968,0.883679323
H,0,3.0383058982,0.8703442968,-0.883679323
H,0,2.2058834922,2.1678929889,0.
C,0,-2.4373575893,1.1010450984,0.
H,0,-3.0383058982,0.8703442968,-0.883679323
H,0,-3.0383058982,0.8703442968,0.883679323
H,0,-2.2058834922,2.1678929889,0.
H,0,0.,1.9023601519,0.

TS3



Charge = 0 Multiplicity = 1

C,0,-1.7970916739,-1.3781540107,0.4653811612
C,0,-2.7498717628,0.7864557642,-0.6069415236
C,0,-0.7019578253,1.0402711865,1.2148347899
C,0,-1.9924062511,-2.3749969121,-0.4848192384
C,0,-2.0460658292,-1.7876485812,1.7713536941
C,0,-3.0975917434,0.9119164099,-1.9444657701
C,0,-3.7629135999,1.1586706084,0.2732568377
C,0,0.3207545162,0.5063932217,1.9920409284
C,0,-0.7917328317,2.4251587236,1.2853572065
C,0,-2.3514340174,-3.6805222583,-0.1882428626
C,0,-2.3986338841,-3.0845485272,2.1200335008
C,0,-4.3190607369,1.4088293988,-2.3862431864
C,0,-4.9957189986,1.6540874884,-0.1126442312
C,0,1.2066208422,1.2600554812,2.7427781857
C,0,0.0779579109,3.2270808359,2.0153642736
C,0,-2.546099066,-4.043622787,1.132415162
C,0,-5.2774287011,1.7849772437,-1.4642822551
C,0,1.0938914994,2.6399280269,2.7470554488
F,0,-1.8329642598,-2.0977396356,-1.8006700735
F,0,-1.9385407258,-0.9218166357,2.8006125718
F,0,-2.2383449195,0.5572042228,-2.9329846923
F,0,-3.5491080395,1.0525244912,1.6028006052
F,0,0.5577797486,-0.8261303126,1.9745938679
F,0,-1.7165531575,3.0972771078,0.56084677
F,0,-2.4750141403,-4.5968582272,-1.1596060669
F,0,-2.590270155,-3.4196683349,3.4036577449
F,0,-4.5686412968,1.5291002079,-3.6982470169
F,0,-5.9146489793,2.0060271872,0.796039248
F,0,2.2284096351,0.6745783953,3.397420397
F,0,-0.0141536586,4.5643361231,1.9613615908
F,0,-2.8584295466,-5.304920462,1.4511908114
F,0,-6.4589930169,2.2634473377,-1.8669021596
F,0,1.9924759315,3.3924148346,3.3978561811
C,0,2.0545198698,-2.4595962523,-0.0144068366
C,0,2.0097412197,-2.3827220662,-1.4013856078
C,0,1.4286646843,-3.4655164072,0.6926394944

C,0,1.3390608947,-3.3049199608,-2.1760785142
C,0,0.760266341,-4.4219889628,-0.0802196415
H,0,1.4497684684,-3.5015442127,1.7762043053
C,0,0.7154725844,-4.3443860923,-1.4766853214
H,0,1.2919809142,-3.218312596,-3.2561312683
H,0,0.2513914657,-5.2400590051,0.4198925525
H,0,0.1728680619,-5.1010792174,-2.0329149033
C,0,0.6312863716,1.3451838401,-1.2222922337
C,0,0.0340071291,2.3947052833,-1.9348919917
C,0,0.5747440664,3.66879977,-1.8687824999
C,0,1.6872501955,3.8834688891,-1.0617278028
C,0,2.2715751675,2.7933880513,-0.4216846659
N,0,1.7946445383,1.5342632713,-0.5507129085
H,0,0.1091904223,4.4935790751,-2.4002015
H,0,-0.8688410934,2.20596558,-2.5013809768
H,0,2.0975697495,4.8771257985,-0.9129198361
C,0,-0.0751024502,0.0391316124,-1.0653840352
H,0,-0.3685391088,-0.376573122,-2.0296062712
H,0,0.5975878499,-0.6599113379,-0.574570121
C,0,3.4681950187,3.0377627553,0.4659163679
H,0,4.4175104937,3.0365506178,-0.091786816
H,0,3.3949915358,4.0318227088,0.9140971733
H,0,3.5217034193,2.3148047697,1.2869860134
B,0,-1.3651415037,0.1418327154,0.0006080236
B,0,3.1015003682,-0.6746281069,-0.6436082083
O,0,2.7794184479,-1.3749261439,0.4739857584
O,0,2.6964998656,-1.2423466088,-1.8129789015
C,0,5.3217032648,-0.3222953781,0.3221285126
C,0,6.3842325712,-1.0533779354,-0.1226701718
C,0,6.6756910586,-1.1042719976,-1.494395579
C,0,5.9376280874,-0.3793720821,-2.4466696915
C,0,4.8487199234,0.3442372571,-2.0644469412
N,0,4.4263738009,0.243015889,-0.6749796191
H,0,7.5336686137,-1.6827444854,-1.825964612
H,0,7.0250036697,-1.5420966529,0.6023734109
H,0,6.2405662987,-0.3618073461,-3.4868766768
C,0,4.991882983,-0.0385482488,1.7343531585
H,0,3.9287646819,0.1490175218,1.88838972
H,0,5.3232866073,-0.8657757983,2.3644733078
H,0,5.5483176186,0.8634466191,2.0291691898
C,0,4.0331330048,1.2170198887,-2.9348716063
H,0,2.976600075,0.9284140591,-2.9281899853
H,0,4.0948149781,2.2524240348,-2.5731986794
H,0,4.4178092576,1.1652144577,-3.9533553659

H,0,4.1036526378,1.1740424888,-0.3487652707