Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

Substitution at *sp*^{3} boron of a six-membered NHC·BH_3: convenient access to a dihydroxyborenium cation

Gargi Kundu,[ab] V. S. Ajithkumar,[ab] K. Vipin Raj,[bc] Kumar Vanka,[bc] Srinu Tothadi[bd] and Sakya S. Sen*[ab]

[a]*Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008 (India);* [b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002 (India);* [c]*Physical and Material Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India;* [d]*Analytical and Environmental Science Division, CSIR-Central Salt & Marine Chemicals Research Institute, Gijubhai Badheka Marg, Bhavnagar-364002 (India).*

Author to whom correspondence should be addressed: E-mail: ss.sen@ncl.res.in

Table of Contents

S1. General procedures and instrumentation

All manipulations were carried out in an inert atmosphere of argon using standard Schlenk techniques and in argon filled glove box. The solvents, especially toluene, tetrahydrofuran, dichloromethane and *n*-hexane were purified by MBRAUN solvent purification system MB SPS-800. Benzene-d_6 was dried and distilled over Na/benzophenone mixture prior to use. Other chemicals were purchased from Sigma Aldrich and TCI Chemicals and were used without further purification. The starting material, 6-SIDipp was synthesized by using literature procedure.[1] The ^{1}H, ^{13}C, ^{11}B NMR and ^{19}F spectra were recorded in C_6D_6 and $CDCl_3$, using a Bruker Advance DPX 200, Bruker Avance DPX 400, or a Bruker Avance DPX 500 spectrometer. Chemical shifts (δ) are given in ppm. NMR spectra were referenced to external $SiMe_4$ (^{1}H and ^{13}C), $BF_3{\cdot}OEt_2$ (^{11}B), $CFCl_3$ (^{19}F) respectively . Mass spectra (ESI-MS) were obtained using a Q Exactive Thermo Scientific at the CSIR National Chemical Laboratory, Pune. Elemental analyses were performed at the CSIR National Chemical Laboratory, Pune, India.

S2. Synthetic procedure and spectroscopic characterization of 1-9

1: $BH_3{\cdot}SMe_2$ (0.05 ml, 0.70 mmol) was added to a solution of 6-SIDipp (0.2 g, 0.50 mmol) in 5 ml toluene solvent at -36 °C. The resulting mixture was stirred for 2 hours at room temperature. Colorless crystals of **1** were isolated from the concentrated toluene solution with a yield of 0.15 g (70 %).

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 0.25 (s, 3 H, BH_3), 1.30 (d, J = 6.97 Hz, 12 H, CH(CH_3)$_2$), 1.36 (d, J = 6.72, 12H, CH(CH_3)$_2$), 2.33 (q, J = 5.88 Hz, 2H, NCH$_2$CH_2CH$_2$N), 3.06 (sept, J = 6.88 Hz, 4 H, CH(CH$_3$)$_2$), 3.52 (t, J = 5.87 Hz, 4H, NCH_2CH$_2$CH_2N), 7.18 (d, J = 7.70 Hz, 4H, Ar-H), 7.32 (t, J = 7.70 Hz, 2 H, Ar-H) ppm.

$^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$): δ = 20.5, 23.5, 25.3, 28.7, 49.3, 124.1, 128.2, 142.0, 144.3 ppm.

$^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$): δ = -31.3 (q, 1B, BH_3) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{43}BN_2$ $[M+H]^+$ 419.3592, found 419.3409.

Elemental Analysis: calcd. C, 80.36; H, 10.36; N, 6.69; found: C, 80.41; H, 10.53; N, 6.61.

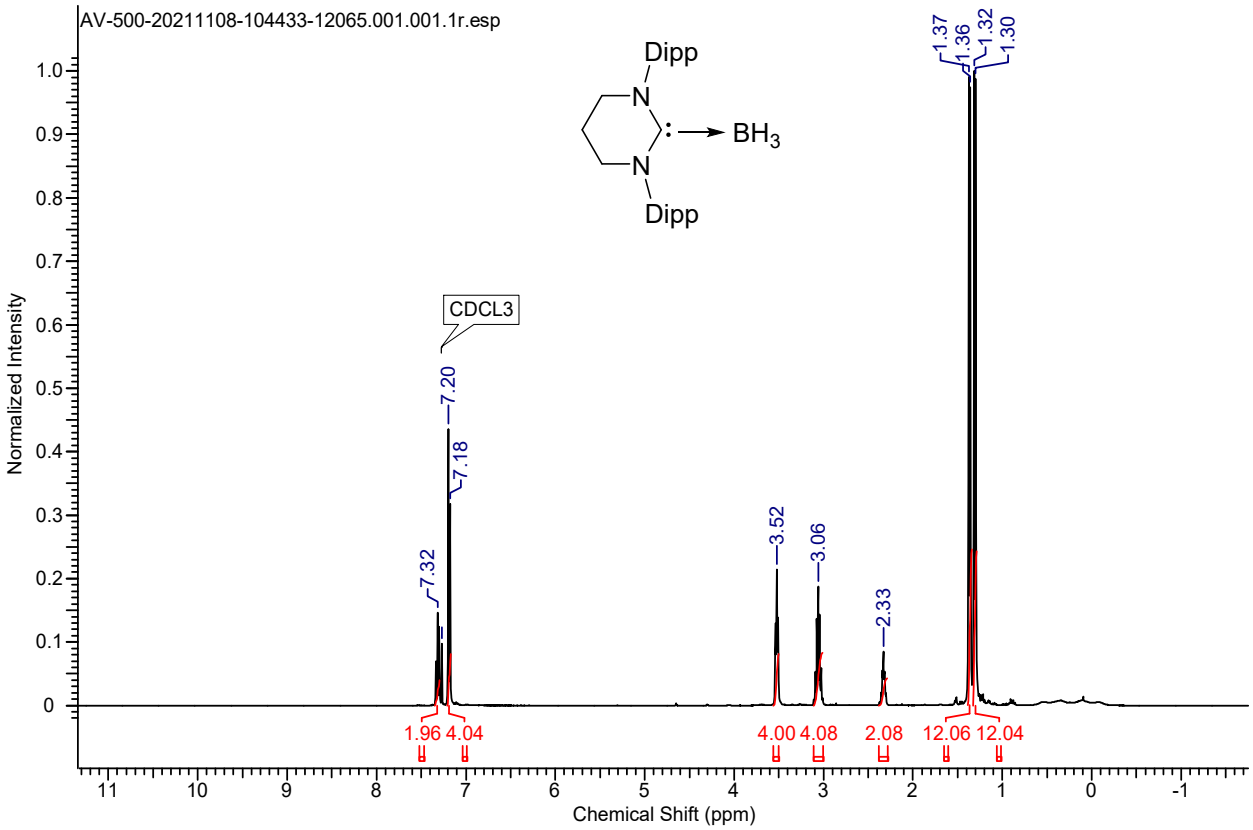

Figure S1. ^{1}H NMR spectrum of **1**.

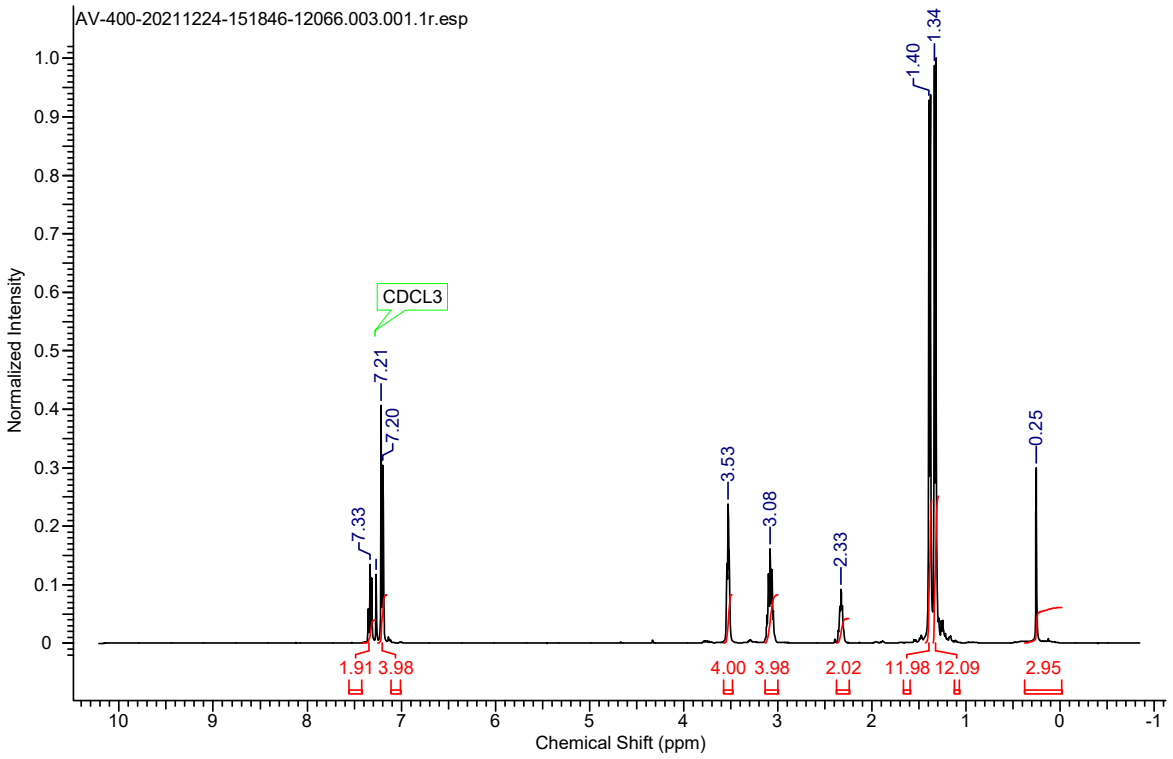

Figure S2.[1]H {11B} NMR spectrum of **1**

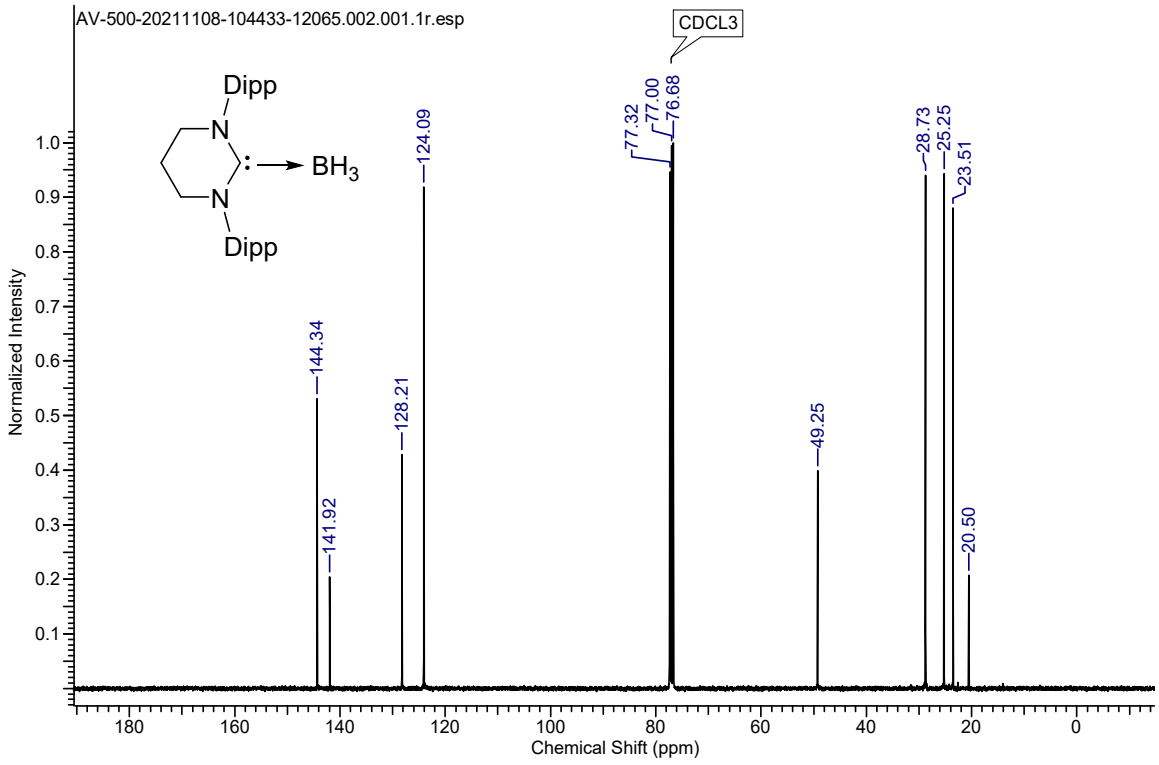

Figure S3.[13]C NMR spectrum of **1**.

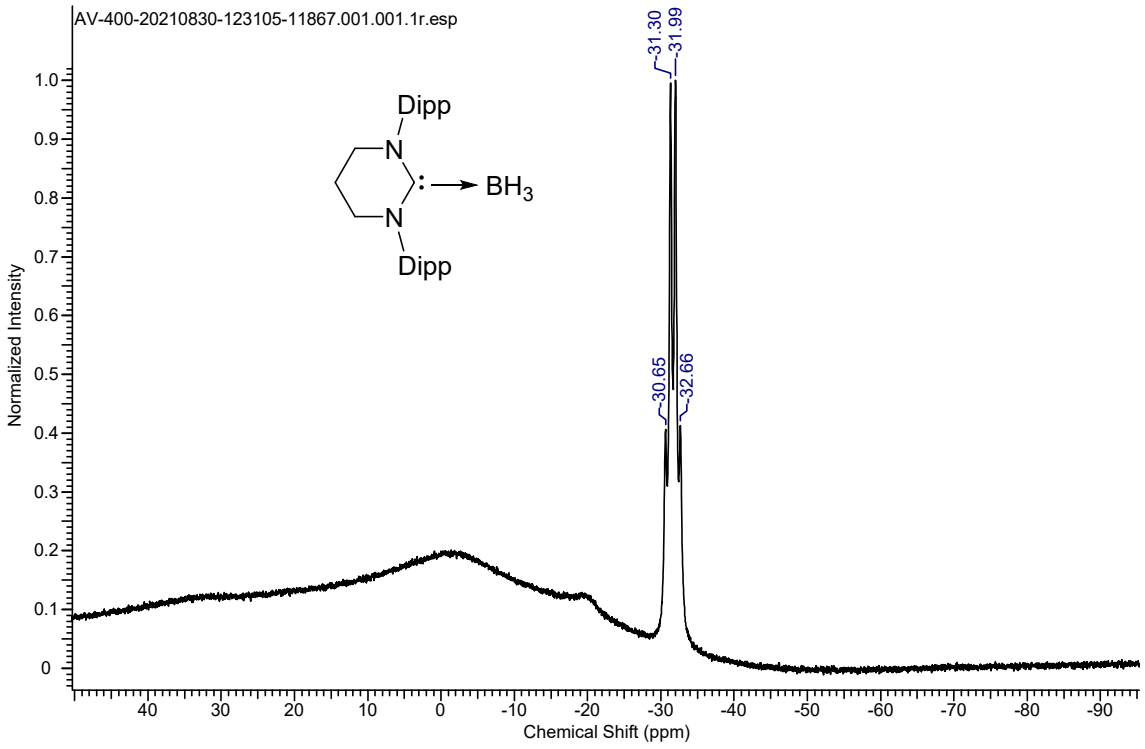

Figure S4.^{11}B NMR spectrum of **1**.

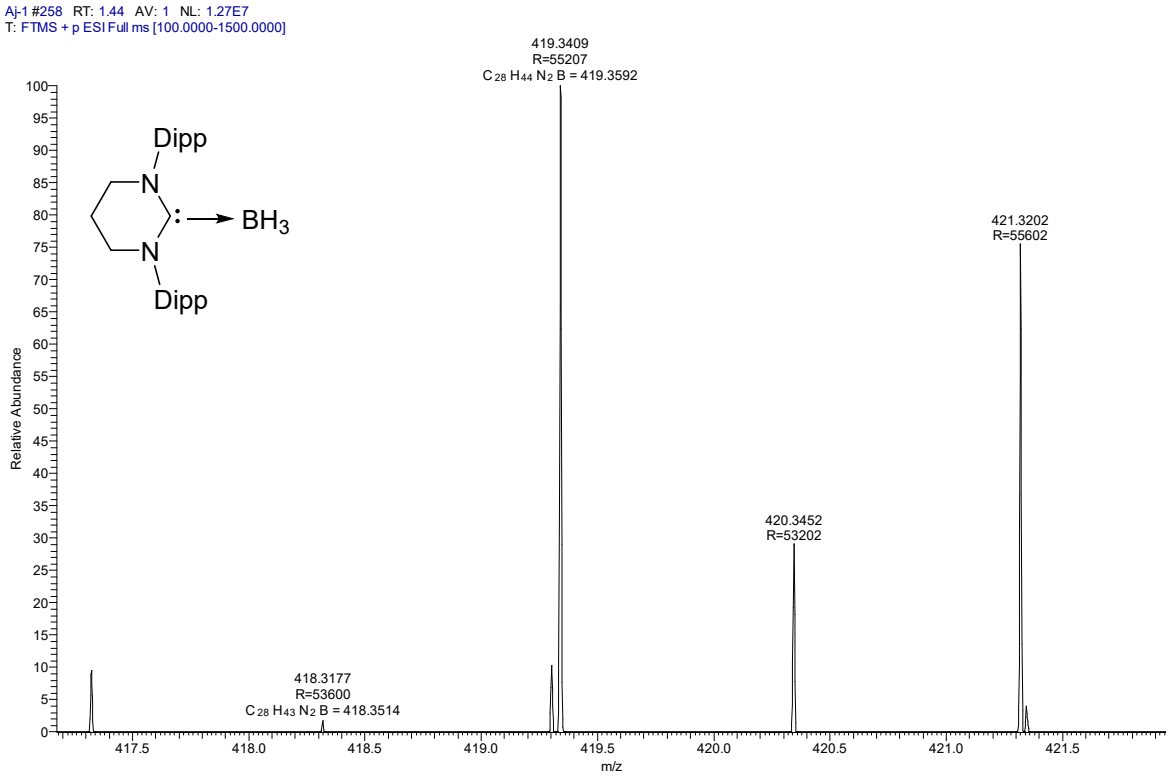

Figure S5. ESI-MS spectrum of **1**.

2: 0.5 equivalent of Iodine (I_2) (0.061 g, 0.24 mmol) and **1** (0.2 g, 0.48 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 1 h at room temperature. The toluene solution was concentrated and filtered through cannula. Colorless crystals of **6** were isolated after keeping the solution at 4 ˚C for a day with a yield of 0.22 g (85 %).

^{1}H {^{11}B} NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.28 (d, J = 6.88 Hz, 12 H, CH(CH_3)$_2$), 1.47 (d, J = 6.63 Hz, 12 H, CH(CH_3)$_2$), 1.60 (s, 2 H, BH_2I), 2.30 (quintet, J = 5.40 Hz, 2 H, NCH$_2$CH_2CH$_2$N), 3.14 (sept, J = 6.16 Hz, 4 H, CH(CH$_3$)$_2$), 3.64 (t, J = 5.67 Hz, 4 H, NCH_2CH$_2$CH_2N), 7.19 (m, 4H, Ar-H), 7.33 (t, J = 7.75 Hz, 2H, Ar-H) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 19.5, 24.0, 26.1, 28.6, 50.9, 124.4, 128.8, 140.8, 144.5 ppm.

^{11}B{^{1}H} NMR (127 MHz, 298 K, $CDCl_3$): δ = -30.2 (bs, 1B, BH$_2$I) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{42}N_2BI$ $[M+H]^+$ 545. 2558, found 545. 3156.

Elemental Analysis: Calcd. C, 61.78; H, 7.78; N, 5.15; found C, 61.72; H, 7.68; N, 5.13.

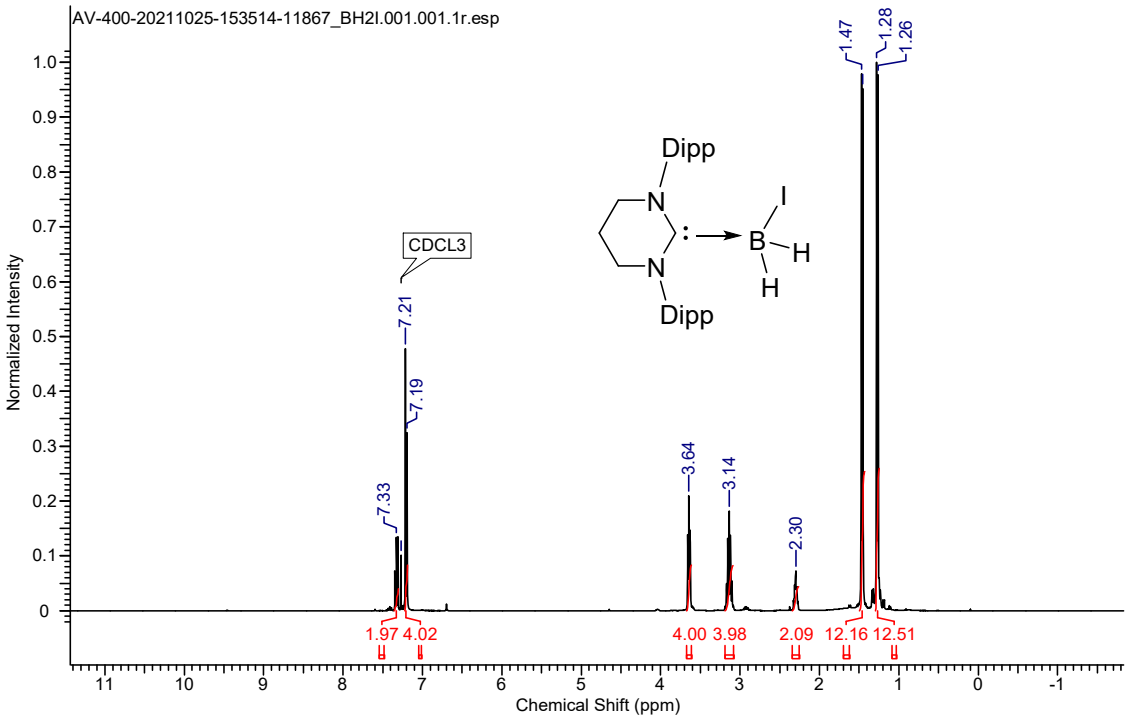

Figure S6.[1]H NMR spectrum of **2**.

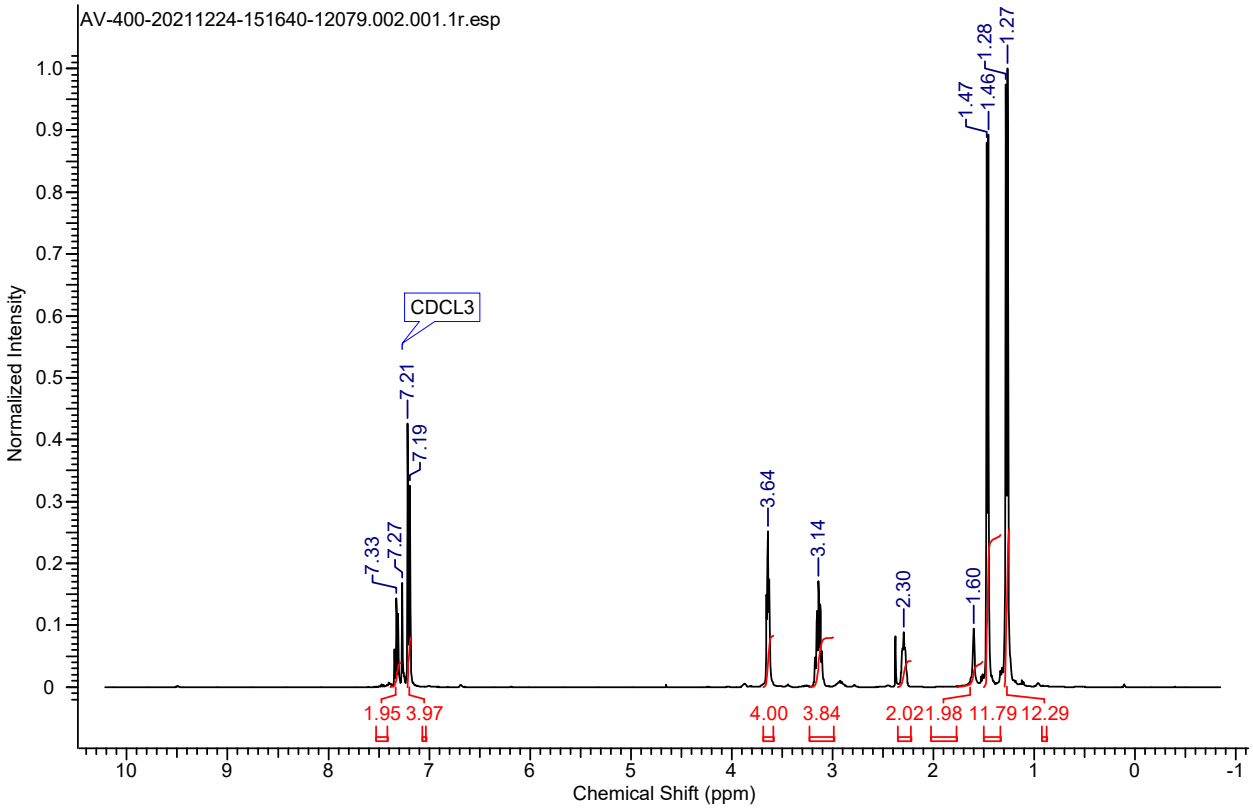

Figure S7.[1]H {[11]B} NMR spectrum of **2**.

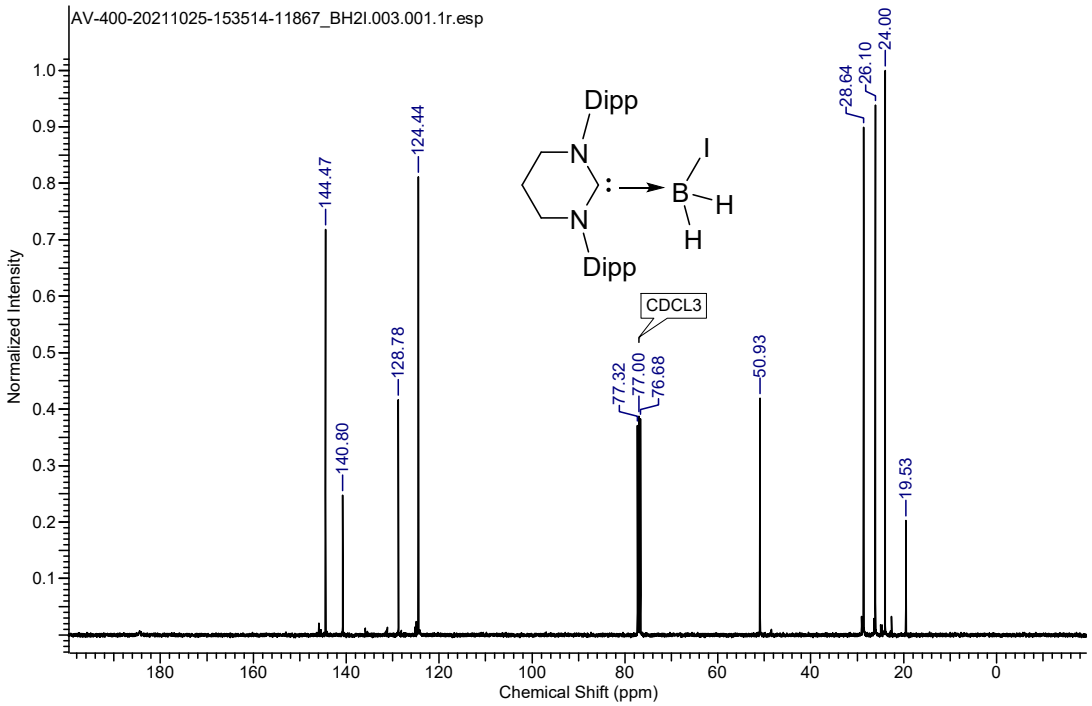

Figure S8. ^{13}C NMR spectrum of **2**.

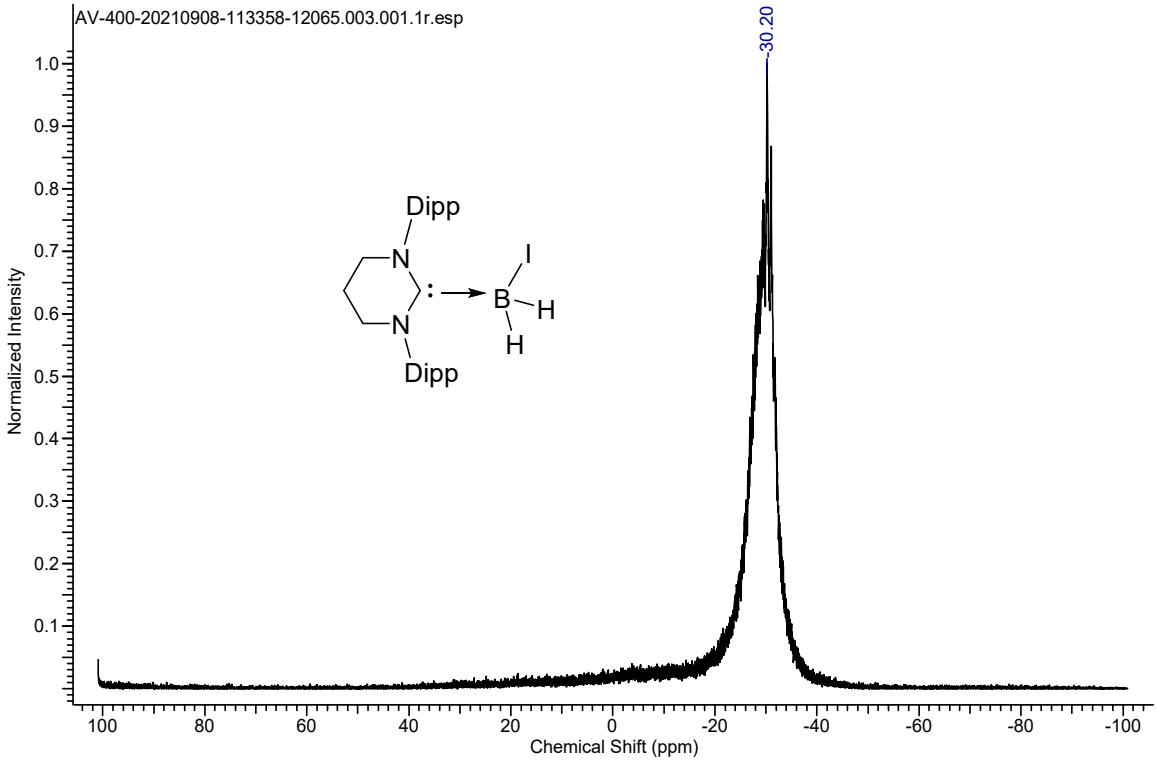

Figure S9. ^{13}B NMR spectrum of **2**.

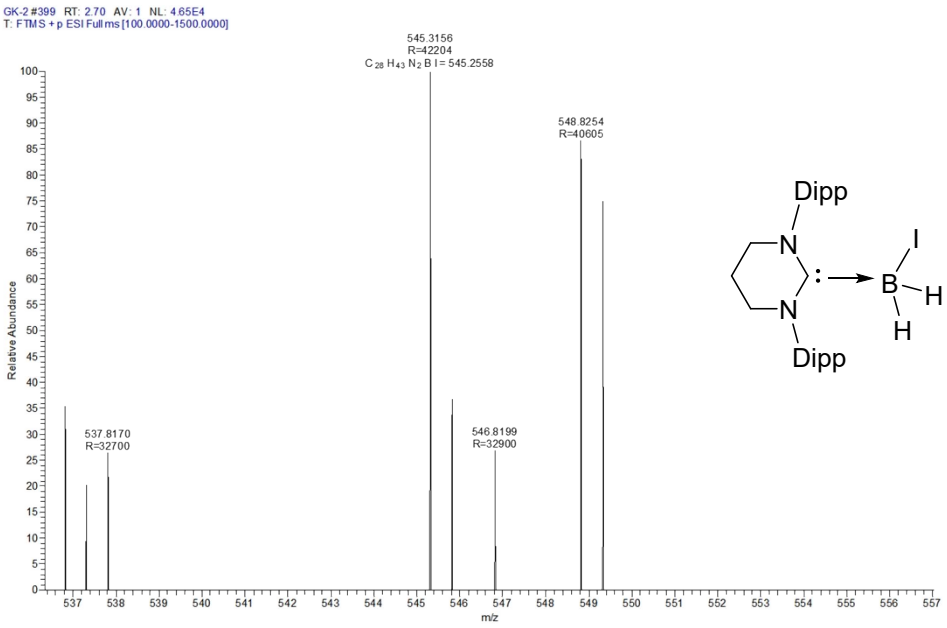

Figure S10. ESI-MS spectrum of **2**.

3: 1.0 equivalent of iodine (I_2) (0.12 g, 0.48 mmol) and **1** (0.2 g, 0.48 mmol) were taken in a Schlenk flask and 5 ml of benzene was added to the reaction mixture. The reaction was run for an hour at room temperature. The benzene solution was concentrated and filtered through cannula. Colorless crystals of **7** were isolated after storing the solution at 4 ˚C for a day with a yield of 0.3 g (88 %).

^{1}H {^{11}B} NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.29 (d, J = 6.88 Hz, 12H, CH(CH_3)$_2$), 1.51 (d, J = 6.65 Hz, 12 H, CH(CH_3)$_2$), 2.38 (s, 1H, BHI$_2$), 2.40 (quintet, J =5.63 Hz, 2H, NCH$_2$CH_2CH$_2$N), 3.25 (sept, J = 6.75 Hz, 4H, CH(CH$_3$)$_2$), 3.72 (t, J = 5.62 Hz, 4H, NCH_2CH$_2$CH_2N), 7.22 (m, 4H, Ar-H), 7.37 (t, J = 7.75 Hz, 2H, Ar-H) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 20.2, 24.5, 26.3, 28.9, 52.6, 125.1, 129.4, 140.8, 145.0 ppm.

^{11}B{^{1}H} NMR (128 MHz, 298 K, $CDCl_3$): δ = -39.4 (bs, 1B, BHI$_2$) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{41}N_2BI_2$ $[M+H]^+$ 671.1525, found 670.8353.

Elemental Analysis: Calcd. C, 50.18; H, 6.17; N, 4.18; found C, 50.15; H, 6.12; N, 4.24.

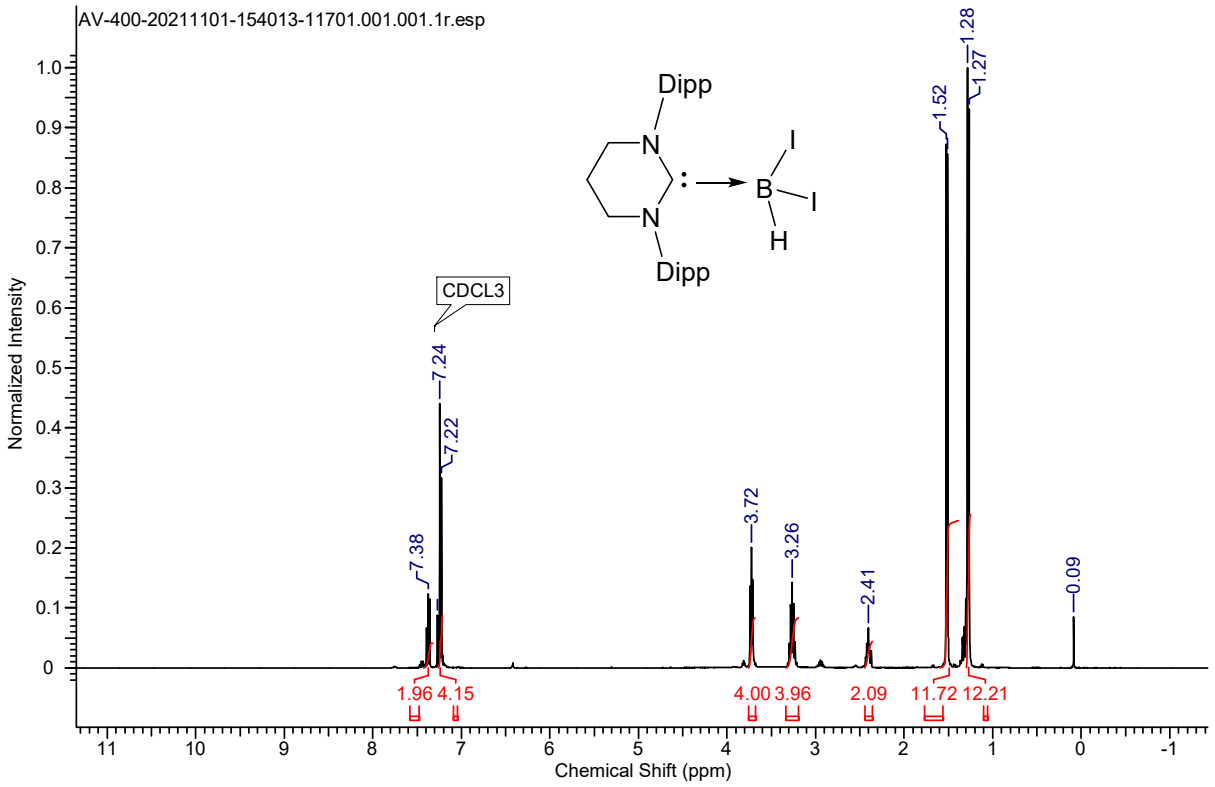

Figure S11. ^{1}H NMR spectrum of **3**.

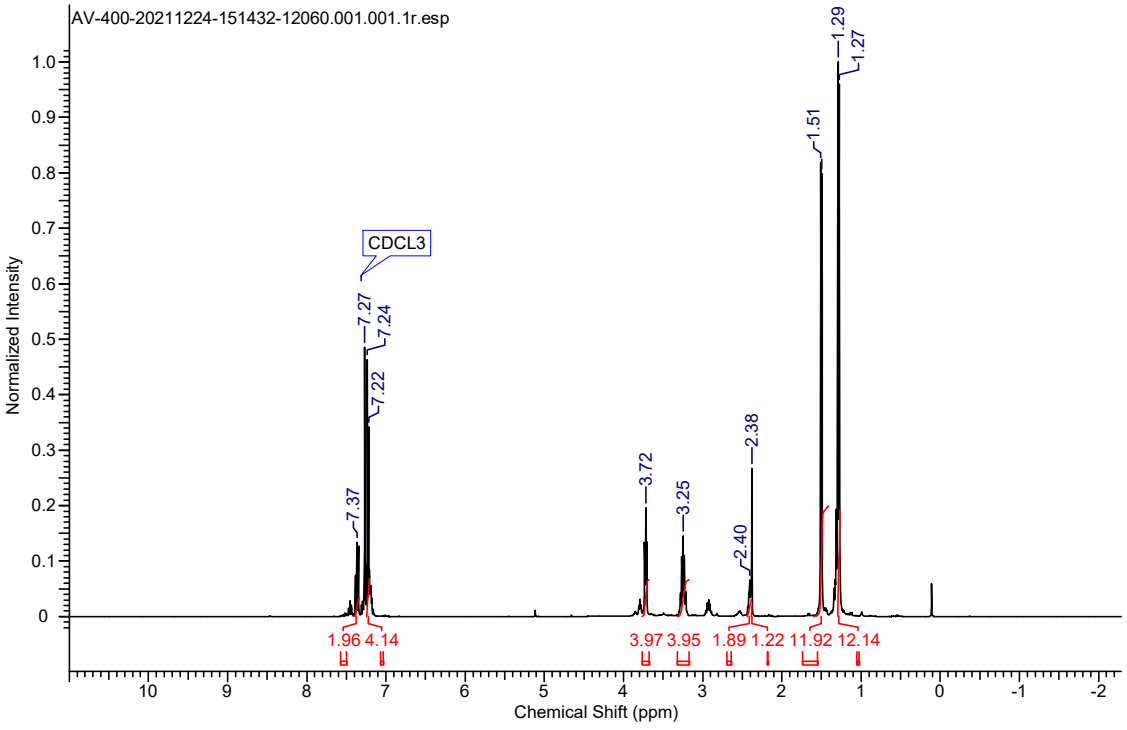

Figure S12. $^{1}H\{^{11}B\}$ NMR spectrum of **3**.

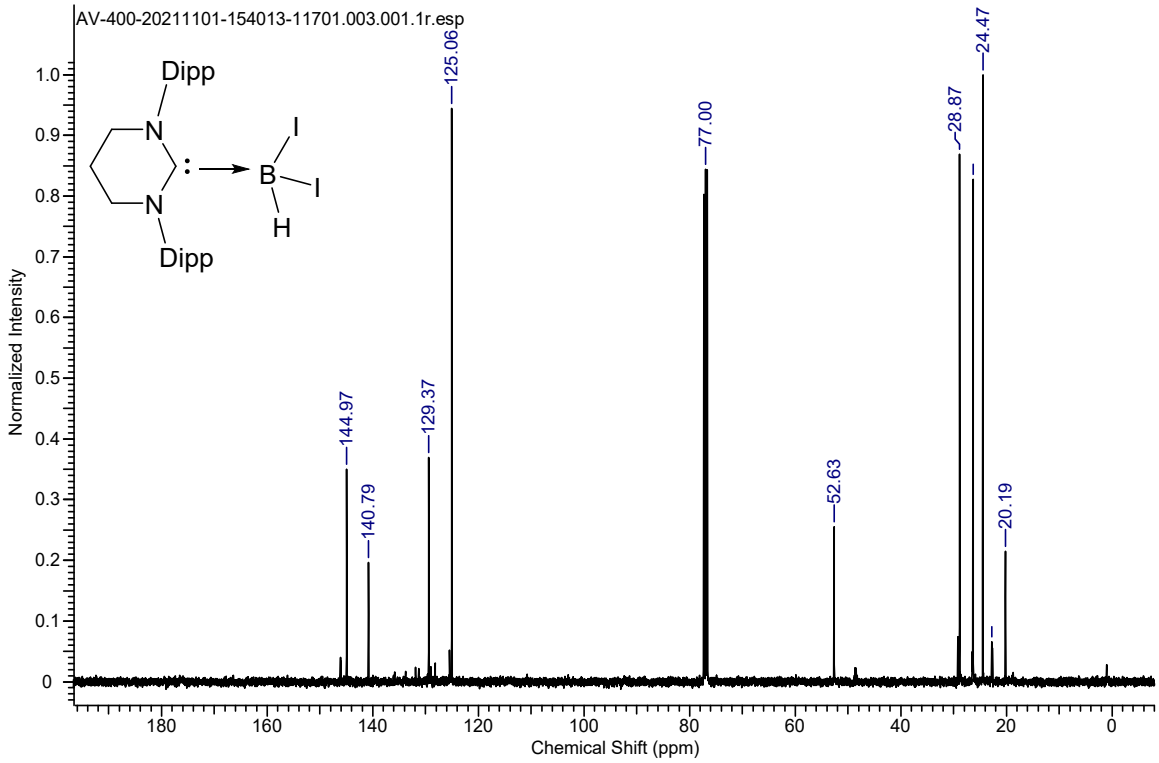

Figure S13. ^{13}C NMR spectrum of **3**.

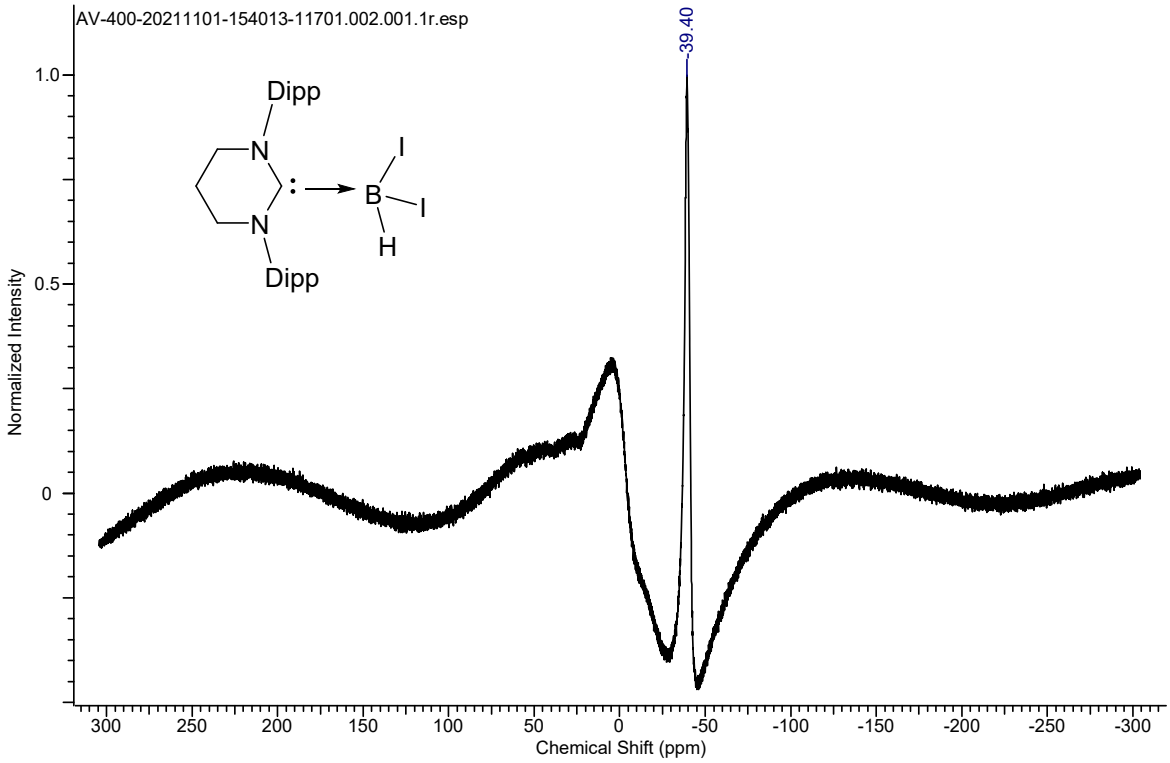

Figure S14. ^{11}B NMR spectrum of **3**.

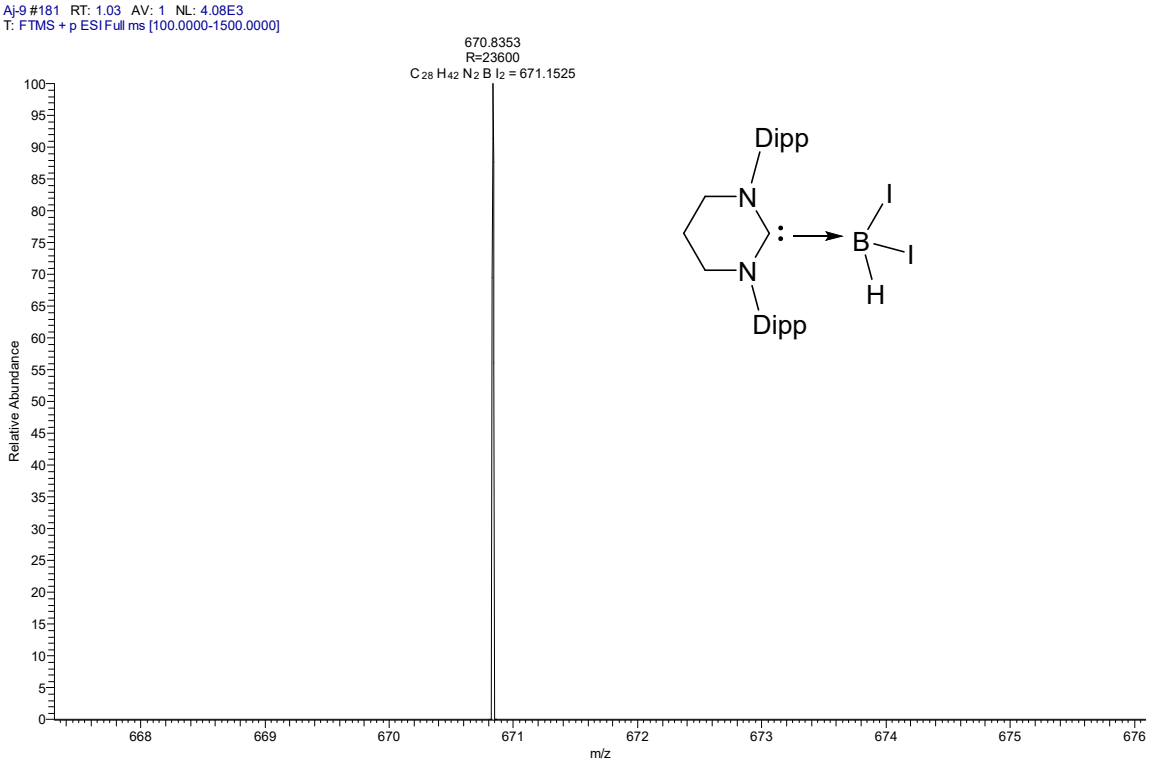

Figure S15. ESI-MS spectrum of **3**.

4: One equivalent of $AgOSO_2CF_3$ (0.10 g, 0.37 mmol) and **2** (0.2 g, 0.37 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 4 h at room temperature. The yellow precipitate of AgI was filtered through frit and the reaction mixture was concentrated. Colorless crystals of **4** were isolated after keeping the solution at room temperature for a day with a yield of 0.12 g (55 %).

$^1H\{^{11}B\}$ NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.31 (d, J = 6.88 Hz, 12H, $CH(CH_3)_2$), 1.36 (d, J = 6.63 Hz, 12H, $CH(CH_3)_2$), 2.34 (quintet, J = 5.50 Hz, 2H, $NCH_2CH_2CH_2N$), 2.37 (bs, 2H, $BH_2OSO_2CF_3$), 2.98 (sept, J = 6.75 Hz, 4H, $CH(CH_3)_2$), 3.56 (t, J = 5.75 Hz, 4H, $NCH_2CH_2CH_2N$), 7.18 (m, 4H, Ar-*H*), 7.35 (t, J = 7.75 Hz, 2H, Ar-*H*) ppm.

$^{13}C\{^1H\}$ NMR (101 MHz, 298 K, $CDCl_3$): δ = 23.6, 26.2, 26.1, 29.0, 51.9, 124.3, 129.1, 140.1, 144.9 ppm.

$^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$): δ = -7.1 (bs, 1B, $BH_2OSO_2CF_3$) ppm.

$^{19}F\{^{1}H\}$ NMR (377 MHz, 298 K, $CDCl_3$): δ = -78.2 (s, 3F, $BH_2OSO_2CF_3$) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{29}H_{42}N_2BF_3SO_3$ $[M+Na]^+$ 579.2839, found 597.2588.

Elemental Analysis: Calcd. C, 61.48; H, 7.47; N, 4.94; found C, 61.32; H, 7.62; N, 4.88.

.

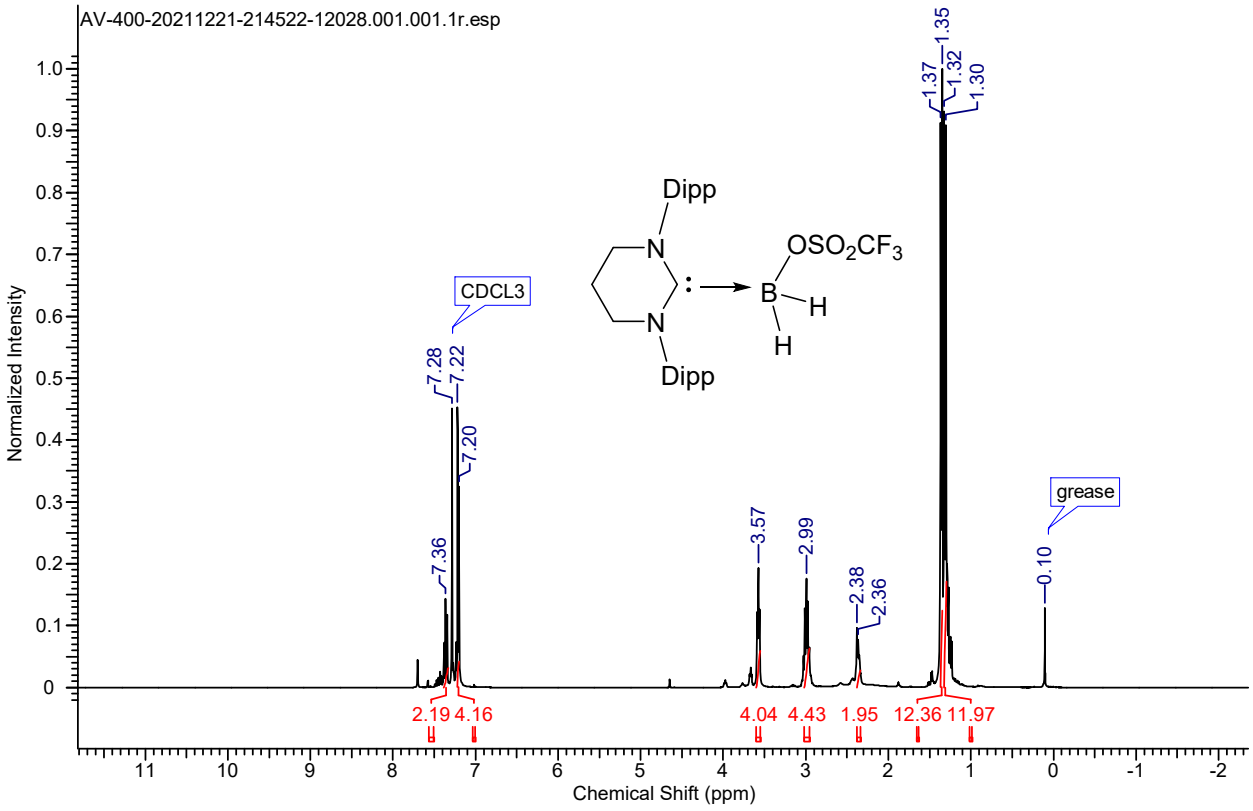

Figure S16. ^{1}H NMR spectrum of **4**.

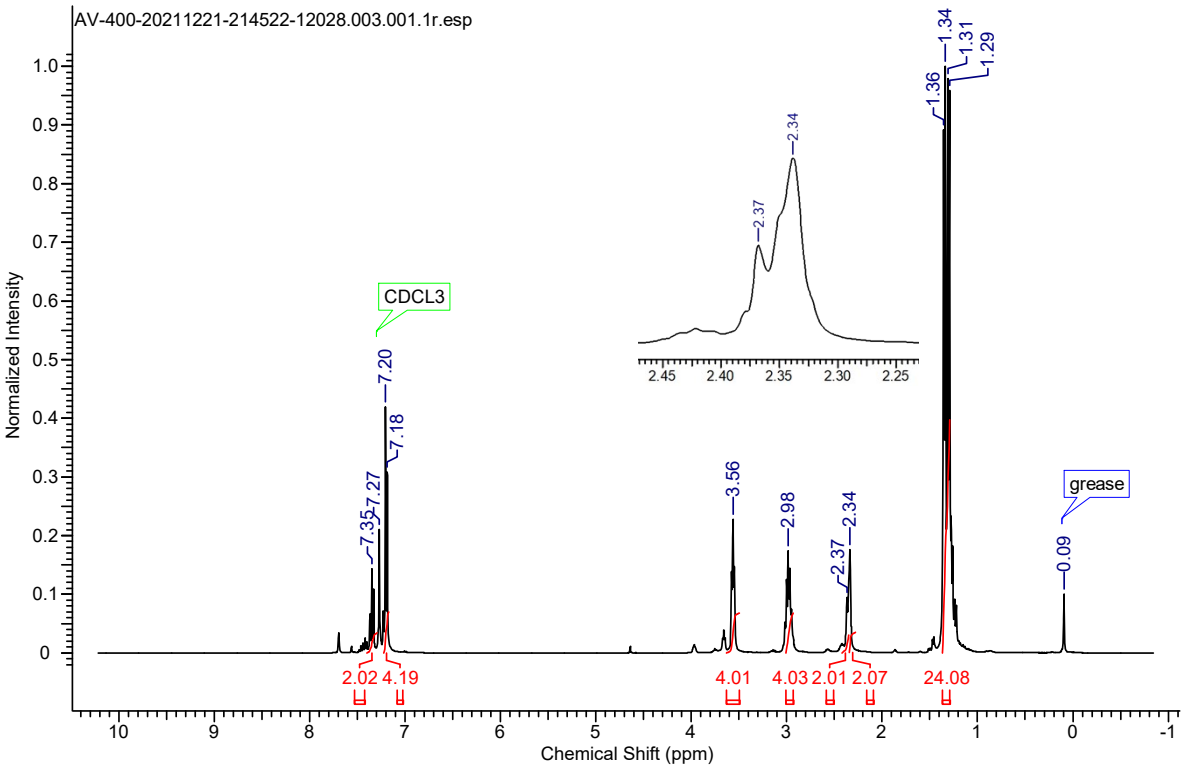

Figure S17. ^{1}H $\{^{11}B\}$ NMR spectrum of **4**.

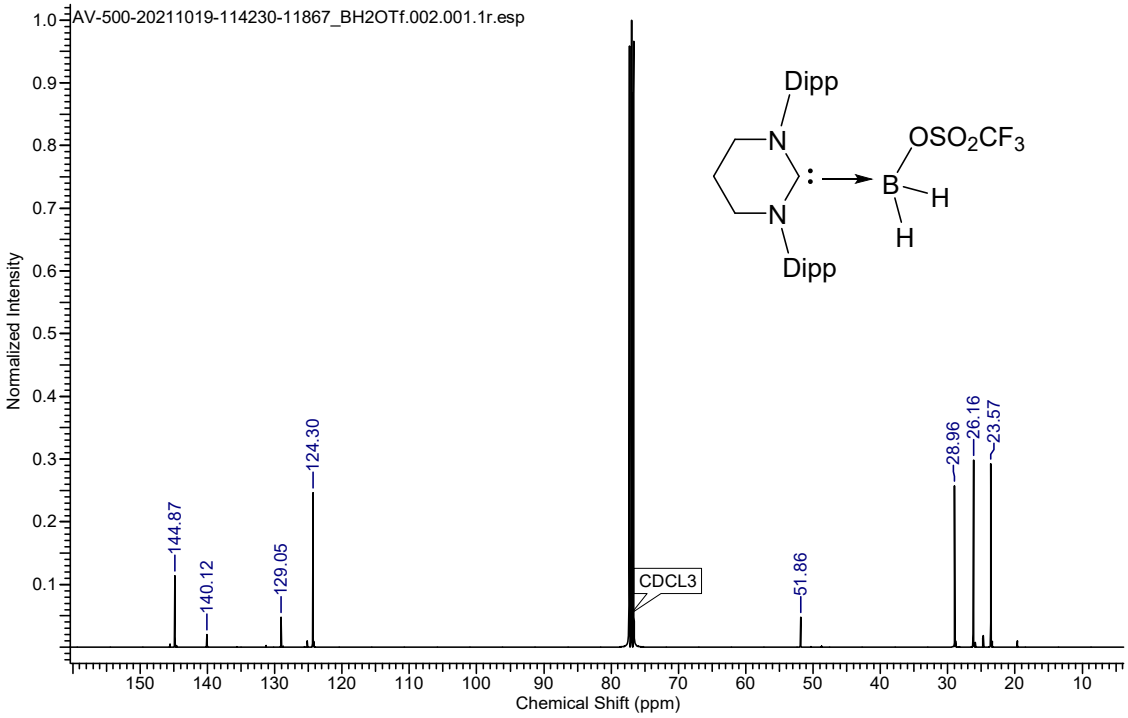

Figure S18. ^{13}C NMR spectrum of **4**.

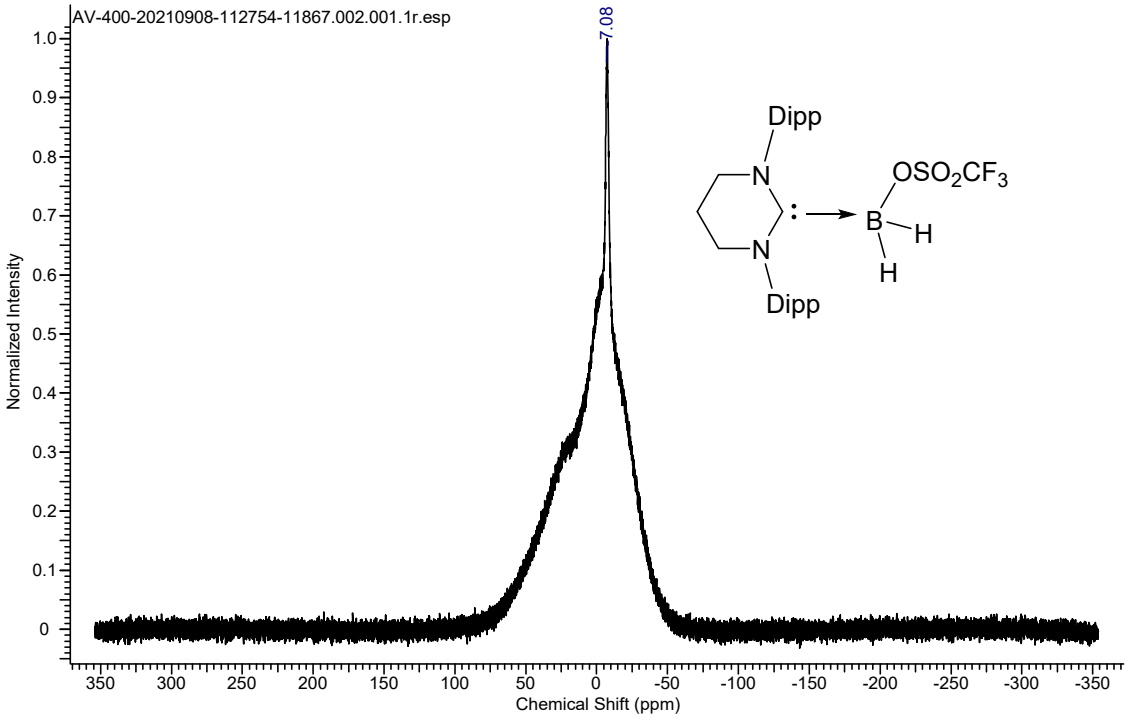

Figure S19. ^{11}B NMR spectrum of **4**.

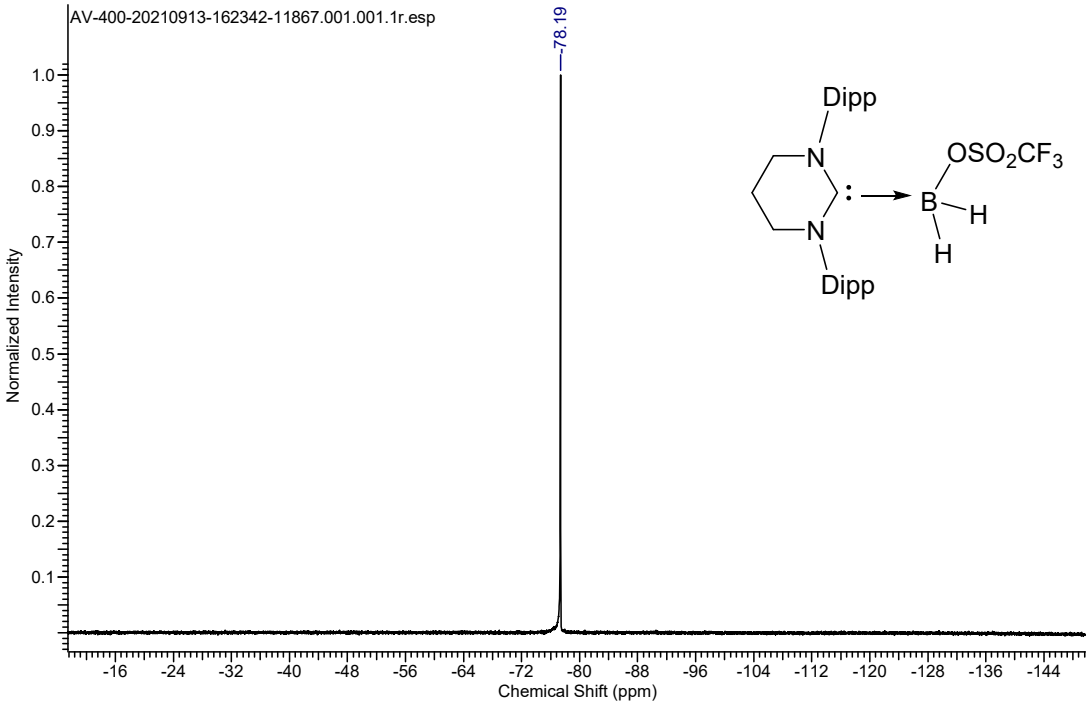

Figure S20. ^{19}F NMR spectrum of **4**.

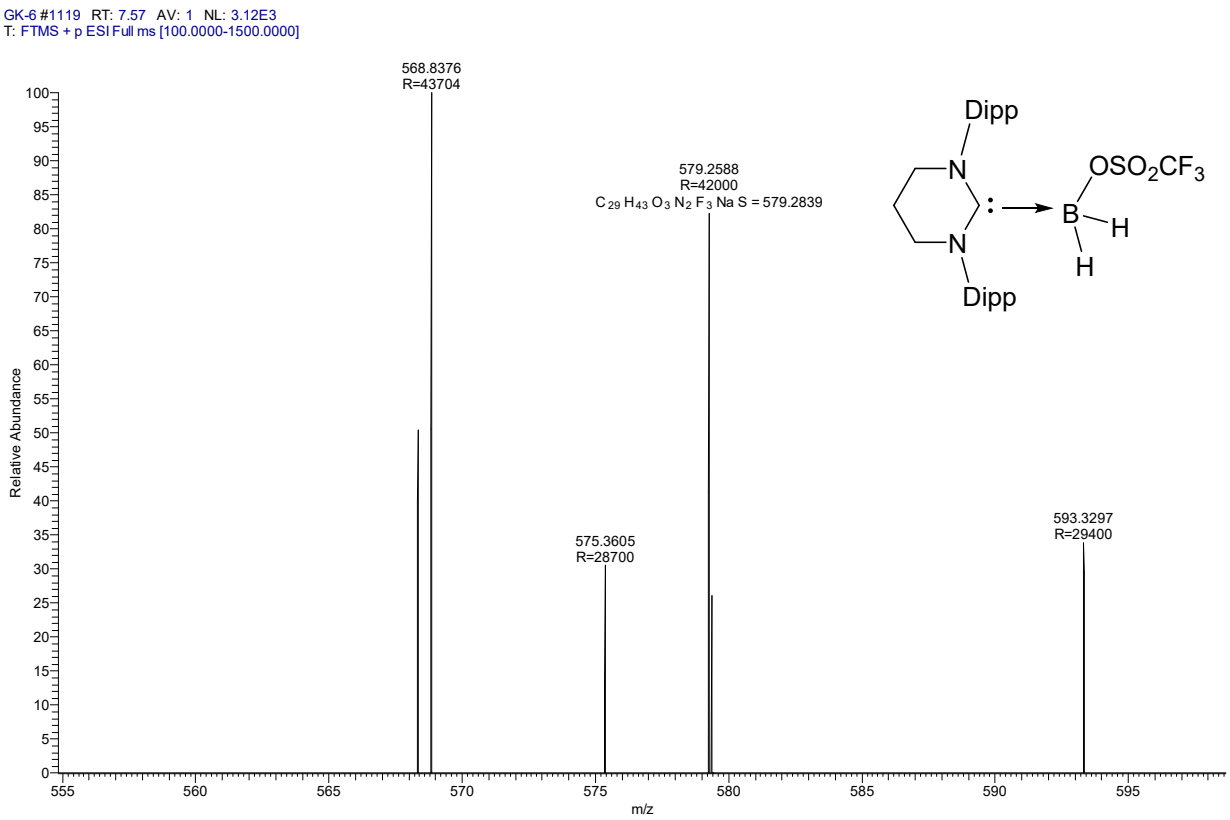

Figure S21. ESI-MS spectrum of **4**.

5: One equivalent of $AgNO_3$ (0.07 g, 0.38 mmol) and **2** (0.2 g, 0.37 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 4 h at room temperature. The yellow precipitate of AgI was filtered through frit and the reaction mixture was concentrated. Colorless crystals of **5** were isolated after keeping the solution at room temperature for a day with a yield of 0.085 g (48 %).

$^{1}H\{^{11}B\}$ NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.28 (d, J = 6.88 Hz, 12H, $CH(CH_3)_2$), 1.38 (d, J = 6.75 Hz, 12H, $CH(CH_3)_2$)), 2.32 (s, 2H, BH_2ONO_2), 2.37 (m, 2H, $NCH_2CH_2CH_2N$), 3.04 (sept, J = 6.88 Hz, 4H, $CH(CH_3)_2$), 3.59 (t, J = 5.88 Hz, 4H, $NCH_2CH_2CH_2N$), 7.19 (m, 4H, Ar-*H*), 7.33 (t, J = 7.75 Hz, 2H, Ar-*H*) ppm.

$^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$): δ = 19.8, 23.2, 25.9, 28.9, 50.2, 124.3, 125.2, 129.0, 139.9, 144.4 ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{42}N_2BN_3O_3$ $[M+Na]^+$ 507.3375, found 507.3315.

Elemental Analysis: Calcd. C, 70.14; H, 8.83; N, 8.76; found C, 70.24; H, 8.79; N, 8.71.

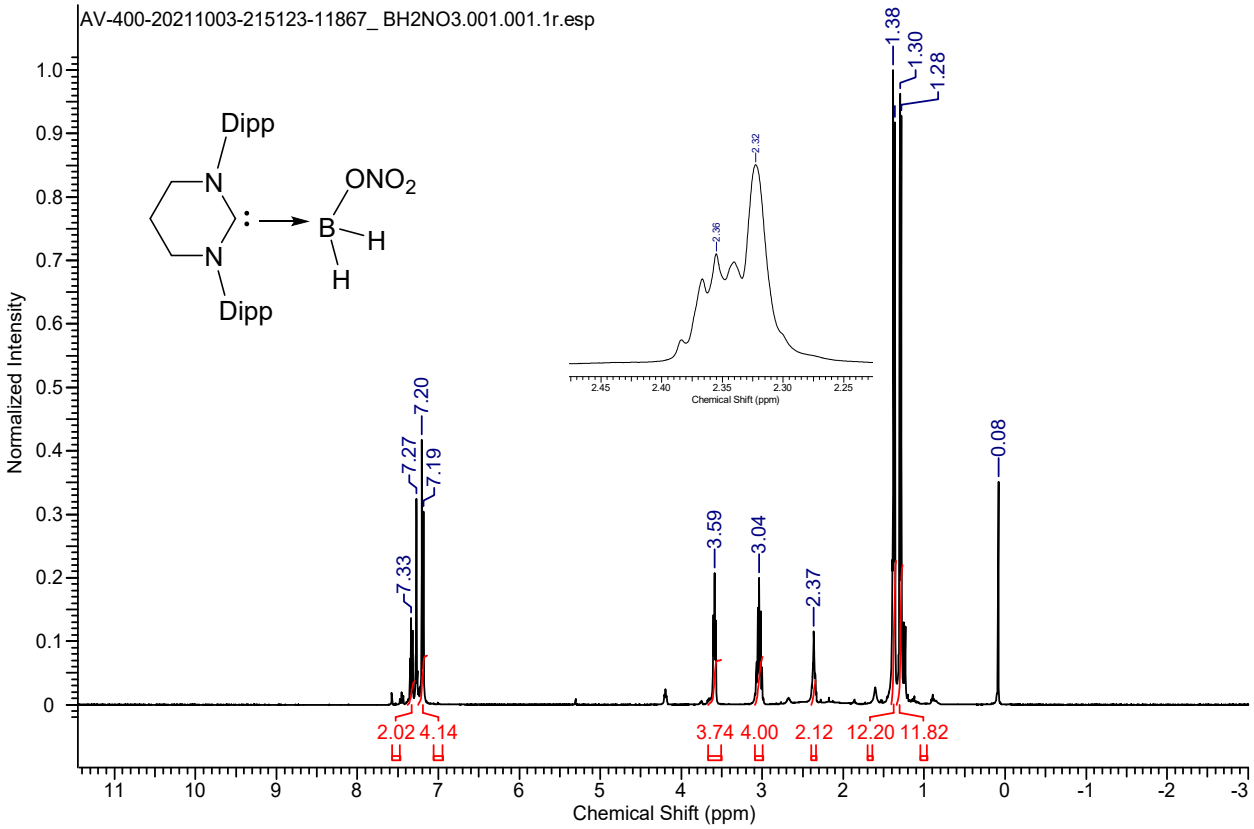

Figure S22. ^1H $\{^{11}B\}$ NMR spectrum of **5**.

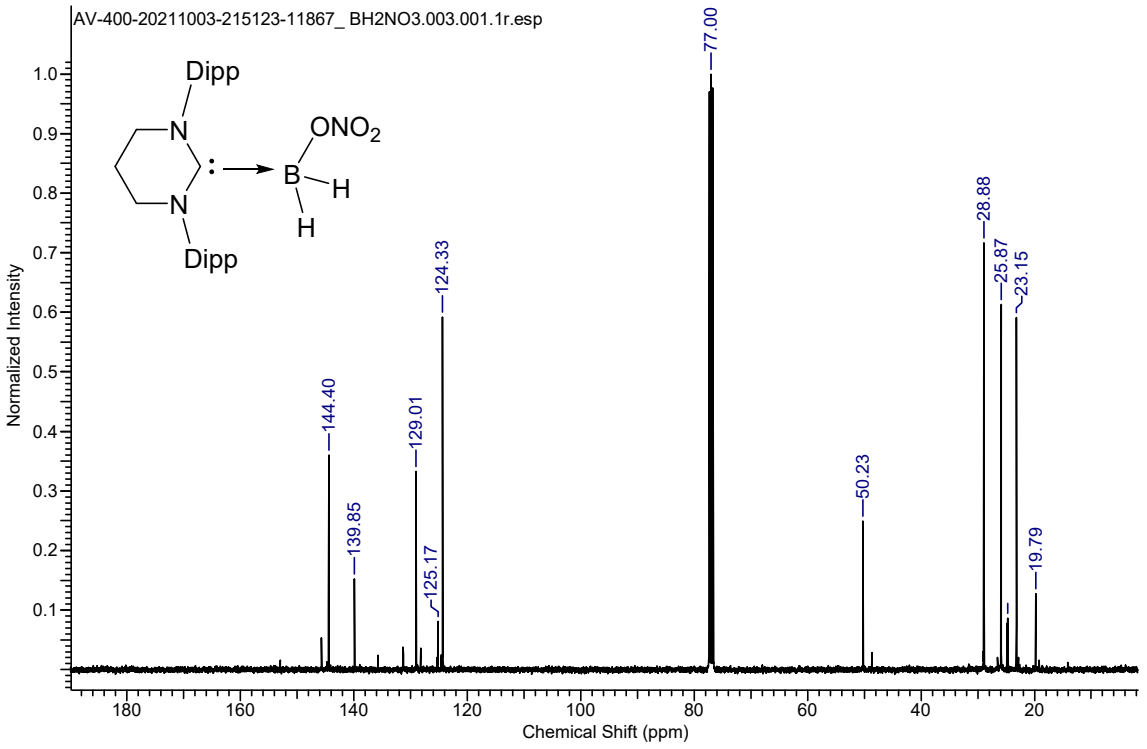

Figure S123. ^{13}C NMR spectrum of **5**.

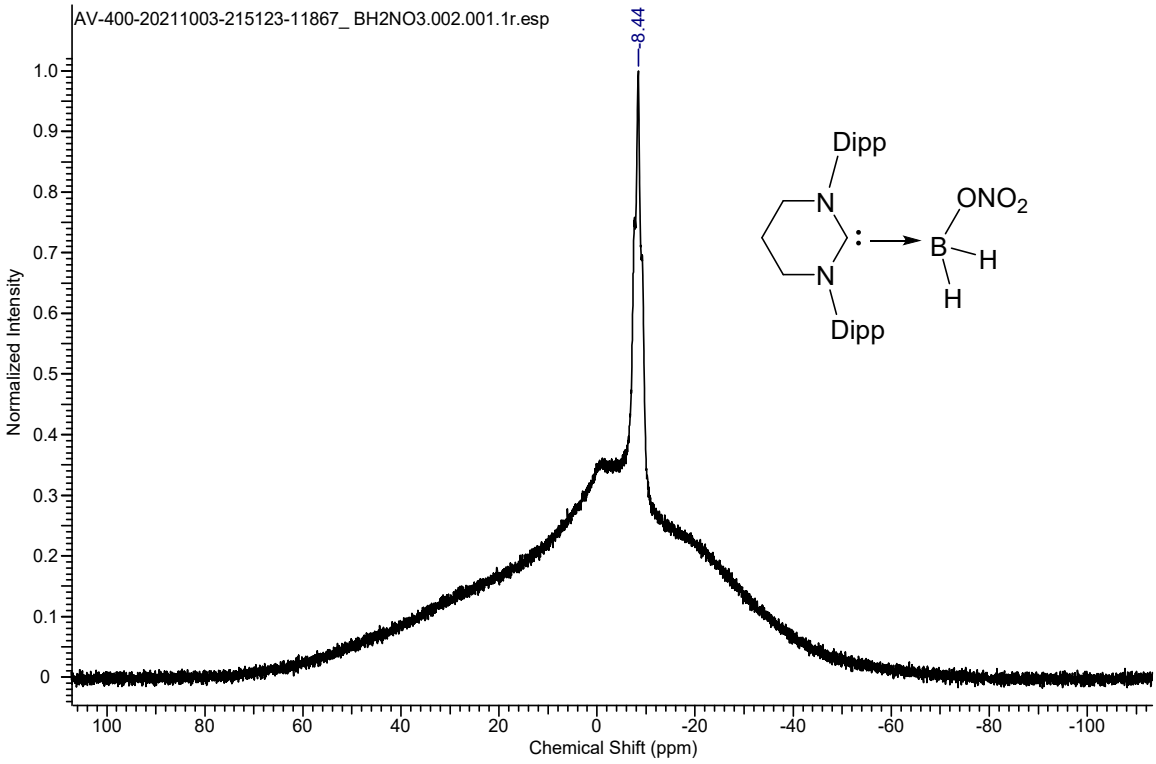

Figure S24. ^{11}B NMR spectrum of **5**.

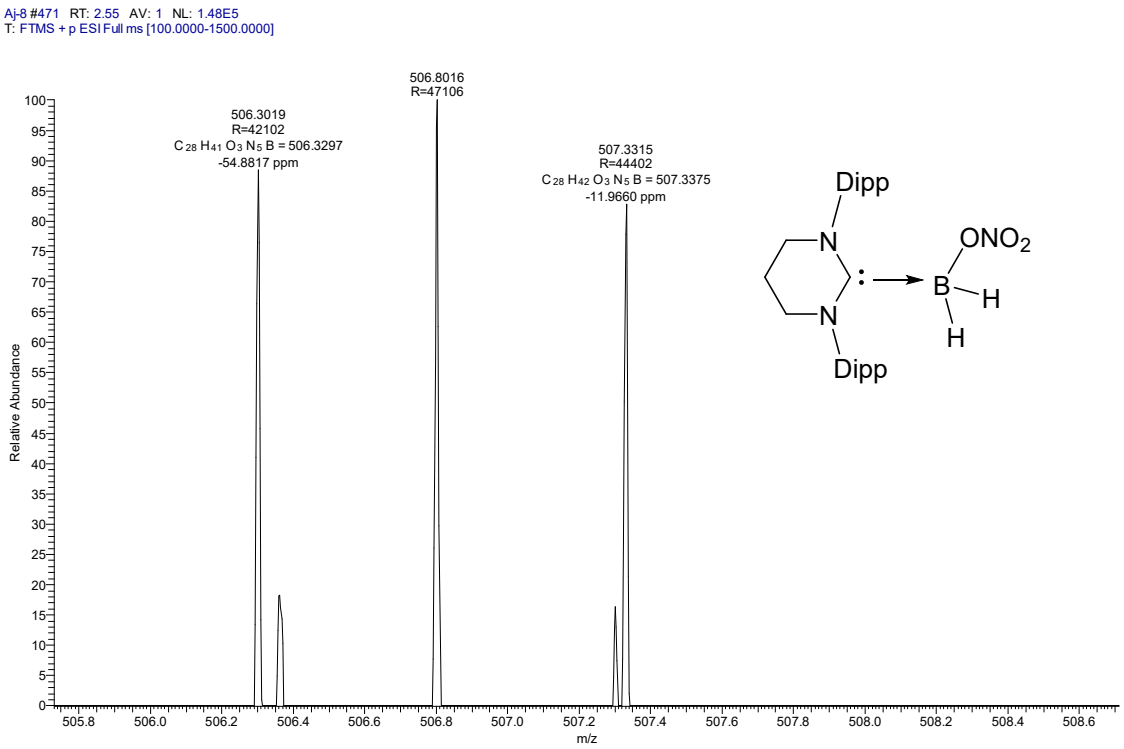

Figure S25. ESI-MS spectrum of **5**.

6: Two equivalents of $AgOSO_2CF_3$ (0.23 g, 0.90 mmol) and **3** (0.3 g, 0.45 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 4 h at room temperature. The yellow precipitate of AgI was filtered through frit and the reaction mixture was concentrated. Colorless crystals of **6** were isolated after keeping the solution at -36 ˚C temperature for 3 days with a yield of 0.17 g (54 %).

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.28 (d, J = 6.88 Hz, 12H, $CH(CH_3)_2$), 1.31 (d, J = 6.63 Hz, 12H, $CH(CH_3)_2$), 2.34 (s, 1H, $BH(OSO_2CF_3)_2$), 2.46 (quintet, J = 5.25 Hz, 2H, $NCH_2CH_2CH_2N$), 2.96 (sept, J = 6.75 Hz, 4H, $CH(CH_3)_2$), 3.68 (t, J = 5.75 Hz, 4H, $NCH_2CH_2CH_2N$), 7.20 (m, 4H, Ar-*H*), 7.42 (t, J = 7.75 Hz, 2H, Ar-*H*) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 22.4, 26.3, 29.1, 48.2, 124.9, 130.1, 136.0, 146.1 ppm.

^{11}B{^{1}H} NMR (128 MHz, 298 K, $CDCl_3$): δ = -3.24 (bs, 1B, $BH(OSO_2CF_3)_2$) ppm.

$^{19}F\{^{1}H\}$ NMR (377 MHz, 298 K, $CDCl_3$): δ = -78.9 (s, 2*3F, $BH(OSO_2CF_3)_2$) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{30}H_{41}N_2BF_6S_2O_6$ $[M+Na]^+$ 715.2476, found 715.2108.

Elemental Analysis: Calcd. C, 50.42; H, 5.78; N, 3.92; found C, 50.32; H, 5.65; N, 3.88.

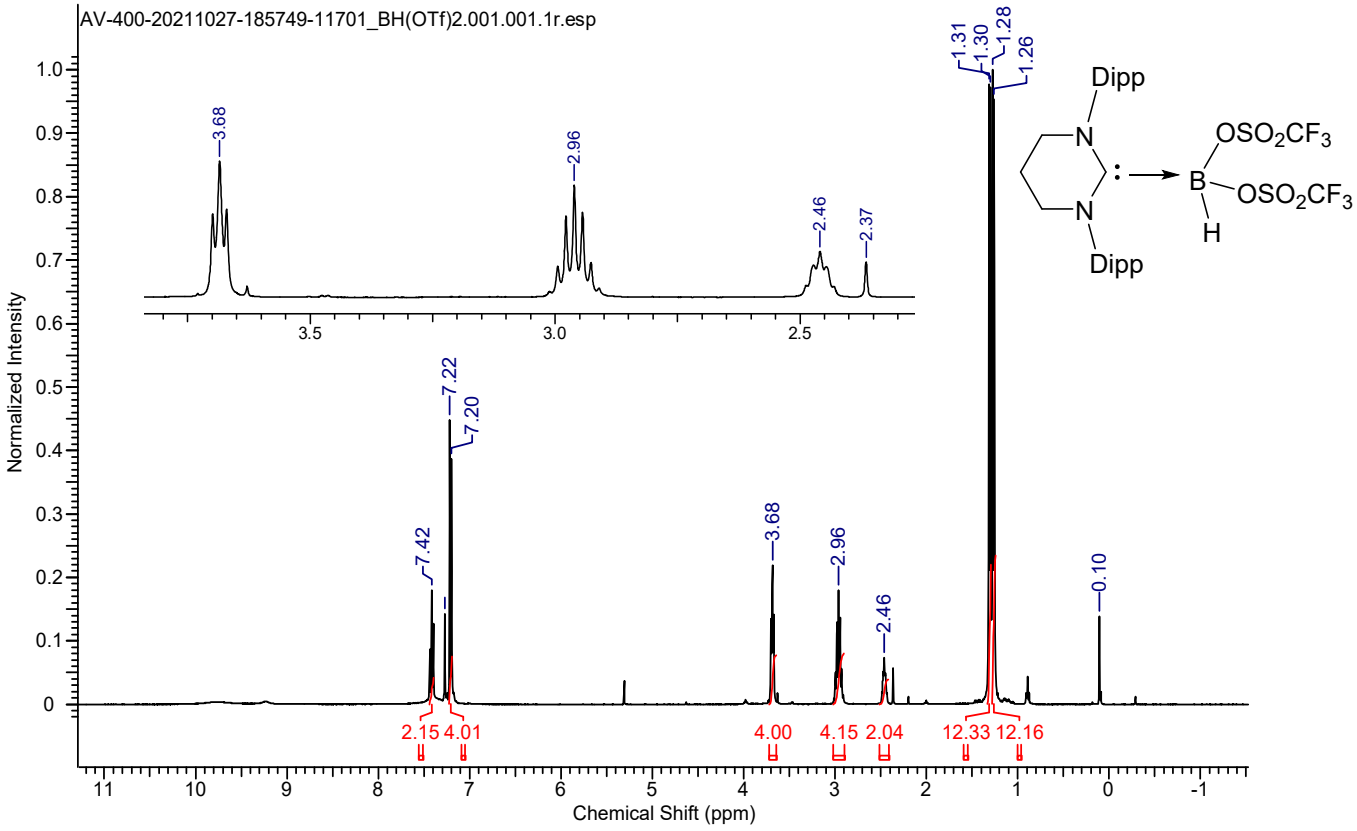

Figure S26.^{1}H $\{^{11}B\}$ NMR spectrum of **6**.

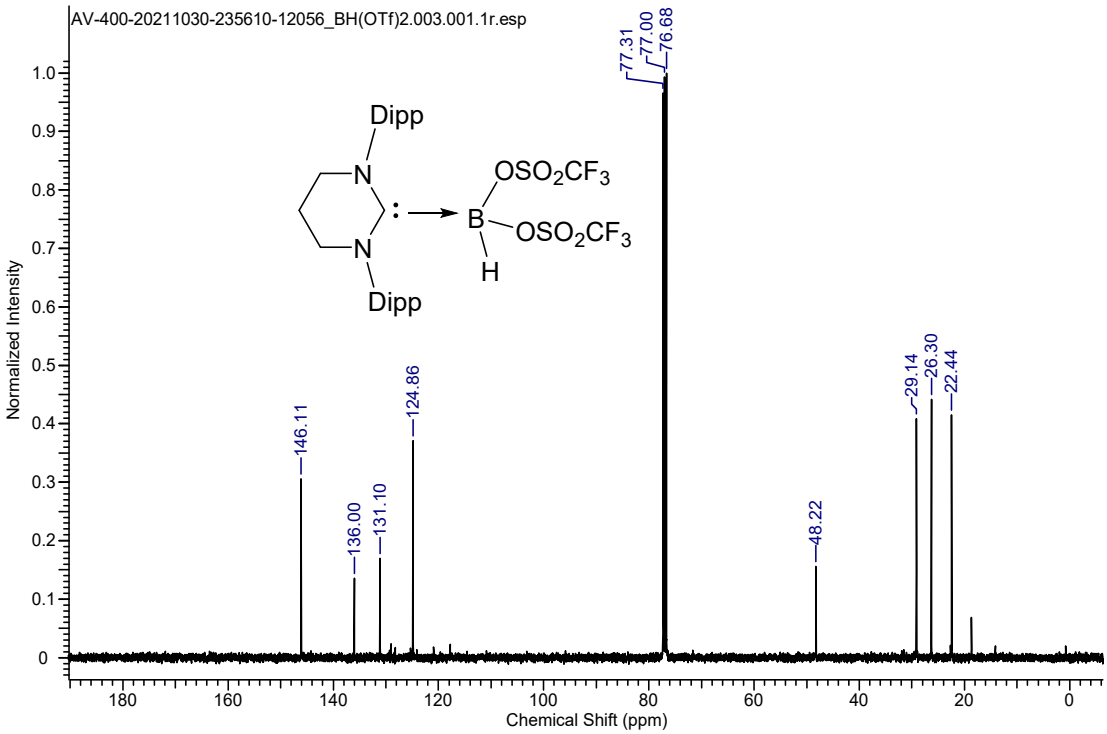

Figure S27.[13]C NMR spectrum of **6**.

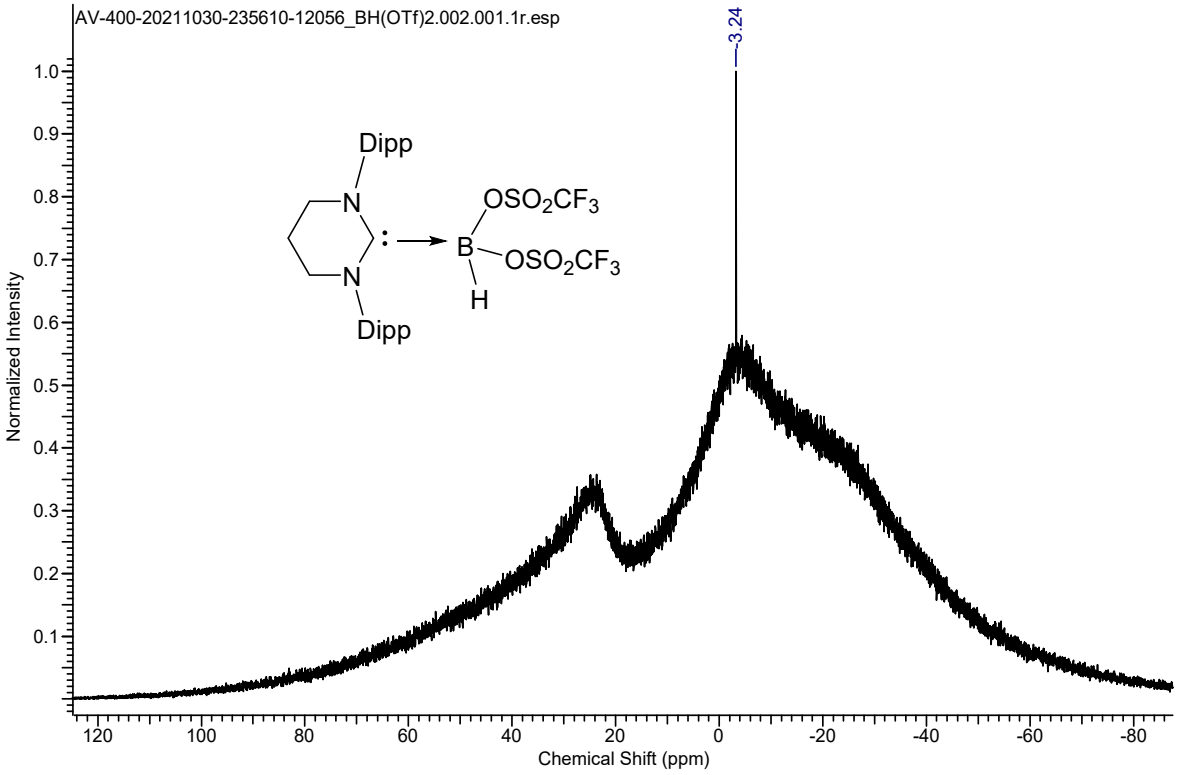

Figure S28. [11]B NMR spectrum of **6**.

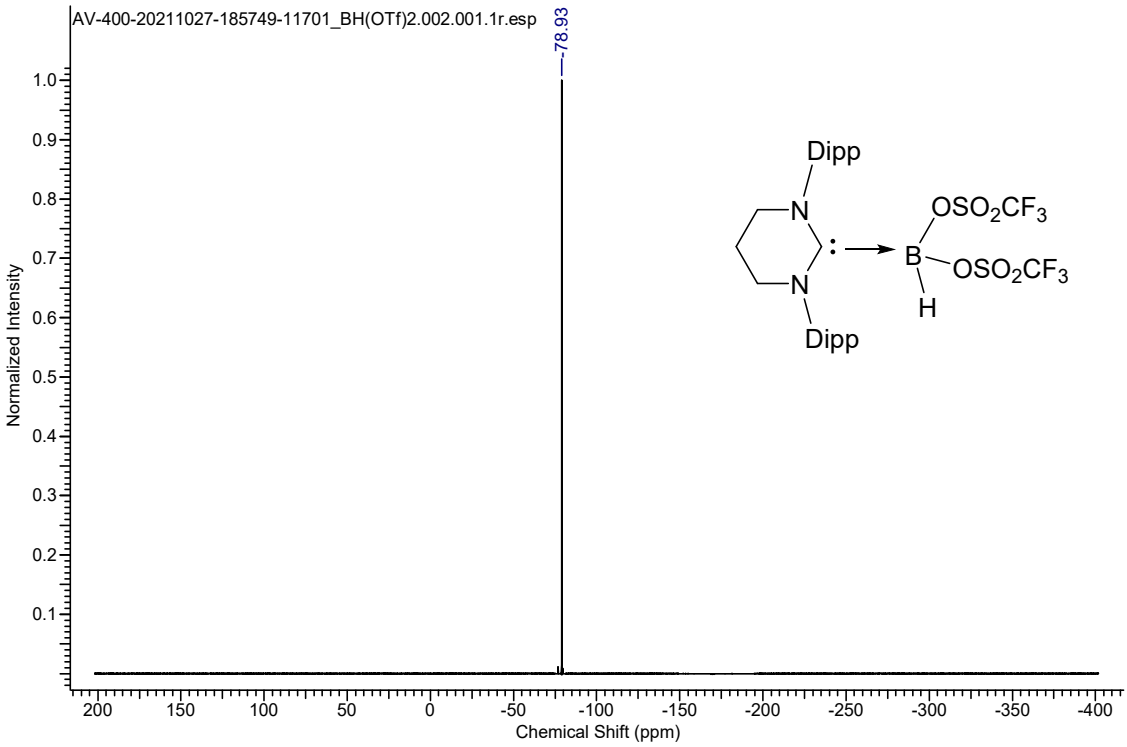

Figure S29.[19]F NMR spectrum of **6**.

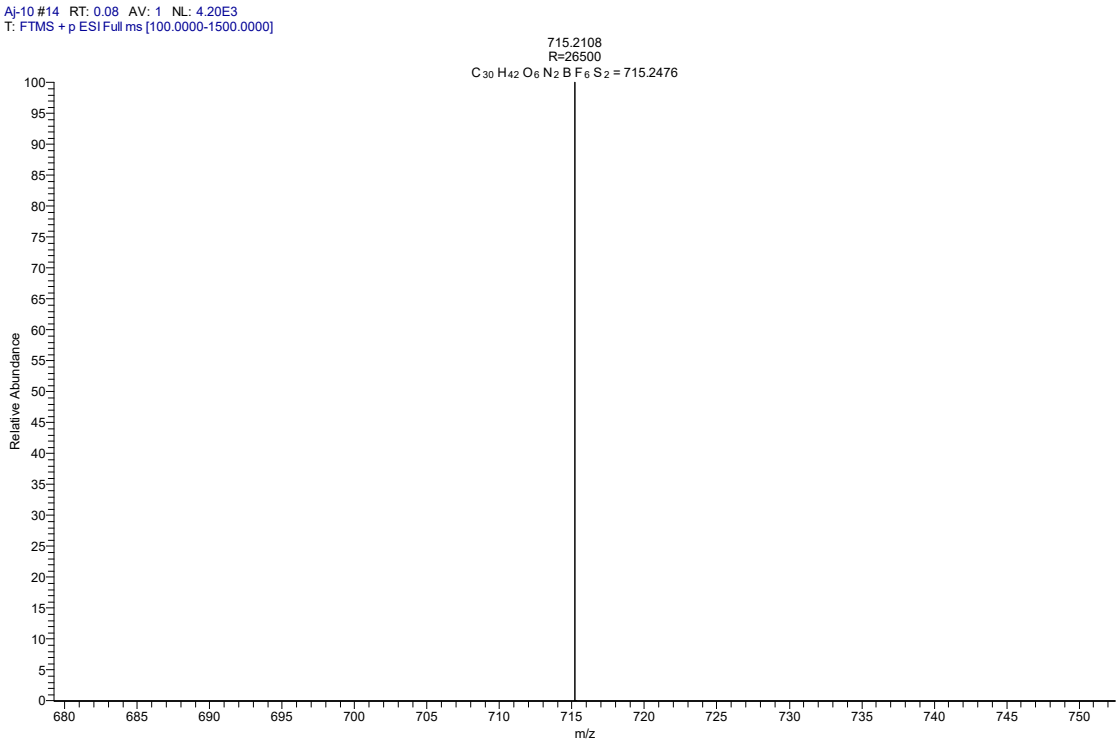

Figure S30. ESI-MS spectrum of **6**.

7: Two equivalents of $AgNO_3$ (0.152 g, 0.90 mmol) and **3** (0.3 g, 0.45 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 12 h at room temperature. The yellow precipitate of AgI was filtered through frit and the reaction mixture was concentrated. Colorless crystals of **7** were isolated after keeping the solution at 4 ˚C temperature for a day with a yield of 0.11 g (46 %).

$^{1}H\{^{11}B\}$NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.27 (d, J = 6.88 Hz, 12H, $CH(CH_3)_2$), 1.39 (d, J = 6.75 Hz, 12H, $CH(CH_3)_2$), 2.37, (s, 1H, $BH(NO_3)_2$), 2.39 (m, 2 H, $NCH_2CH_2CH_2N$), 3.06 (sept, J = 6.88 Hz, 4H, $CH(CH_3)_2$), 3.67 (t, J = 5.75 Hz, 4H, $NCH_2CH_2CH_2N$), 7.23 (m, 4H, Ar-*H*), 7.38 (t, J = 7.75 Hz, 2 H, Ar-*H*) ppm.

$^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$): δ = 14.1, 22.6, 26.5, 29.0, 31.6, 51.3, 124.4, 124.6, 129.7, 144.7 ppm.

$^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$): δ = -0.98 (bd, 1B, $BH(NO_3)_2$ ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{41}N_4BO_6$ [M] 540.3114, found 540.3331.

Elemental Analysis: Calcd. C, 62.23; H, 7.65; N, 10.37; found C, 60.24; H, 7.29; N, 9.89.

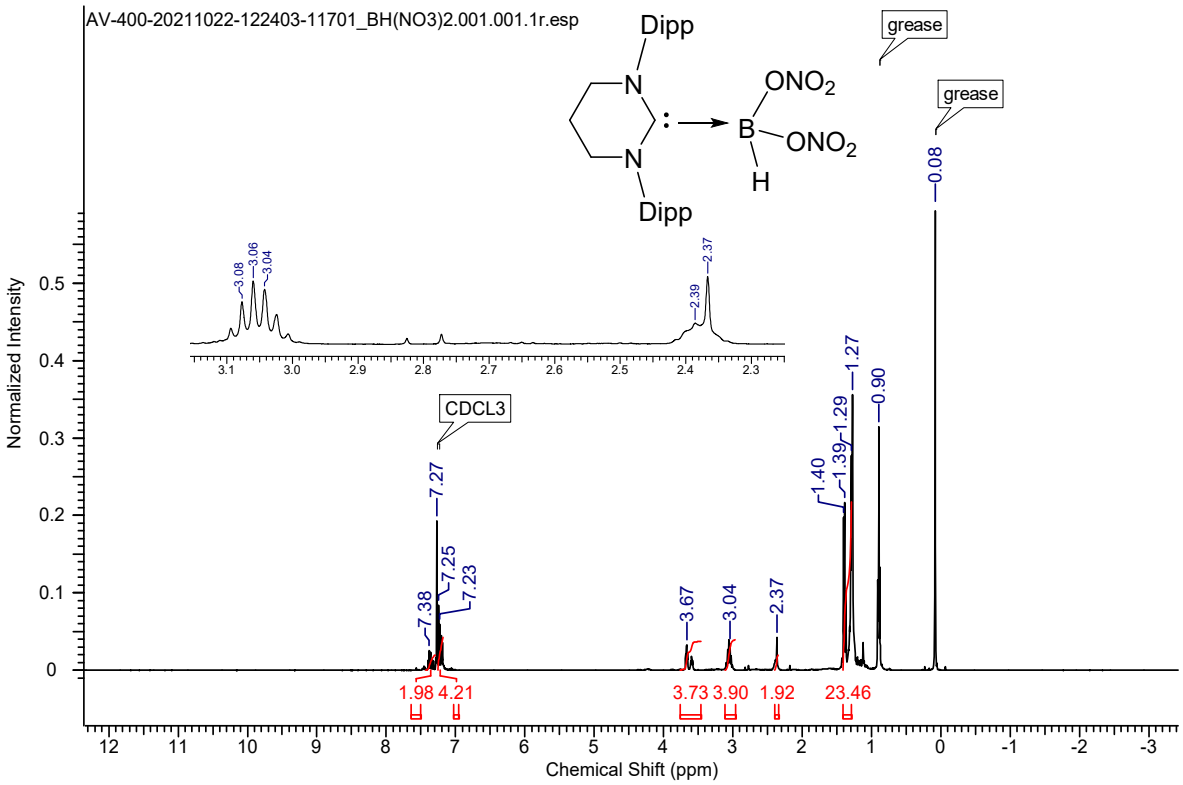

Figure S31.$^{1}H\{^{11}B\}$ NMR spectrum of **7**.

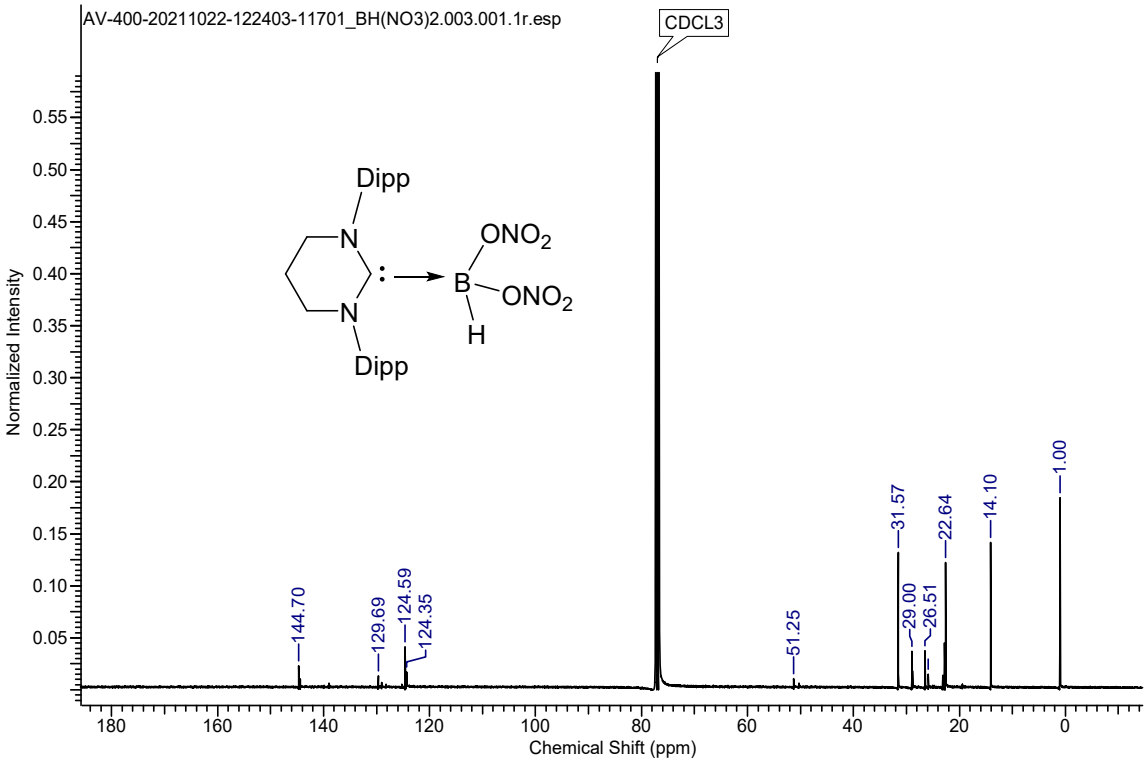

Figure S32. ^{13}C NMR spectrum of **7**.

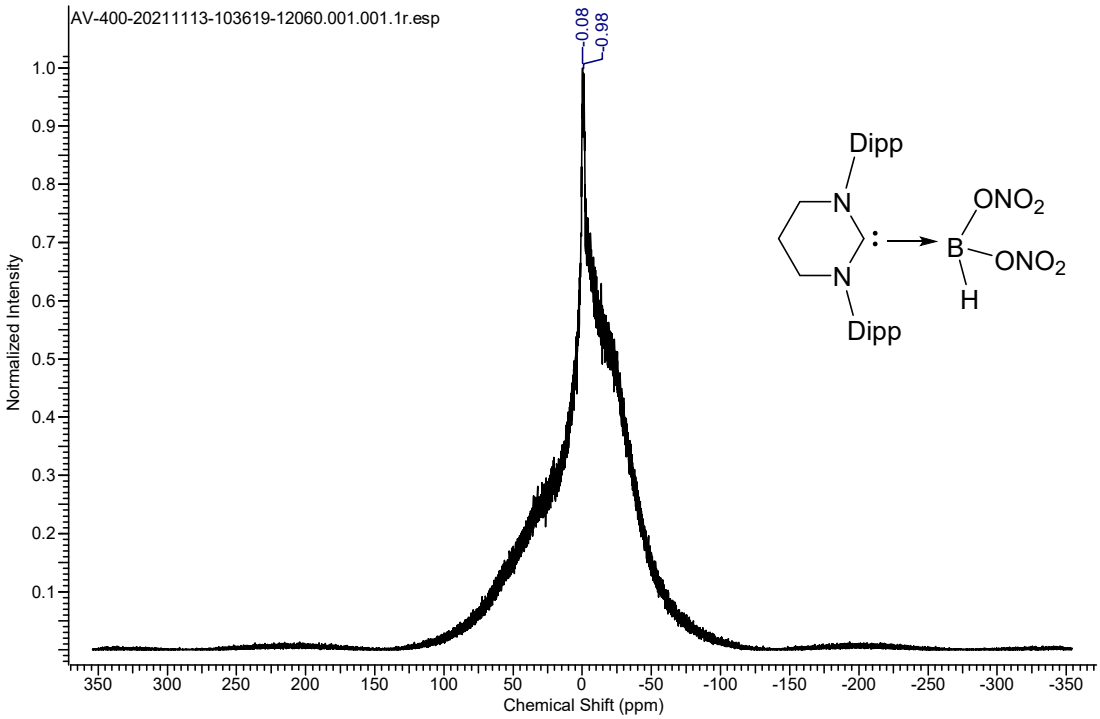

Figure S33.[11]B NMR spectrum of **7**.

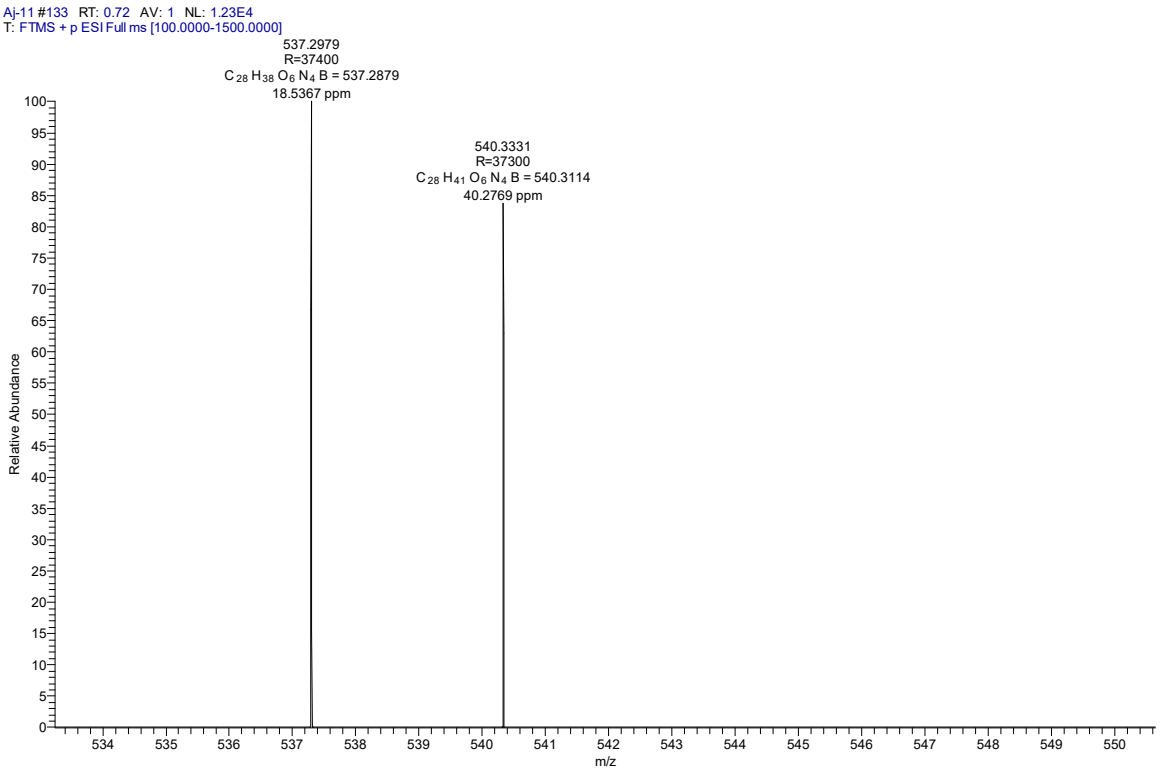

Figure S34. ESI-MS spectrum of **7**.

8 and **9**: 1.2 equivalent of bromine-water (Br_2/H_2O) (0.05 uL, 0.58 mmol) was added to the toluene solution (5 ml) of **1** (0.2 g, 0.48 mmol) at low temperature. The reaction was run for 3 h at room temperature. The toluene solution was concentrated and filtered through cannula. Colorless crystals of **8** were isolated after keeping the solution at 4 ˚C for a day with a yield of 0.14 g (55%). The remaining solution was again further kept for recrystallization and colorless crystal of **9** were isolated with 7% (16 mg) yield.

Analytical data for **8**:

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.26 (d, J = 5.88 Hz, 12H, CH(CH_3)$_2$), 1.32 (d, J = 6.38 Hz, 12 H, CH(CH_3)$_2$), 2.48 (bs, 2H, NCH$_2$CH_2CH$_2$N), 2.95 (sept, J = 5.88 Hz, 4H, CH(CH$_3$)$_2$), 3.71 (bs, 4H, NCH_2CH$_2$CH_2N), 4.50 (s, 2H, B-(OH)$_2$), 7.19 (m, 4H, Ar-H), 7.38 (t, J = 7.58 Hz, 2H, Ar-H) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 19.2, 22.9, 26.8, 29.3, 33.8, 49.1, 125.1, 129.0, 129.2, 131.3, 136.3, 137.9, 146.3 ppm.

^{11}B{^{1}H} NMR (127 MHz, 298 K, $CDCl_3$): δ = 25.4 (bs, 1B, B(OH)$_2$) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $C_{28}H_{42}BO_2N_2$ [M+H]$^+$ 449.3334, found 449.3254.

Elemental Analysis: Calcd. C, 63.53; H, 8.00; N, 5.29; found C, 63.42; H, 8.31; N, 5.38.

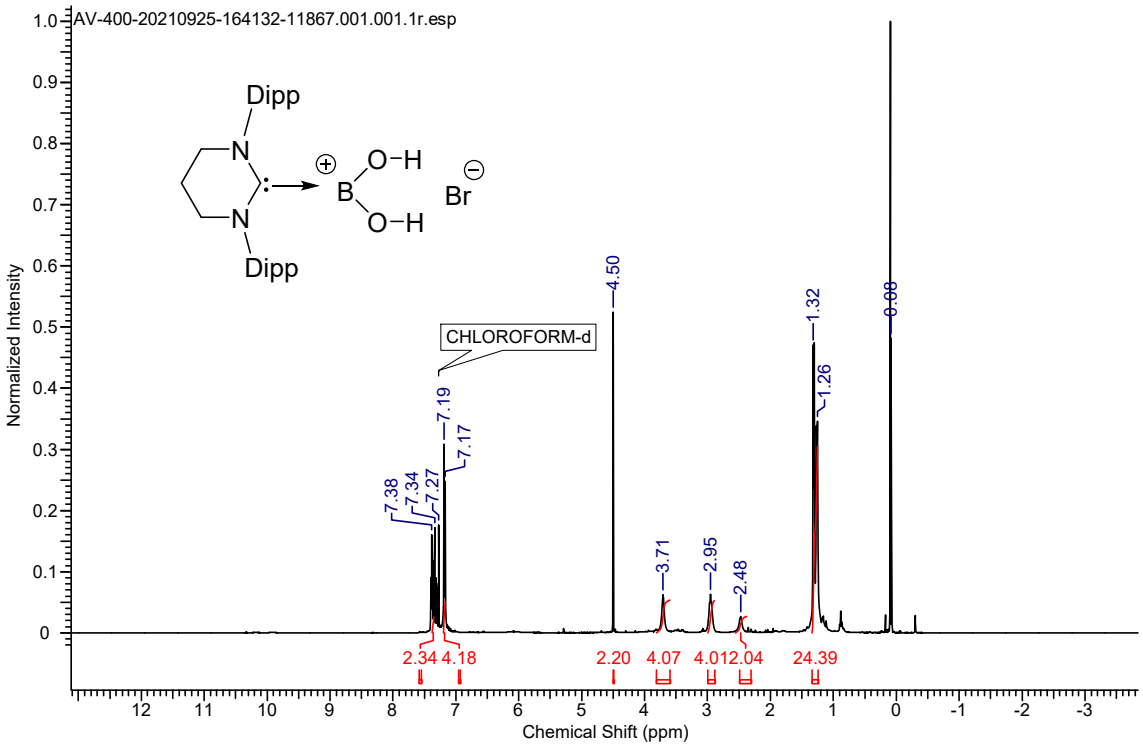

Figure S35. $^{1}H\{^{11}B\}$ NMR spectrum of **8**.

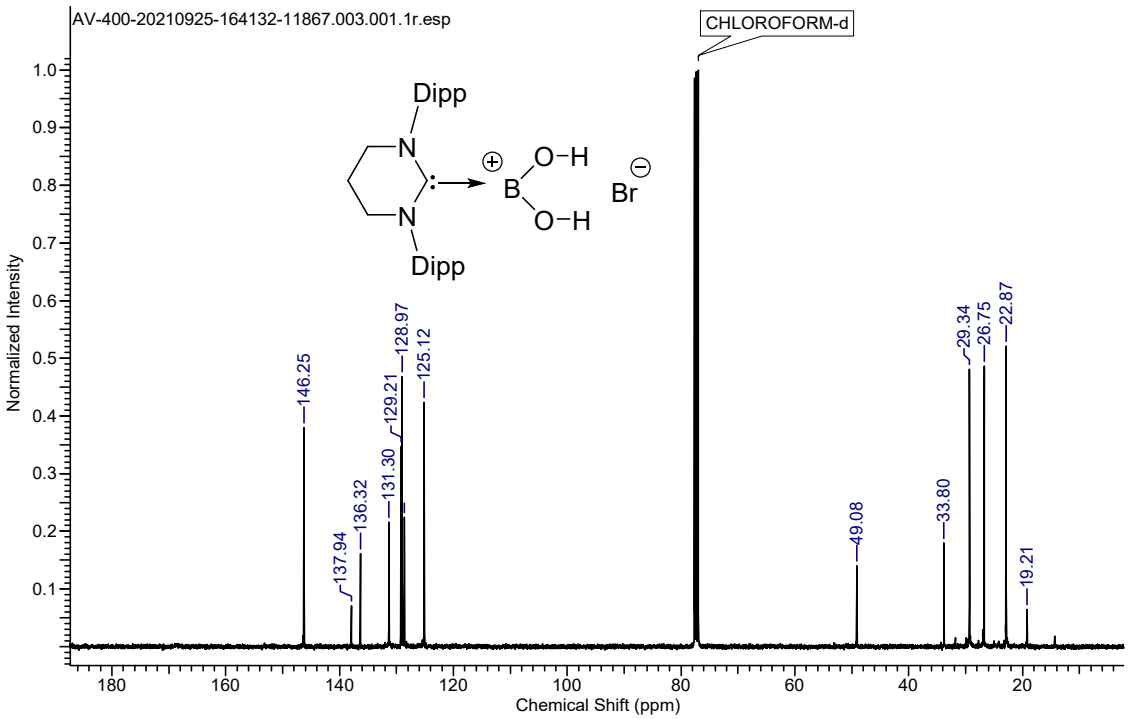

Figure S36. ^{13}C NMR spectrum of **8**.

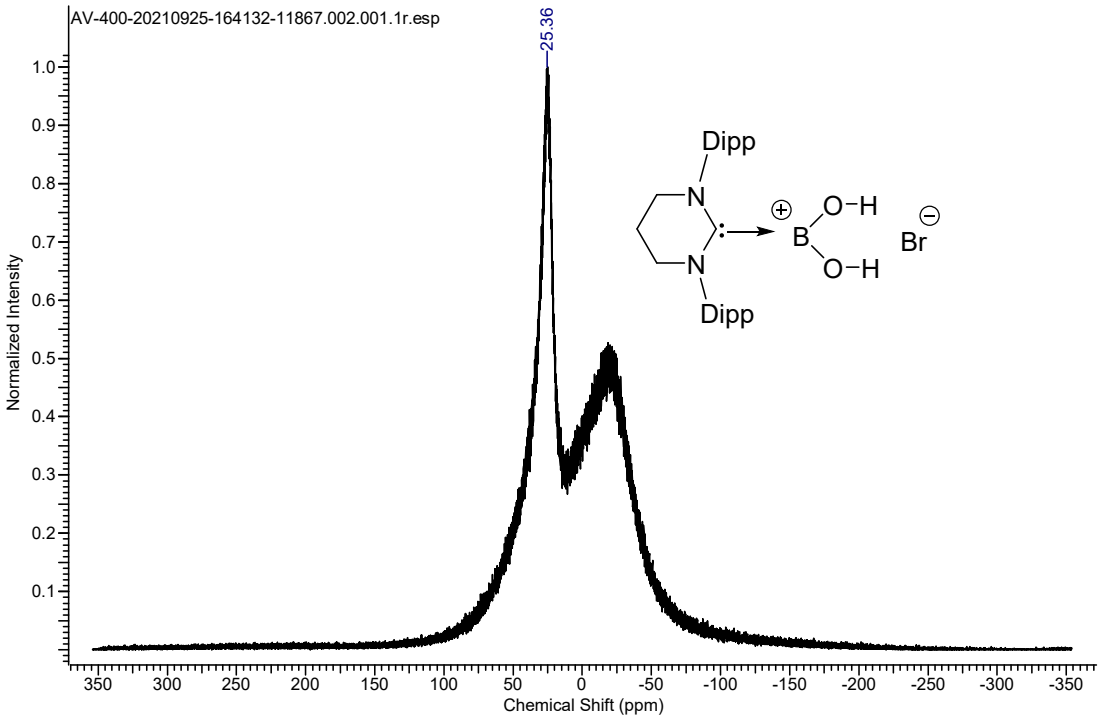

Figure S37. ^{11}B NMR spectrum of **8**.

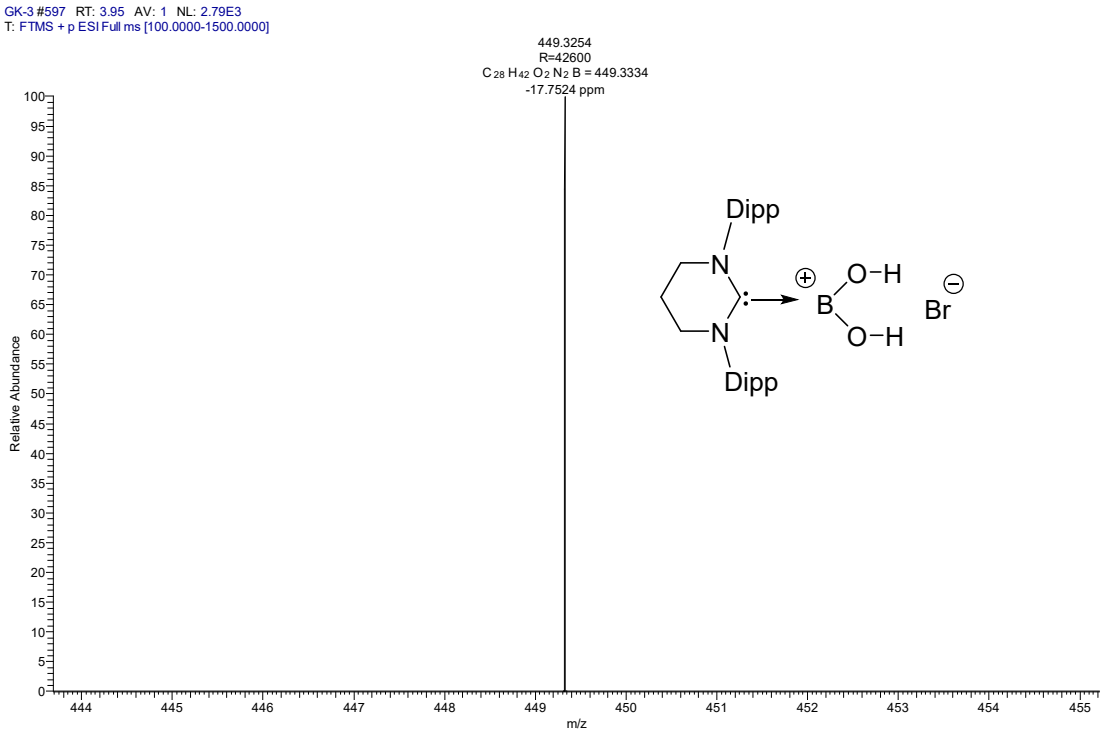

Figure S38. HRMS spectrum of **8**.

Analytical data for **9**:

^{1}H {^{11}B}NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.27 (d, J = 6.85 Hz, 12H, $CH(CH_3)_2$), 1.42 (d, J = 6.72 Hz, 12H, $CH(CH_3)_2$), 2.36 (quintet, J = 4.75 Hz, 2H, $NCH_2CH_2CH_2N$), 3.16 (sept, J = 6.75 Hz, 4H, $CH(CH_3)_2$), 3.63 (t, J = 5.62 Hz, 4H, $NCH_2CH_2CH_2N$), 7.19 (m, 4H, Ar-*H*), 7.34 (t, J = 7.5, 2H, Ar-*H*) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 19.6, 23.5, 26.1, 28.9, 51.9, 124.2, 125.1, 129.0, 131.2, 140.1, 144.8 ppm.

^{11}B{^{1}H} NMR (127 MHz, 298 K, $CDCl_3$): δ = -5.2 (s, 1B, $B(OH)_3$) ppm.

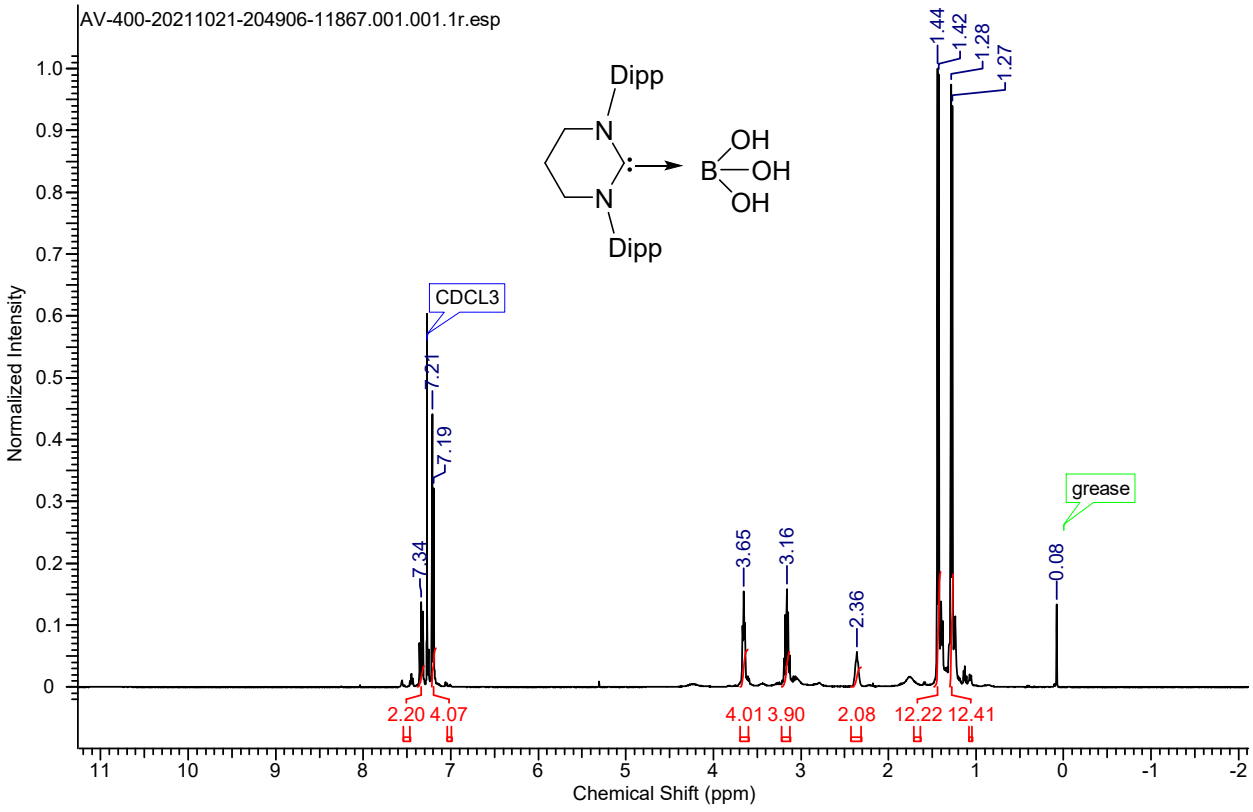

Figure S39. ^{1}H{^{11}B} NMR spectrum of **9**.

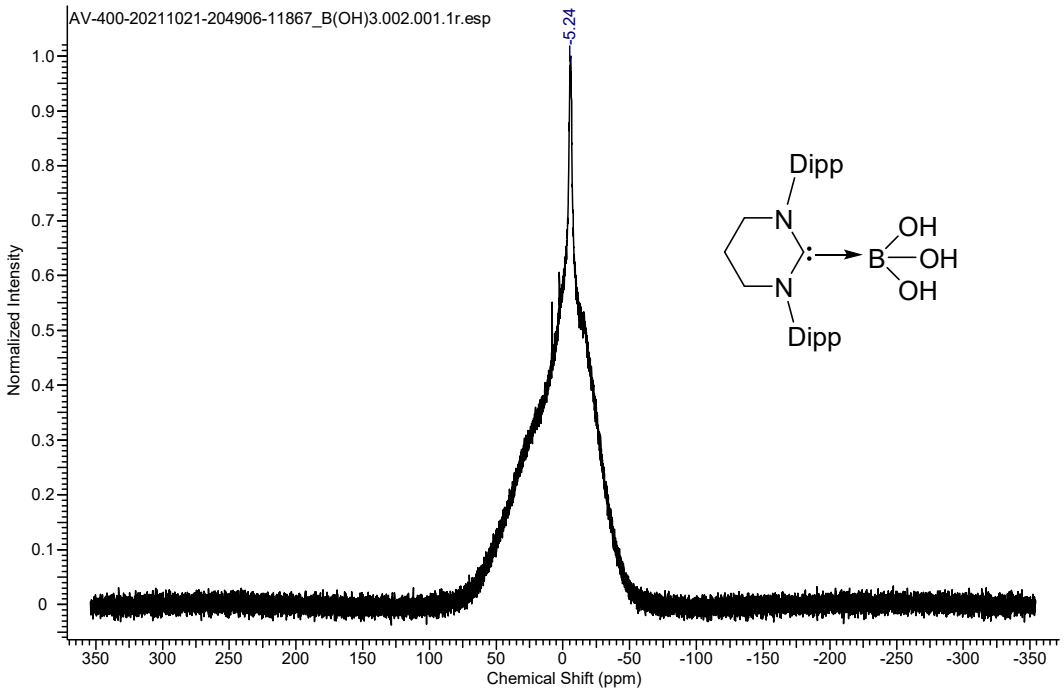

Figure S40. ^{11}B NMR spectrum of **9**.

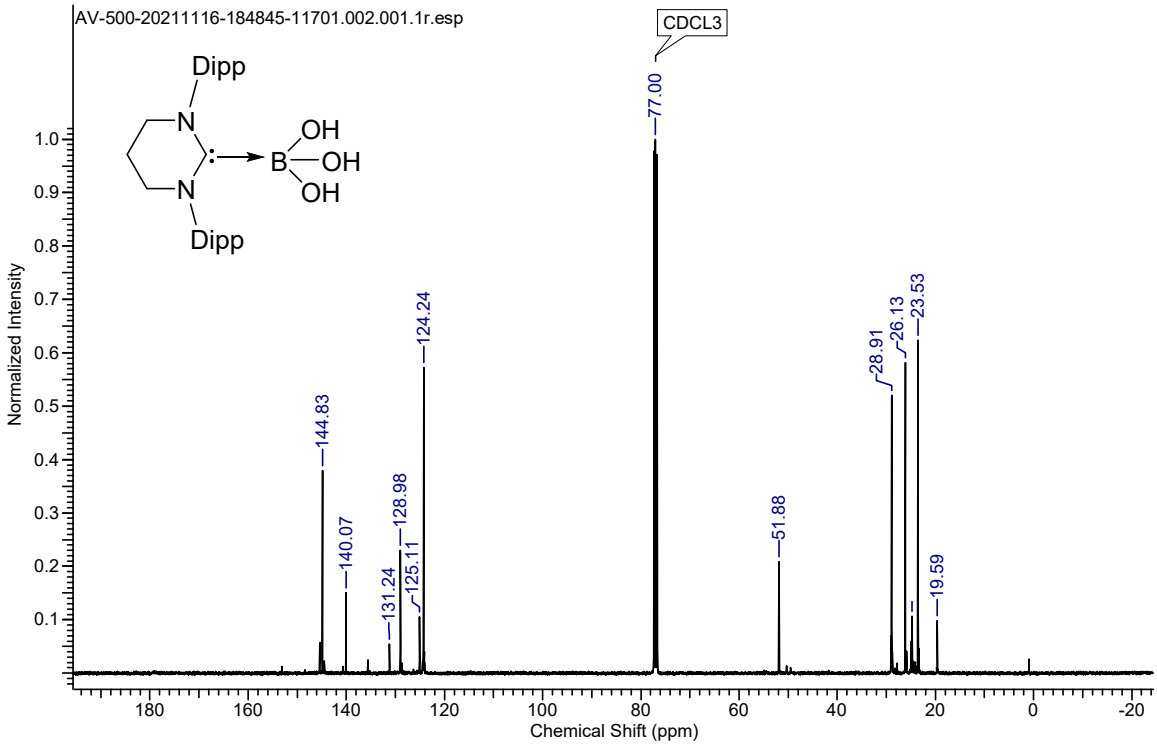

Figure S41. ^{13}C NMR spectrum of **9**.

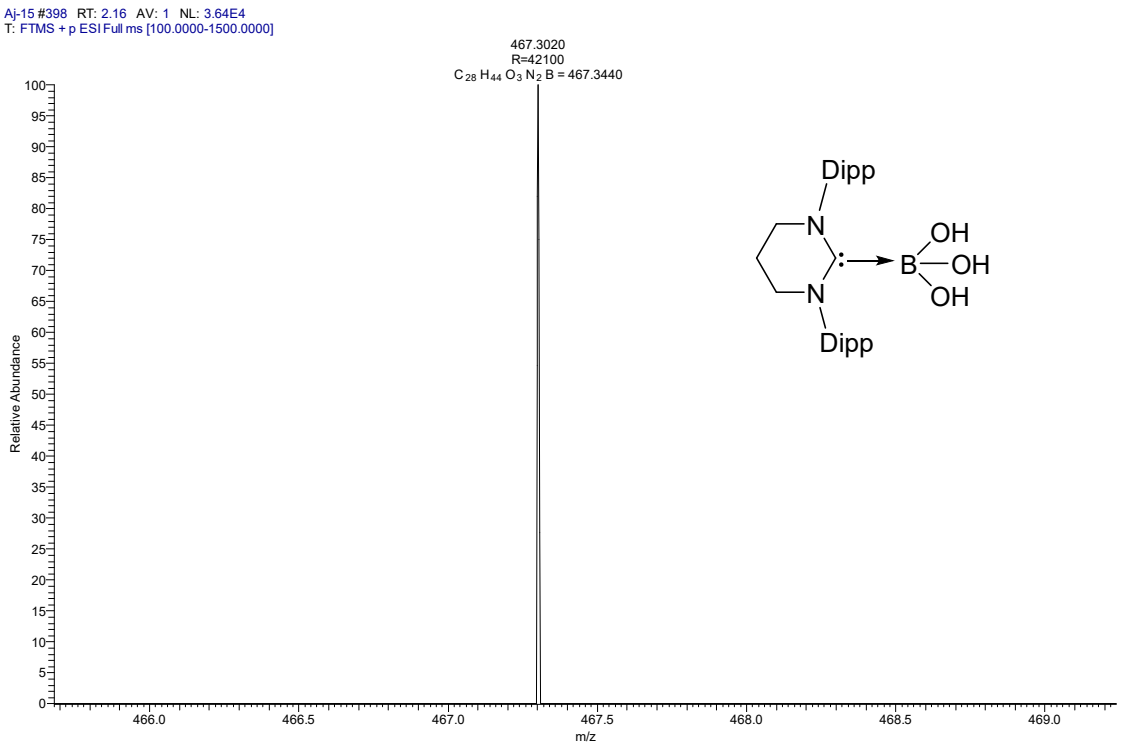

Figure S42. ESI-MS spectrum of **9**.

S3 Synthetic procedure and spectroscopic characterization of 5-IDipp·BH_3 reactivity with 1 and 1.2 equivalent of iodine

With 1 equivalent of iodine: 1 equivalent of Iodine (I_2) (0.13 g, 0.50 mmol) and IPr-BH_3 (0.2 g, 0.50 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 1 h at room temperature. The toluene solution was concentrated and filtered through cannula. Yellow mixture crystals of **6** were isolated after keeping the solution at 4 ˚C for a day. From the NMR It can be said that in case of IDipp carbene double iodination is not selective. It gives all the three iodine substituted products (IDipp-BH_2I, IDipp-BHI_2, IDipp-BI_3); which can be clearly seen from the ^1H and ^{11}B NMRs.

$^1H\{^{11}B\}$ NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.13 (d, J = 6.85 Hz, 12 H, $CH(CH_3)_2$), 1.14 (d, 12 H, J = 6.85 Hz, $CH(CH_3)_2$), 1.24 (d, J = 6.85 Hz, 12 H, $CH(CH_3)_2$), 1.30 (d, J= 6.72 Hz, 12 H,

CH(CH_3)$_2$), 1.35 (d, J = 6.72 Hz, 12 H, CH(CH_3)$_2$), 1.41 (d, J = 6.60 Hz, 12 H, CH(CH_3)$_2$), 2.42 (sept, J = 6.85 Hz, 4 H, CH(CH$_3$)$_2$), 2.60 (sept, J = 6.72 Hz, 4 H, CH(CH$_3$)$_2$), 2.69 (sept, J = 6.85 Hz, 4 H, NCH_2CH$_2$CH_2N), 7.15- 7.60 (m, *Ar-H*) 7.13 (s, 2 H, CH=CH), 7.92 (s, 2 H, CH=CH), 9.35 (s, 2 H, CH=CH) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, CDCl$_3$): δ = 19.18, 22.66, 23.29, 24.12, 25.82, 28.17, 28.61, 47.79, 53.42, 124.11, 126.09, 128.65, 131.20, 134.87, 141.09, 143.49, 143.85, 144.87 ppm.

^{11}B{^{1}H} NMR (127 MHz, 298 K, CDCl$_3$): δ = -33.4 (bs, 1B, BH$_2$I), -44.2 (bs, 1B, BHI$_2$), 19.7 (bs, 1B, BI$_3$) ppm.

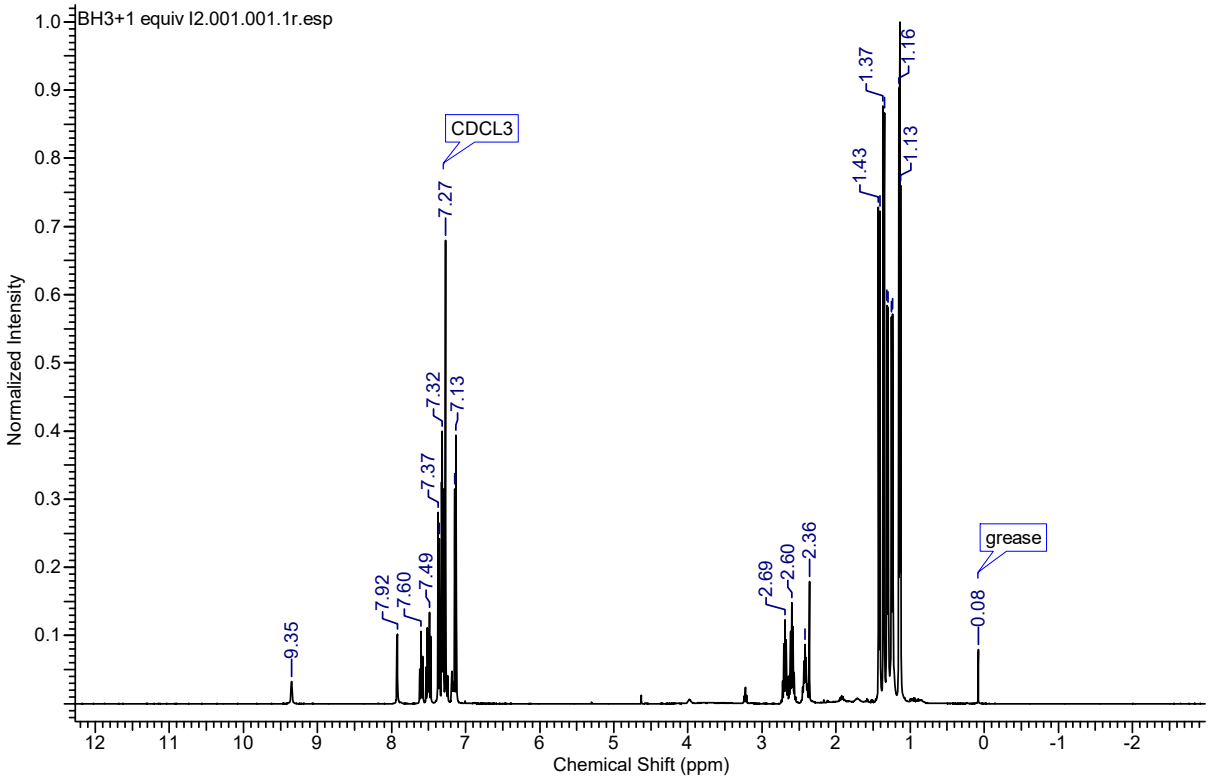

Figure S43. ^{1}H{^{11}B} NMR spectrum.

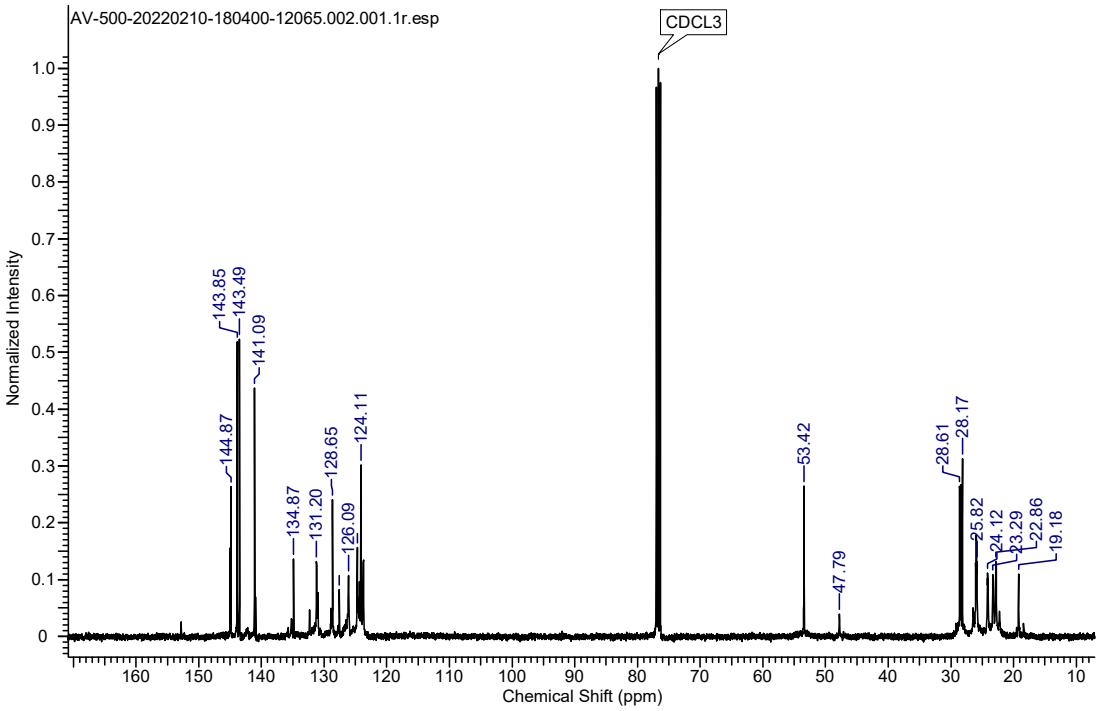

Figure S44. ^{13}C NMR spectrum.

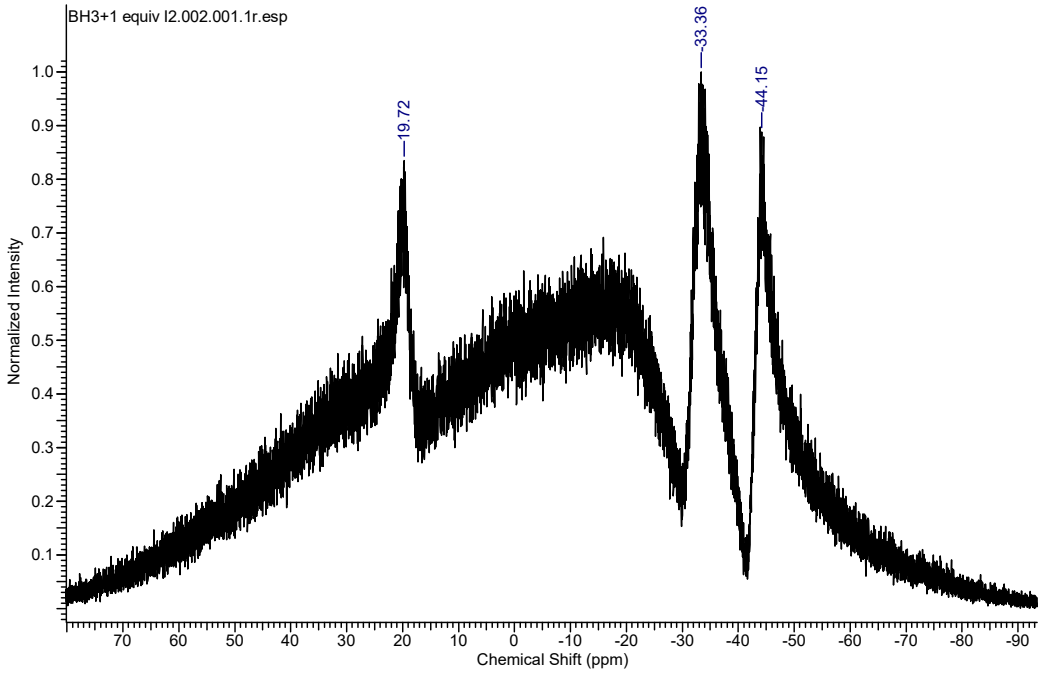

Figure S45. ^{11}B NMR spectrum.

With 1.2 equivalent of iodine: 1.2 equivalent of Iodine (I_2) (0.150 g, 0.60 mmol) and IPr-BH_3 (0.2 g, 0.50 mmol) were taken in a Schlenk flask and 5 ml of toluene was added to the reaction mixture. The reaction was run for 1 h at room temperature. The toluene solution was concentrated and filtered through cannula. Yellow mixture crystals of **6** were isolated after keeping the solution at 4 ˚C for a day. Similar mixture of all the three iodo substituted IDipp-boranes are seen in the ^{1}H and the ^{11}B NMRs

^{1}H $\{^{11}B\}$ NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.14 (d, J = 6.72 Hz, 12 H, $CH(CH_3)_2$), 1.15 (d, 12 H, J = 6.85 Hz, $CH(CH_3)_2$), 1.23 (d, J = 6.85 Hz, 12 H, $CH(CH_3)_2$), 1.28 (d, J = 6.72 Hz, 12 H, $CH(CH_3)_2$), 1.35 (d, J = 6.72 Hz, 12 H, $CH(CH_3)_2$), 1.41 (d, J = 6.72 Hz, 12 H, $CH(CH_3)_2$), 2.41 (sept, J = 6.72 Hz, 4 H, $CH(CH_3)_2$), 2.60 (sept, J = 6.85 Hz, 4 H, $CH(CH_3)_2$), 2.69 (sept, J = 6.85 Hz, 4 H, $NCH_2CH_2CH_2N$), 7.17- 7.59 (m, *Ar-H*) 7.15 (s, 2 H, C*H*=C*H*), 7.92 (s, 2 H, C*H*=C*H*), 9.46 (s, 2 H, C*H*=C*H*) ppm.

$^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$): δ = 22.97, 25.94, 29.13, 123.16, 124.03, 124.40, 130.58, 130.98, 133.24, 144.54, 145.51 ppm.

$^{11}B\{^{1}H\}$ NMR (127 MHz, 298 K, $CDCl_3$): δ = -33.0 (bs, 1B, BH_2I), -44.2 (bs, 1B, BHI_2), 19.1 (bs, 1B, BI_3) ppm.

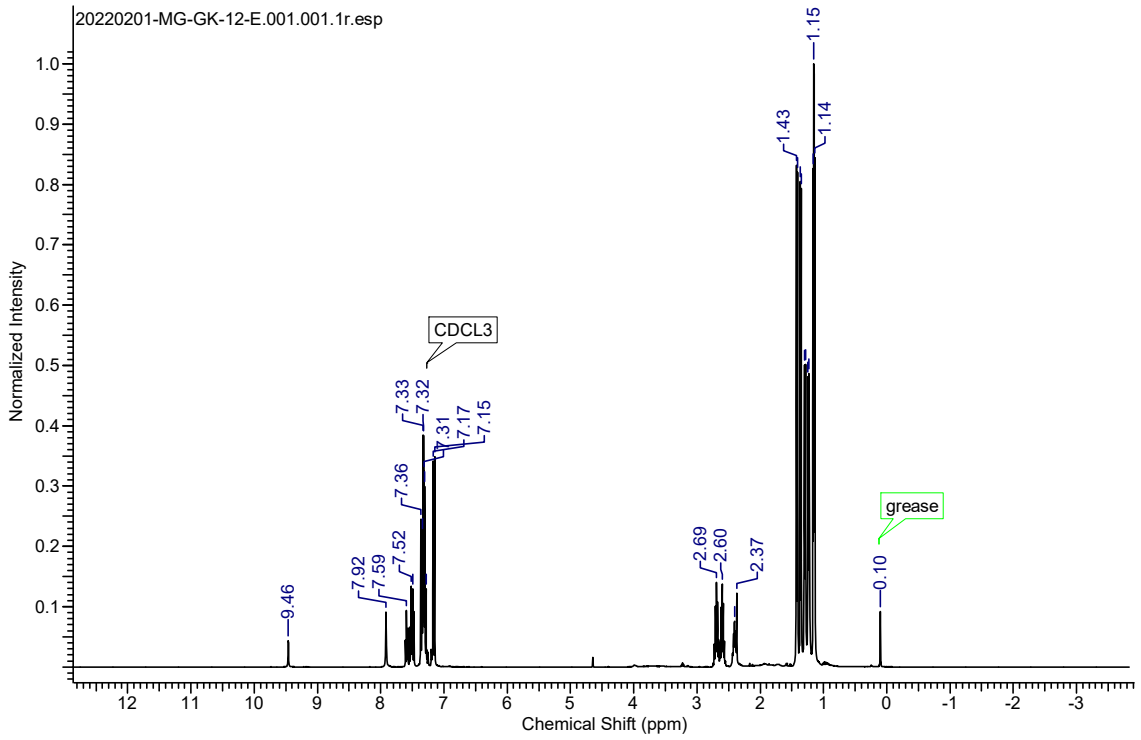

Figure S46. $^{1}H\{^{11}B\}$ NMR spectrum.

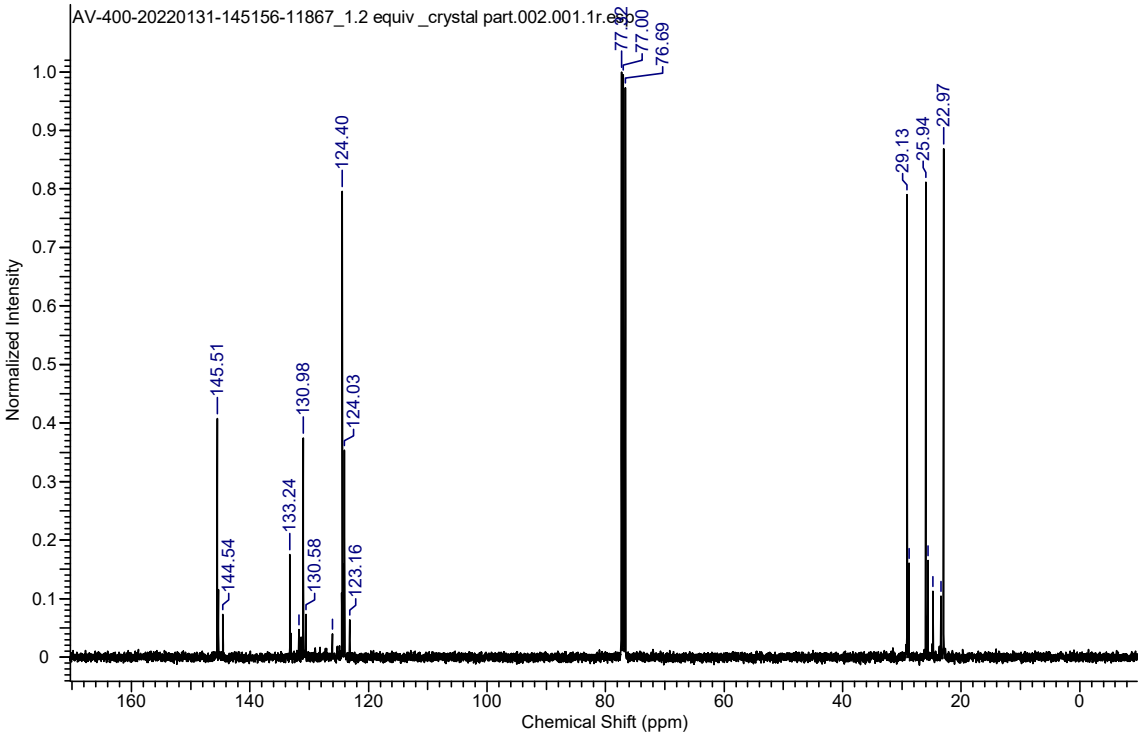

Figure S47. ^{13}C NMR spectrum.

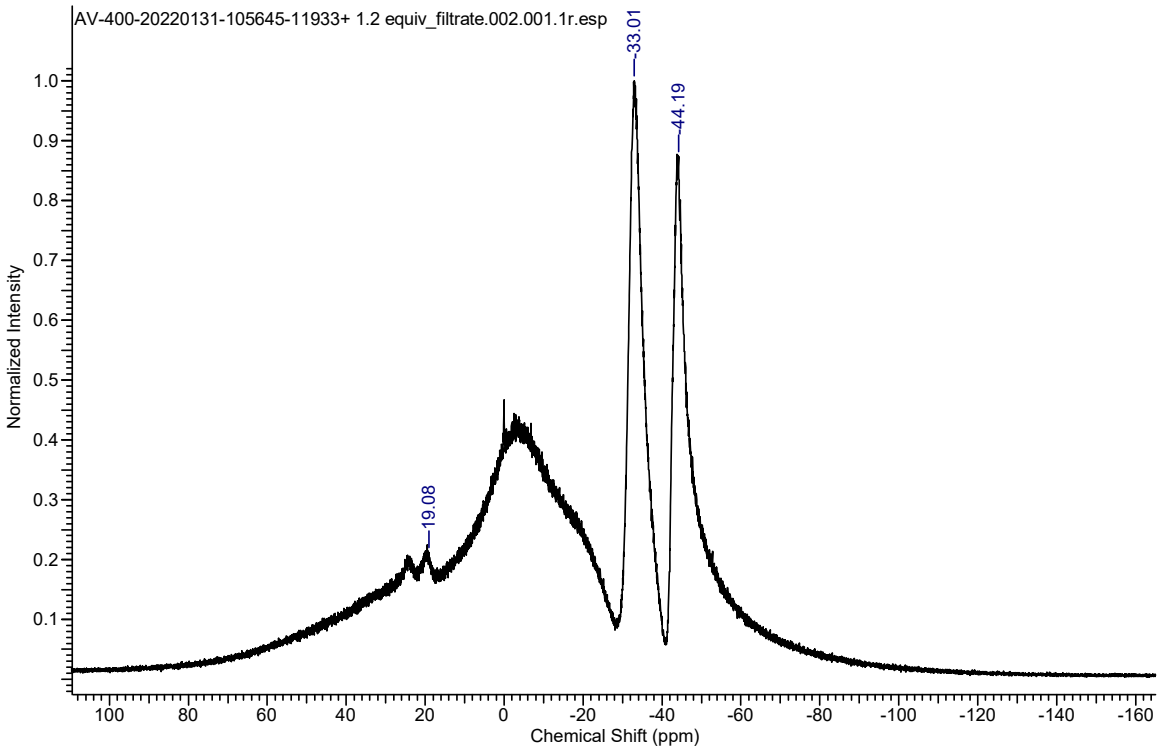

Figure S48. ^{11}B NMR spectrum.

S4. Crystal picture and bond lengths (Å), bond angles (degree) of 9

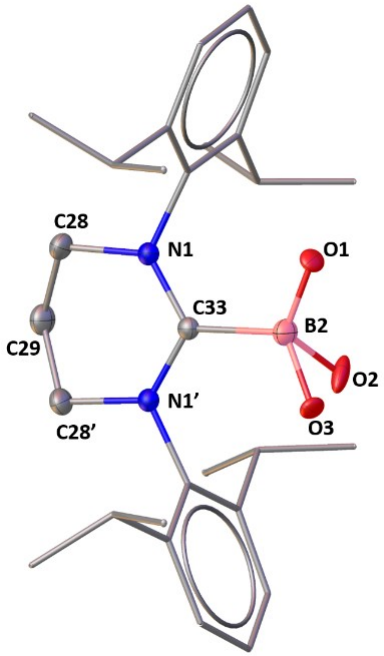

Figure S49**.** The molecular structures of **9**. Selected bond lengths [Å], angles [deg]: N1-C33 1.3338(17), C33-B2 1.683(4), B2-O1 1.326(5), B2–O2 1.282(4), B2-O3 1.381(4); N1–C33–N1', 118.74(19), C33-B2-O1 110.6(3), O1-B2-O2 115.1(4).

S5. The cyclic voltammogram of 8

All experiments were carried out under an atmosphere of argon in degassed and anhydrous acetonitrile solution containing n-Bu_4NPF_6 (0.1 M) at a scan rate of 0.70 Vs^{-1}. The set up consisted of a glassy carbon working electrode (surface area = 0.04 cm^2), Pt counter electrode, Ag/AgCl reference electrode and 0.1 M n-Bu_4NPF_6 solution in acetonitrile as the electrolyte.

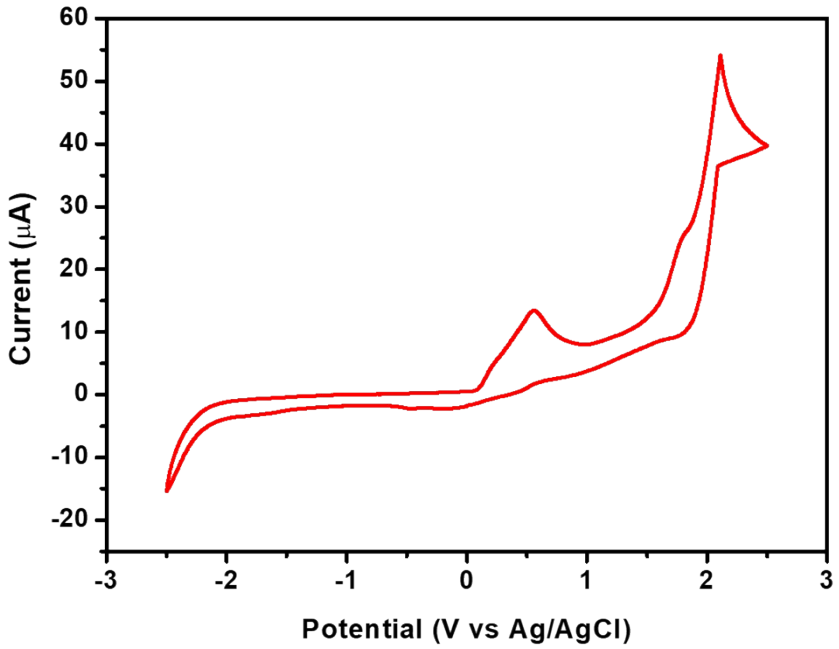

Figure S50. The cyclic voltammogram of **8** were recorded at 0.7 V s^{-1}.

S6. Crystallographic data for the structural analysis of compounds 1-4 and 6-9

Single crystals of **1-4** and **6-9** were mounted on a Bruker SMART APEX II single crystal X-ray CCD diffractometer having graphite monochromatised (Mo-Kα = 0.71073 Å) radiation at low temperature 100 K and 298 K. The X-ray generator was operated at 50 kV and 30 mA. The X-ray data acquisition was monitored by APEX2 program suit. The data were corrected for Lorentz-polarization and absorption effects using SAINT and SADABS programs which are an integral part of APEX2 package.[2] The structures were solved by direct methods and refined by full matrix least squares, based on F^2, using SHELXL Crystal structures were refined using Olex2-1.0 software. Anisotropic refinement was performed for all non-H atom. The C-H hydrogen atoms were calculated using the riding model.[3] The structures were examined using the ADSYM subroutine of PLATON to assure that no additional symmetry could be applied to the models. The molecular weight of each structure mentioned herein has been calculated considering the solvent molecules trapped in the crystal. Crystallographic information is available at www.ccdc.cam.ac.uk/data or as part of Supporting Information.

1. ($C_{28}H_{43}BN_2$), colorless, 0.12 × 0.12 × 0.07 mm^3, orthorhombic, space group '*P bcn*', a = 19.167(2) Å, b = 14.1542(17) Å, c = 39.176(5) Å, $\alpha = \beta = \gamma = 90$, V = 10628(2) Å^3, Z = 16, T = 100(2) K, $2\theta_{max}$ = 48.22°, D_{calc} (g cm^{-3}) = 1.046, $F(000)$ = 3680, μ (mm^{-1}) = 0.059, 465420 reflections collected, 10905 unique reflections (R_{int} = 0.1436), 8657 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6275, T_{max} = 0.7454, 599 refined parameters, S = 1.145, $R1$ = 0.0644, $wR2$ = 0.1465 (all data R = 0.0902, $wR2$ = 0.1612), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.295, $\Delta\rho_{min}$= -0.483 (eÅ^{-3}). CCDC: 2102132

2. ($C_{28}H_{42}BIN_2 * C_7H_7$), colorless, 0.25 × 0.15 × 0.12 mm^3, monoclinic, space group '*C* 2/*c*', a = 30.7004(15) Å, b = 13.6937(5) Å, c = 18.6768(8) Å, $\alpha = \gamma = 90$, β = 118.551(3), V = 6896.9(5)

Å^3, Z = 8, T = 100 (2) K, 2θ_{max} = 66.64°, D_{calc} (g cm^{-3}) = 1.224, $F(000)$ = 2648, μ (mm^{-1}) = 0.952, 325196 reflections collected, 16717 unique reflections (R_{int} = 0.0516), 14908 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6797, T_{max} = 0.7471, 379 refined parameters, S = 1.124, $R1$ = 0.0345, $wR2$ = 0.0929 (all data R = 0.0409, $wR2$ = 0.1005), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 3.047, $\Delta\rho_{min}$= -2.301 (eÅ^{-3}). CCDC: 2125724.

3. ($C_{28}H_{41}BI_2N_2$), colorless, 0.1 × 0.06 × 0.05 mm^3, monoclinic, space group '$P2_1/n$', a = 9.5036(4) Å, b = 19.9724(6) Å, c = 16.0540(6) Å, $\alpha = \gamma = 90$, β = 103.2450(10), V = 2966.15(19) Å^3, Z = 4, T = 100.(2) K, 2θ_{max} = 68.59 °, D_{calc} (g cm^{-3}) = 1.501, $F(000)$ = 1336, μ (mm^{-1}) = 2.43, 119156 reflections collected, 10349 unique reflections (R_{int} = 0.0482), 9558 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.5564, T_{max} = 0.7467, 306 refined parameters, S = 1.222, $R1$ = 0.0350, $wR2$ = 0.1352 (all data R = 0.0431, $wR2$ = 0.1510), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 2.177, $\Delta\rho_{min}$= -3.068 (eÅ^{-3}). CCDC: 2123602.

4. ($C_{29}H_{42}BF_3N_2O_3S$), colorless, 0.24 × 0.12 × 0.1 mm^3, triclinic, space group 'P -1', a = 9.601(6) Å, b = 9.604(6) Å, c = 18.081(11) Å, α =97.88(2), β = 90.02(2), γ = 108.16(3), V = 1567.4(17) Å^3, Z = 2, T = 100.(2) K, 2θ_{max} = 60.42 °, D_{calc} (g cm^{-3}) = 1.200, $F(000)$ = 604, μ (mm^{-1}) = 0.152, 102707 reflections collected, 11185 unique reflections (R_{int} = 0.0811), 7314 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6558, T_{max} = 0.7465, 360 refined parameters, S = 1.076, $R1$ = 0.0579, $wR2$ = 0.1627 (all data R = 0.1096, $wR2$ = 0.1912), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.719, $\Delta\rho_{min}$= -1.218 (eÅ^{-3}). CCDC: 2123596

6. ($C_{30}H_{41}BF_6N_2O_6S_2$), colorless, 0.22 × 0.12 × 0.09 mm^3, monoclinic, space group '$P2_1/c$', a = 17.311(3) Å, b = 11.1748(15) Å, c = 17.490(3) Å, $\alpha = \gamma = 90$, β = 96.691(7), V = 3360.5(9) Å^3, Z = 4, T = 100.(2) K, 2θ_{max} = 50.48°, D_{calc} (g cm^{-3}) = 1.412, $F(000)$ = 1496, μ (mm^{-1}) = 0.236, 113806 reflections collected, 12070 unique reflections (R_{int} = 0.0487), 9829 observed ($I > 2\sigma(I)$)

reflections, multi-scan absorption correction, T_{min} = 0.6731, T_{max} = 0.7467, 432 refined parameters, S = 1.129, $R1$ = 0.0361, $wR2$ = 0.1029 (all data R = 0.0537, $wR2$ = 0.1211), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.918, $\Delta\rho_{min}$= -0.884 (eÅ^{-3}). CCDC: 2123605

7. ($C_{28}H_{41}BN_4O_6$), colorless, 0.22 × 0.11 × 0.08 mm^3, monoclinic, space group '$P2_1/c$', a = 18.736(3) Å, b = 8.3227(19) Å, c = 18.866(3) Å, $\alpha = \gamma = 90$, β = 96.145(5), V = 2925.0(10) Å^3, Z = 4, T = 100.(2) K, $2\theta_{max}$ = 62.78 °, D_{calc} (g cm^{-3}) = 1.227, $F(000)$ = 1160, μ (mm^{-1}) = 0.086, 90856 reflections collected, 9543 unique reflections (R_{int} = 0.0487), 7541 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6465, T_{max} = 0.7462, 432 refined parameters, S = 1.152, $R1$ = 0.0637, $wR2$ = 0.1651 (all data R = 0.0875, $wR2$ = 0.1820), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.683, $\Delta\rho_{min}$= -0.476 (eÅ^{-3}). CCDC: 2123606

8. ($C_{28}H_{42}BBrN_2O_2$), colorless, 0.15 × 0.12 × 0.06 mm^3, orthorhombic, space group '$P\ nma$', a = 16.517(10) Å, b = 20.453(9) Å, c = 8.264(3) Å, $\alpha = \beta = \gamma = 90$, V = 2792(2) Å^3, Z = 4, T = 100.(2) K, $2\theta_{max}$ = 42.30 °, D_{calc} (g cm^{-3}) = 1.259, $F(000)$ = 1120, μ (mm^{-1}) = 1.499, 64957 reflections collected, 2527 unique reflections (R_{int} = 0.194), 1755 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6212, T_{max} = 0.7457, 173 refined parameters, S = 1.071, $R1$ = 0.0412, $wR2$ = 0.0855 (all data R = 0.0795, $wR2$ = 0.1063), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.558, $\Delta\rho_{min}$= -0.659 (eÅ^{-3}). CCDC: 2123612

9. ($C_{28}H_{40}BN_2O_4$), colorless, 0.15 × 0.10 × 0.08 mm^3, orthorhombic, space group '$P\ nma$', a = 12.325(3) Å, b = 20.525(5) Å, c = 10.920(3) Å, $\alpha = \beta = \gamma = 90$, V = 2762.4(12) Å^3, Z = 4, T = 293(2) K, $2\theta_{max}$ = 59.66 °, D_{calc} (g cm^{-3}) = 1.153, $F(000)$ = 1036, μ (mm^{-1}) = 0.076, 215531 reflections collected, 4981 unique reflections (R_{int} = 0.100), 3797 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6965, T_{max} = 0.7463, 176 refined parameters, S = 1.110,

$R1 = 0.0979$, $wR2 = 0.2878$ (all data $R = 0.1463$, $wR2 = 0.3238$), maximum and minimum residual electron densities; $\Delta\rho_{max} = 0.720$, $\Delta\rho_{min} = -1.319$ (eÅ^{-3}). CCDC: 2123642

S7. Details of theoretical calculations for the fromation of 3

All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.5 suite of programs,[4] using the PBE functional,[5] along with dispersion correction (DFT-D3).[6] The def-TZVP basis set[7] has been employed. The resolution of identity (RI),[8] along with the multipole accelerated resolution of identity (marij)[9] approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent correction was incorporated with optimization calculations using the COSMO model,[10] with toluene (ε = 2.374) as the solvent. The values reported are ΔG values, with zero-point energy corrections, internal energy and entropic contributions were included through frequency calculations on the optimized minima, with the temperature taken to be 298.15 K. The translational entropy term in the calculated structures was corrected through a free volume correction introduced by Mammen *et al.*[11] This volume correction is to account for the unreasonable enhancement in translational entropy that is generally observed in computational software. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition state structures.

Energy profile for the disubstitution reaction of 5-IDipp·BH_3:

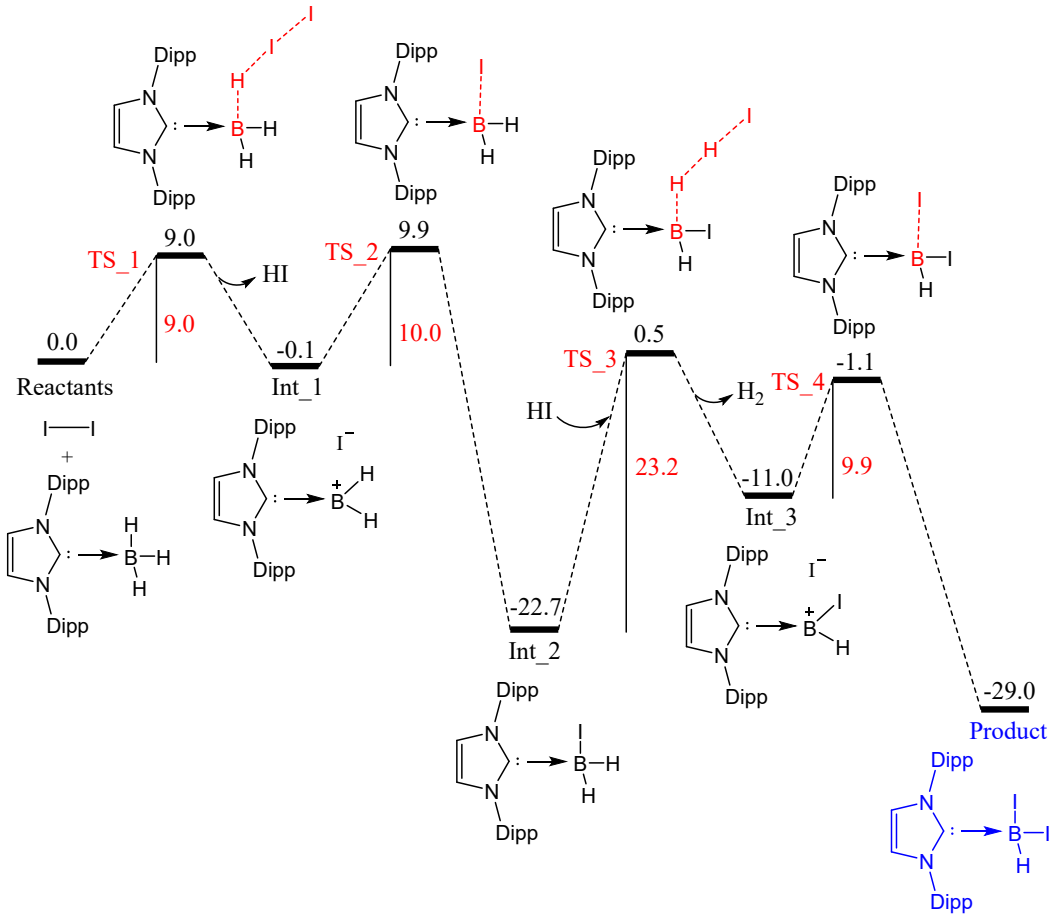

Figure S51. The free energy profile for the disubstitution reaction of 5-IDipp·BH_3 by the iodine molecule. Values are in kcal/mol.

S8. References

1. M. Iglesias, D. J. Beetstra, J. C. Knight, L.-L. Ooi, A. Stasch, S. Coles, L. Male, M. B. Hursthouse, K. J. Cavell, A. Dervisi and I. A. Fallis, *Organometallics*., 2008, **27**, 3279–3289.

2. APEX3, SAINT-Plus and SADABS; Bruker AXS Inc.: Madison, WI, USA, **2006**. (b) Apex CCD and SAINT v8.30C; Bruker AXS Inc.: Madison, WI, USA, **2013**.

3. (a) G. M. Sheldrick, A short history of SHELX. *Acta Crystallogr., Sect. A*: Found. Crystallogr., 2008, **64**, 112–122; (b) L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Crystallogr.*, 2015, **48**, 3–10; (c) L. Krause, R. Herbst-Irmer and D. Stalke, *J. Appl. Crystallogr.,* 2015, **48**, 1907–1913.

4. TURBOMOLE V7.5 2020, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.org.

5. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett*., 1996, **77**, 3865–3868.

6. S. Grimme, J. Antony, S. Ehrlich and H. A. Krieg, *J. Chem. Phys.,* 2010, **132**, 154104 (1-19).

7. K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor Chem Acta.,* 1997, **97**, 119–124.

8. K. Eichkorn, O. Treutler, H. Öhm, M. Haser and R. Ahlrichs, *Chem. Phys. Lett*., 1995, **240**, 283–289.

9. M. Sierka, A. Hogekamp and R. Ahlrichs, *J. Chem. Phys*., 2003, **118**, 9136–9148.

10. A. Klamt and G. Schuurmann, *J. Chem. Soc., Perkin Trans.*, 1993, **2**, 799–805.

11. M. Mammen, E. I.Shakhnovich, J. M.; Deutch and G. M. Whitesides, *J. Org. Chem.,* 1998, **63**, 3821–3830.

S9. PBE-D3/def-TZVP optimized geometries for the structures shown in Figure 3 and S51.

(1) I_2

2

I	0.090450	0.000000	-0.453342
I	0.090450	0.000000	-3.176822

(2) 1

74

N	1.195545	-0.059297	-0.621936
N	0.028123	-0.144512	1.373210
C	0.005885	-0.126709	0.020648
C	1.257414	-0.070023	-2.065164
C	-1.181067	-0.314017	2.146885
C	1.275144	1.160509	-2.755133
C	1.151859	2.494469	-2.032265
H	0.886488	2.279855	-0.986314
C	-2.957934	0.648876	3.452893
H	-3.486164	1.519517	3.847274
C	1.524689	-1.286383	-4.126595
H	1.617612	-2.229423	-4.669491
C	1.379810	-1.306208	-2.732398
C	-1.816954	0.833854	2.661561
C	-1.630671	-1.617757	2.432731
C	1.373530	-2.634346	-1.988522
H	1.113253	-2.427864	-0.939413
C	1.422284	1.127310	-4.148432
H	1.433533	2.064208	-4.709204
C	-2.774827	-1.751111	3.232326
H	-3.157888	-2.748747	3.458396
C	2.500537	-0.014882	0.062351
H	3.196099	0.534061	-0.585749
H	2.894420	-1.040329	0.173502
C	2.354763	0.653465	1.418488
H	2.101003	1.717081	1.285357
H	3.300465	0.600295	1.974685
C	1.548531	-0.082965	-4.830127
H	1.662199	-0.088249	-5.916208
C	0.026550	3.366145	-2.611219
H	0.248661	3.682362	-3.641952
H	-0.096754	4.275872	-2.004095
H	-0.926836	2.820393	-2.611696
C	-1.330666	2.235892	2.323483
H	-0.348986	2.140501	1.835299
C	-3.434704	-0.631471	3.737213
H	-4.326634	-0.756555	4.354766
C	2.491591	3.253928	-2.040172
H	3.302348	2.657768	-1.595165
H	2.406894	4.193045	-1.472301
H	2.791304	3.506461	-3.068978
C	1.253190	-0.050924	2.190485
H	1.567556	-1.065104	2.493616
H	0.994596	0.497276	3.107542
C	2.768607	-3.285498	-2.016418
H	3.060163	-3.539127	-3.047276
H	2.774368	-4.214078	-1.425479
H	3.537772	-2.612292	-1.609784
C	0.307960	-3.597587	-2.534638
H	-0.685580	-3.129472	-2.515380
H	0.272386	-4.510237	-1.920745
H	0.530106	-3.901285	-3.569003
C	-0.946788	-2.855006	1.868561
H	-0.050844	-2.524297	1.321386
C	-1.142966	3.105872	3.575555
H	-2.100836	3.297079	4.082215
H	-0.714509	4.081545	3.300827
H	-0.469602	2.626689	4.302456
C	-2.271058	2.905271	1.304424
H	-2.363259	2.289935	0.398993
H	-1.883785	3.895228	1.017320
H	-3.275823	3.043372	1.733134
C	-1.854918	-3.570230	0.853169
H	-2.768649	-3.947149	1.338189
H	-1.328936	-4.429204	0.408718
H	-2.146324	-2.884882	0.045803
C	-0.485610	-3.812074	2.980160
H	0.179989	-3.306583	3.696029
H	0.058146	-4.666049	2.547991
H	-1.341364	-4.213463	3.543432
B	-1.359452	-0.166939	-0.818966
H	-2.330675	-0.202002	-0.090013
H	-1.373856	0.830481	-1.531949
H	-1.321125	-1.146218	-1.554561

(3) TS_1

76

N	0.279304	2.057901	2.622848
N	-1.455908	0.832390	3.566205
C	-0.788252	1.253779	2.495143
C	0.956630	2.440781	1.400842
C	-2.560018	-0.099644	3.463261
C	0.578284	3.648702	0.766387
C	-0.524540	4.542235	1.313199
H	-1.036787	3.993820	2.118308
C	-4.922328	-0.499963	3.349849
H	-5.948615	-0.138747	3.258908
C	2.661288	2.031694	-0.244894
H	3.468921	1.419905	-0.650746
C	2.004191	1.618750	0.920748
C	-3.867210	0.421053	3.378287
C	-2.283504	-1.479260	3.551680
C	2.434449	0.348398	1.638136
H	1.676679	0.114253	2.401636
C	1.271885	4.009035	-0.394739
H	1.001700	4.928107	-0.918327
C	-3.376825	-2.354112	3.515969
H	-3.208552	-3.431805	3.521368
C	0.788213	2.533135	3.919145
H	1.235861	3.522131	3.754277
H	1.586019	1.855761	4.266186
C	-0.359328	2.589550	4.917344
H	-1.057940	3.392637	4.637226
H	0.024534	2.815730	5.920692
C	2.301635	3.211741	-0.894228
H	2.828415	3.512996	-1.801885
C	-1.583134	4.884537	0.251366
H	-1.162690	5.506491	-0.552801
H	-2.406985	5.449794	0.711223
H	-2.003424	3.977261	-0.203873
C	-4.148565	1.916493	3.314764
H	-3.186155	2.448736	3.374430
C	-4.680167	-1.871109	3.415275
H	-5.510007	-2.576745	3.355161
C	0.068740	5.826171	1.923973
H	0.807816	5.603928	2.707646
H	-0.727683	6.442175	2.367271
H	0.572806	6.427203	1.152099
C	-1.086249	1.252233	4.935551
H	-0.463449	0.462670	5.387723
H	-2.018272	1.308907	5.512321
C	3.775328	0.572181	2.363645
H	4.578112	0.781570	1.641066
H	4.055971	-0.326032	2.933427
H	3.724842	1.421385	3.061499
C	2.516628	-0.862475	0.695849
H	1.571450	-1.021029	0.158979
H	2.734990	-1.772326	1.273337
H	3.317290	-0.741905	-0.048634
C	-0.868844	-2.031080	3.659790

H	-0.168288	-1.180790	3.685855
C	-5.002395	2.376924	4.508811
H	-5.997545	1.909265	4.487518
H	-5.142824	3.468029	4.483140
H	-4.530744	2.112608	5.467279
C	-4.801098	2.314321	1.980059
H	-4.179423	2.011282	1.125970
H	-4.945946	3.404318	1.933859
H	-5.784372	1.835576	1.861030
C	-0.499440	-2.887118	2.436281
H	-1.177860	-3.745194	2.323983
H	0.528372	-3.268094	2.537112
H	-0.566627	-2.304269	1.507711
C	-0.682473	-2.819951	4.968065
H	-0.931828	-2.207742	5.848134
H	0.360076	-3.158530	5.065069
H	-1.326925	-3.710757	4.985093
B	-1.075763	0.944899	0.952320
H	-0.468002	0.070777	0.417706
H	-2.941958	0.334961	-0.123916
I	-3.964771	-4.599525	0.295000
H	-1.648087	1.793395	0.332071
I	-3.246884	-1.333066	-0.048076

(4) HI

2

H	-0.118281	0.000000	-1.731613
I	-0.118281	0.000000	-3.361156

(5) Int_1

74

N	0.807102	-0.179181	-1.502288
N	0.777941	-1.336163	0.528092
C	0.169405	-0.834554	-0.536968
C	-0.088732	0.216398	-2.573640
C	-0.034794	-2.080031	1.469517
C	-0.682513	1.505972	-2.527619
C	-0.350618	2.511217	-1.444056
H	0.239519	2.020354	-0.655075
C	-1.393616	-2.137826	3.450211
H	-1.847740	-1.636692	4.307050
C	-1.218432	-0.305367	-4.639043
H	-1.431366	-0.983441	-5.466546
C	-0.326715	-0.700368	-3.635652
C	-0.595595	-1.392866	2.569097
C	-0.227864	-3.464038	1.249264
C	0.398251	-2.033532	-3.725476
H	0.813503	-2.261991	-2.731418
C	-1.568354	1.838880	-3.561387
H	-2.050002	2.817980	-3.552212
C	-1.028178	-4.156767	2.166988
H	-1.199001	-5.226268	2.030865
C	2.253851	0.083518	-1.474530
H	2.424799	1.072175	-1.922121
H	2.763278	-0.669708	-2.098074
C	2.736897	0.056430	-0.026167
H	2.392157	0.969313	0.492465
H	3.834683	0.066412	-0.006913
C	-1.832096	0.948007	-4.600634
H	-2.522516	1.234685	-5.396605
C	-1.597902	3.092850	-0.761518
H	-2.177444	3.734059	-1.443291
H	-1.275089	3.699565	0.096577
H	-2.260257	2.298744	-0.387797
C	-0.342923	0.080871	2.827086
H	0.292521	0.490241	2.026825
C	-1.607968	-3.500591	3.253471
H	-2.230085	-4.059980	3.955213
C	0.529117	3.638460	-2.019288
H	1.421761	3.240110	-2.525112
H	0.866550	4.281207	-1.193671
H	-0.031934	4.244955	-2.747154
C	2.233341	-1.175376	0.723810
H	2.732353	-2.100164	0.389245
H	2.408354	-1.065403	1.802453
C	1.580425	-1.923002	-4.709030
H	1.216386	-1.721961	-5.727837
H	2.150360	-2.863687	-4.728610
H	2.266156	-1.109235	-4.432925
C	-0.526963	-3.196182	-4.113852
H	-1.396685	-3.258152	-3.445489
H	0.021427	-4.147465	-4.051950
H	-0.894292	-3.096452	-5.145743
C	0.431601	-4.206913	0.096515
H	0.854347	-3.460040	-0.593767
C	0.424416	0.285679	4.144838
H	-0.188096	0.000575	5.014591
H	0.703329	1.345260	4.235130
H	1.348741	-0.310566	4.167968
C	-1.641689	0.903441	2.817108
H	-2.206398	0.751828	1.885569
H	-1.387433	1.970556	2.891855
H	-2.295804	0.636827	3.661382
C	-0.569388	-5.052920	-0.706175
H	-0.978334	-5.876516	-0.102551
H	-0.072372	-5.499012	-1.580086
H	-1.411609	-4.444043	-1.064046
C	1.596463	-5.073794	0.610659
H	2.332957	-4.473620	1.164770
H	2.111446	-5.564102	-0.229015
H	1.227684	-5.857960	1.289157
B	-1.380008	-0.971550	-0.828201
H	-2.127555	-0.131338	-0.422334
H	-1.784734	-1.960127	-1.368338
I	1.653046	3.337382	1.817757

(6) TS_2

74

N	0.748766	-1.103661	-0.655231
N	-0.533762	-0.956834	1.300907
C	-0.433471	-1.226173	-0.022598
C	0.949450	-1.618703	-1.994640
C	-1.595304	-1.504015	2.139544
C	1.283202	-0.717547	-3.034400
C	1.282480	0.789702	-2.855902
H	0.857083	1.028494	-1.868357
C	-3.756127	-1.343893	3.193104
H	-4.695889	-0.809620	3.346523
C	1.202868	-3.493437	-3.495440
H	1.174006	-4.568133	-3.684979
C	0.910598	-3.018964	-2.207492
C	-2.793034	-0.787492	2.337693
C	-1.328410	-2.715537	2.821617
C	0.611628	-4.044391	-1.122491
H	0.411632	-3.515170	-0.179784
C	1.587003	-1.253843	-4.291870
H	1.843642	-0.575212	-5.106850
C	-2.322884	-3.219139	3.672158
H	-2.143573	-4.153551	4.207451
C	1.935524	-0.658470	0.093824
H	2.670440	-0.296496	-0.633418
H	2.377493	-1.530700	0.609178
C	1.516639	0.424012	1.077648
H	1.101539	1.281090	0.523059
H	2.382184	0.770786	1.657463
C	1.547438	-2.626573	-4.527199
H	1.780489	-3.020226	-5.518490
C	0.363499	1.468340	-3.885589
H	0.752990	1.361729	-4.909776
H	0.279546	2.538170	-3.651414
H	-0.650240	1.046795	-3.847001
C	-3.060068	0.550855	1.684733
H	-2.205167	0.811779	1.044043
C	-3.530640	-2.548376	3.852536

H	-4.292110	-2.962203	4.516746
C	2.701876	1.378723	-2.936378
H	3.390136	0.919543	-2.210416
H	2.667132	2.459096	-2.734280
H	3.135562	1.233954	-3.938546
C	0.462816	-0.132204	2.021201
H	0.912671	-0.752726	2.811108
H	-0.094990	0.681161	2.510337
C	1.824806	-4.958835	-0.877573
H	2.069992	-5.546242	-1.774697
H	1.612259	-5.665582	-0.062767
H	2.715212	-4.373568	-0.604880
C	-0.645766	-4.861792	-1.466725
H	-1.529483	-4.214447	-1.580879
H	-0.861081	-5.595449	-0.676973
H	-0.517443	-5.413726	-2.409258
C	-0.008611	-3.469444	2.718648
H	0.589271	-3.011861	1.914505
C	-3.179466	1.670864	2.731374
H	-4.073657	1.544551	3.361293
H	-3.245595	2.640857	2.217852
H	-2.299705	1.699128	3.392396
C	-4.296573	0.517054	0.773976
H	-4.221283	-0.281968	0.020643
H	-4.379179	1.473956	0.239145
H	-5.221906	0.354217	1.348671
C	-0.217395	-4.948497	2.356661
H	-0.721100	-5.490775	3.169907
H	0.751177	-5.440177	2.184111
H	-0.830862	-5.057798	1.452659
C	0.798553	-3.350906	4.025907
H	0.964991	-2.302885	4.314272
H	1.778891	-3.838853	3.918268
H	0.265274	-3.839896	4.854981
B	-1.718461	-1.586817	-0.857131
H	-1.747800	-1.249871	-2.001747
H	-2.623452	-2.167868	-0.337850
I	-1.249861	2.687828	-0.711949

(7) Int_2

74

N	0.522329	-1.305415	-0.539541
N	0.587795	0.086794	1.317048
C	-0.138027	-0.653866	0.444995
C	-0.135138	-2.132862	-1.533892
C	0.036831	0.593850	2.560671
C	-0.315753	-1.616870	-2.837749
C	0.071933	-0.194663	-3.227183
H	0.135371	0.395956	-2.299974
C	-0.727827	2.429823	3.917055
H	-1.001733	3.480846	4.026623
C	-0.965420	-4.289581	-2.220857
H	-1.216875	-5.327383	-1.994015
C	-0.441893	-3.473159	-1.209400
C	-0.293758	1.961981	2.667859
C	-0.018117	-0.279503	3.669502
C	-0.192746	-4.060386	0.172485
H	0.023952	-3.228800	0.858298
C	-0.841823	-2.479454	-3.810773
H	-1.002249	-2.106253	-4.823299
C	-0.466464	0.238234	4.891684
H	-0.535823	-0.421091	5.759487
C	1.996931	-1.344350	-0.591562
H	2.287168	-1.623770	-1.609394
H	2.358015	-2.140387	0.083525
C	2.557566	0.001854	-0.174610
H	2.229254	0.779404	-0.881741
H	3.655870	-0.016703	-0.176456
C	-1.164757	-3.800775	-3.510426
H	-1.573831	-4.452914	-4.284898
C	-0.975225	0.480941	-4.126845
H	-0.994398	0.033414	-5.132190
H	-0.728607	1.546434	-4.246843
H	-1.978364	0.410988	-3.687860
C	-0.178676	2.934448	1.501780
H	-0.036910	2.342268	0.584052
C	-0.820140	1.580537	5.017897
H	-1.166846	1.966822	5.978594
C	1.442876	-0.158761	-3.934137
H	2.253167	-0.576919	-3.321068
H	1.713009	0.878225	-4.185620
H	1.405878	-0.735734	-4.870770
C	2.048507	0.297948	1.221843
H	2.544161	-0.349672	1.965576
H	2.249975	1.336226	1.512899
C	1.033314	-4.992264	0.157228
H	0.852479	-5.864244	-0.490028
H	1.248425	-5.361933	1.171572
H	1.930968	-4.480243	-0.219792
C	-1.423915	-4.791976	0.728455
H	-2.299007	-4.128360	0.749102
H	-1.228063	-5.134820	1.755064
H	-1.675062	-5.678530	0.126904
C	0.379536	-1.746701	3.583543
H	0.721282	-1.949091	2.557405
C	1.031888	3.872839	1.677988
H	0.897101	4.513349	2.562972
H	1.138810	4.527448	0.799696
H	1.976851	3.325593	1.809771
C	-1.456612	3.768651	1.313158
H	-2.338650	3.123693	1.213148
H	-1.375630	4.373248	0.397527
H	-1.614153	4.459845	2.155284
C	-0.820008	-2.670681	3.851810
H	-1.202979	-2.535178	4.874640
H	-0.522728	-3.724813	3.742446
H	-1.639226	-2.465892	3.149101
C	1.551504	-2.068962	4.526408
H	2.416352	-1.417157	4.332039
H	1.870779	-3.114037	4.395535
H	1.263933	-1.937023	5.580321
B	-1.730618	-0.804434	0.626284
H	-2.130797	-1.867111	0.229059
H	-2.088439	-0.515774	1.737574
I	-2.750016	0.765426	-0.747112

(8) TS_3

76

N	0.393490	0.383267	2.410094
N	-1.659879	-0.188700	3.359527
C	-0.918657	0.126049	2.292555
C	1.162640	0.795755	1.250295
C	-2.984074	-0.759688	3.179531
C	1.343852	2.180629	1.013187
C	0.725082	3.253322	1.900445
H	-0.146638	2.809389	2.407122
C	-5.373830	-0.565395	3.260489
H	-6.278801	0.022566	3.421433
C	2.577987	0.227148	-0.610972
H	3.062088	-0.515319	-1.247359
C	1.779298	-0.200490	0.458334
C	-4.121715	0.039498	3.431379
C	-3.067703	-2.132162	2.848777
C	1.626761	-1.687229	0.742985
H	0.797829	-1.816750	1.455672
C	2.153636	2.545254	-0.069905
H	2.308536	3.602049	-0.291209
C	-4.347371	-2.677982	2.686076
H	-4.457232	-3.715343	2.368729
C	1.100460	0.199161	3.692418
H	2.002497	0.819481	3.664886
H	1.419155	-0.853529	3.772430
C	0.171230	0.572542	4.837360

H	-0.060639	1.647415	4.795392
H	0.656611	0.370925	5.801515
C	2.766399	1.582431	-0.871462
H	3.394570	1.892844	-1.708707
C	0.222439	4.470296	1.107506
H	1.057010	5.068554	0.712644
H	-0.365993	5.125053	1.766181
H	-0.415167	4.171032	0.265551
C	-4.029136	1.483044	3.907982
H	-3.007010	1.842927	3.703354
C	-5.486445	-1.901067	2.876611
H	-6.470331	-2.342378	2.710327
C	1.721035	3.721324	2.980989
H	2.075242	2.897980	3.615557
H	1.249332	4.471725	3.632969
H	2.603011	4.183504	2.512857
C	-1.101062	-0.251725	4.725876
H	-0.913589	-1.309611	4.971799
H	-1.878226	0.110521	5.409370
C	2.903497	-2.243785	1.402819
H	3.758066	-2.172687	0.712996
H	2.766465	-3.303075	1.665782
H	3.168313	-1.692544	2.317311
C	1.272278	-2.493378	-0.515713
H	0.378264	-2.093870	-1.014001
H	1.070567	-3.540011	-0.247895
H	2.097613	-2.492347	-1.243063
C	-1.849195	-3.038110	2.723496
H	-0.940315	-2.424415	2.833915
C	-4.281170	1.573143	5.427718
H	-5.309062	1.257433	5.661905
H	-4.155092	2.608809	5.777987
H	-3.604084	0.931569	6.009935
C	-5.005614	2.419665	3.177795
H	-4.916464	2.329635	2.087609
H	-4.803570	3.464616	3.455896
H	-6.048469	2.202534	3.452732
C	-1.765560	-3.736333	1.357558
H	-2.654749	-4.350243	1.157115
H	-0.879988	-4.388623	1.322745
H	-1.694527	-3.009908	0.537966
C	-1.840184	-4.069238	3.868333
H	-1.893970	-3.583768	4.854692
H	-0.922790	-4.675839	3.829429
H	-2.699672	-4.750049	3.783631
B	-1.507514	0.176566	0.810949
H	-1.165930	-0.625605	0.002956
H	-3.343664	-1.149015	0.149486
I	-2.558240	1.903629	0.145764
H	-3.804493	-1.718238	-0.108163
I	-5.301688	-3.830849	-0.801215

(9) H_2

2

H	0.493997	0.000000	0.444397
H	0.493997	0.000000	-0.307726

(10) Int_3

74

N	1.313624	0.257587	-1.481868
N	1.512054	-0.660688	0.659093
C	0.793463	-0.348456	-0.416629
C	0.423120	0.421091	-2.615969
C	0.830812	-1.435629	1.679570
C	-0.432985	1.546741	-2.658143
C	-0.316459	2.698605	-1.679211
H	0.294887	2.391420	-0.816036
C	-0.660181	-1.555637	3.560220
H	-1.271682	-1.069491	4.321992
C	-0.494871	-0.455587	-4.654746
H	-0.527269	-1.211476	-5.441242
C	0.434109	-0.579376	-3.617155
C	0.066804	-0.759590	2.659416
C	0.943047	-2.845707	1.626348
C	1.438057	-1.724098	-3.606152
H	1.855506	-1.798377	-2.589411
C	-1.353777	1.604363	-3.717259
H	-2.040888	2.450097	-3.775951
C	0.208662	-3.582723	2.561004
H	0.259906	-4.672688	2.546791
C	2.715165	0.720688	-1.507436
H	2.739615	1.650450	-2.090451
H	3.326949	-0.030306	-2.033075
C	3.202827	0.956805	-0.082322
H	2.703333	1.847566	0.340573
H	4.281930	1.158967	-0.094420
C	-1.390333	0.616058	-4.695891
H	-2.115631	0.683923	-5.509418
C	-1.664189	3.177554	-1.121794
H	-2.277144	3.669283	-1.892750
H	-1.472282	3.905224	-0.320395
H	-2.248484	2.347720	-0.697695
C	0.090435	0.748687	2.817245
H	0.542952	1.207913	1.924467
C	-0.597409	-2.944958	3.507736
H	-1.171412	-3.541887	4.219432
C	0.430835	3.868879	-2.350159
H	1.399268	3.549263	-2.763420
H	0.625620	4.646434	-1.597952
H	-0.164952	4.295467	-3.172473
C	2.924606	-0.255158	0.799298
H	3.567026	-1.111804	0.537789
H	3.089230	-0.015230	1.858361
C	2.598774	-1.412851	-4.572116
H	2.232399	-1.369615	-5.608941
H	3.368818	-2.197047	-4.514640
H	3.072549	-0.446362	-4.347352
C	0.816570	-3.088952	-3.937342
H	-0.026414	-3.317824	-3.271851
H	1.571398	-3.880345	-3.818670
H	0.457157	-3.131357	-4.976082
C	1.858203	-3.548930	0.632657
H	2.110720	-2.830073	-0.162509
C	0.992657	1.126538	4.009180
H	0.555067	0.779792	4.958347
H	1.108885	2.219352	4.037555
H	1.995856	0.683890	3.916269
C	-1.300701	1.375685	2.982855
H	-1.987246	1.064123	2.182198
H	-1.199312	2.469450	2.940091
H	-1.759034	1.110862	3.948335
C	1.207616	-4.762036	-0.048998
H	1.001558	-5.569477	0.668577
H	1.886088	-5.167351	-0.814276
H	0.263538	-4.488023	-0.538731
C	3.170009	-3.961571	1.330140
H	3.662743	-3.106828	1.815376
H	3.871278	-4.399015	0.603651
H	2.969905	-4.714313	2.107378
B	-0.782569	-0.538470	-0.357503
H	-1.414001	0.369517	0.087175
I	1.504203	4.144186	1.471816
I	-1.890157	-2.237976	-0.975720

(11) TS_4

74

N	0.554590	-0.995065	-0.629915
N	-0.748980	-0.561404	1.273879
C	-0.632163	-1.022223	0.010042
C	0.745109	-1.723922	-1.872986
C	-1.812745	-0.943171	2.200162
C	1.049903	-1.008758	-3.058029
C	1.067146	0.506885	-3.148041
H	0.648828	0.924564	-2.219042

C	-3.899466	-0.500303	3.324500
H	-4.791764	0.114892	3.451780
C	1.005637	-3.824300	-3.042572
H	1.001093	-4.914136	-3.049590
C	0.737540	-3.146380	-1.845015
C	-2.948437	-0.121145	2.365275
C	-1.588583	-2.072544	3.024605
C	0.582119	-3.966969	-0.570432
H	-0.002961	-3.385885	0.155486
C	1.334138	-1.747801	-4.214022
H	1.567337	-1.213950	-5.136522
C	-2.567605	-2.398258	3.972994
H	-2.419803	-3.269525	4.613398
C	1.731303	-0.361877	-0.005770
H	2.405693	-0.054439	-0.812191
H	2.262277	-1.109165	0.608191
C	1.261716	0.815473	0.832119
H	0.765538	1.556724	0.183713
H	2.114835	1.297620	1.327092
C	1.306675	-3.138738	-4.215616
H	1.521687	-3.691521	-5.132304
C	0.160529	1.009389	-4.284453
H	0.546121	0.713730	-5.272326
H	0.100367	2.105292	-4.247101
H	-0.862409	0.626080	-4.172170
C	-3.163046	1.150090	1.573965
H	-2.385517	1.224156	0.799000
C	-3.719902	-1.629121	4.118292
H	-4.471902	-1.904816	4.860452
C	2.497986	1.043663	-3.340034
H	3.190200	0.699257	-2.556315
H	2.488119	2.143347	-3.324836
H	2.913049	0.721127	-4.307621
C	0.284593	0.312536	1.878869
H	0.796641	-0.253972	2.672629
H	-0.252033	1.145587	2.355053
C	1.968704	-4.232323	0.048572
H	2.588221	-4.824468	-0.641669
H	1.873198	-4.794934	0.988984
H	2.508240	-3.298700	0.262273
C	-0.169860	-5.287713	-0.789878
H	-1.134833	-5.124482	-1.290155
H	-0.364346	-5.771007	0.176952
H	0.414957	-5.997075	-1.392959
C	-0.335155	-2.934467	2.955648
H	0.256489	-2.618310	2.083747
C	-3.020189	2.390701	2.473476
H	-3.825699	2.437876	3.223779
H	-3.066368	3.297522	1.853198
H	-2.060376	2.397383	3.012287
C	-4.514164	1.169219	0.843259
H	-4.647058	0.273446	0.219907
H	-4.552999	2.046587	0.182262
H	-5.359330	1.226897	1.547180
C	-0.684547	-4.420187	2.770182
H	-1.191182	-4.823048	3.658967
H	0.227947	-5.014413	2.616614
H	-1.350095	-4.568525	1.908963
C	0.543195	-2.741055	4.205994
H	0.809999	-1.685411	4.360133
H	1.473365	-3.321868	4.114976
H	0.016205	-3.084145	5.108955
B	-1.844567	-1.482152	-0.898766
H	-1.885807	-1.064979	-2.011383
I	-1.620248	2.582721	-1.424996
I	-3.380703	-2.830456	-0.319785

(12) Product

74

N	1.035292	-1.113269	-1.012936
N	1.296433	0.368792	0.750741
C	0.473412	-0.397542	-0.007493
C	0.320133	-2.022018	-1.895885
C	1.022211	0.773839	2.122572
C	0.118908	-1.650071	-3.244409
C	0.503604	-0.283951	-3.799746
H	0.660352	0.391295	-2.944288
C	0.511348	2.470647	3.752078
H	0.195841	3.486658	3.996154
C	-0.555268	-4.226964	-2.327262
H	-0.819952	-5.227598	-1.981409
C	-0.005541	-3.313010	-1.419337
C	0.640645	2.101144	2.405780
C	1.346983	-0.144563	3.150238
C	0.231185	-3.743325	0.020297
H	0.457996	-2.845556	0.611803
C	-0.436104	-2.606303	-4.108230
H	-0.608785	-2.342800	-5.152808
C	1.196547	0.277337	4.476690
H	1.418704	-0.419957	5.286901
C	2.500551	-1.137849	-1.186626
H	2.710458	-1.566881	-2.170909
H	2.939894	-1.810613	-0.428721
C	3.040440	0.270174	-1.026245
H	2.588122	0.930027	-1.781334
H	4.129925	0.294239	-1.163849
C	-0.768410	-3.882290	-3.660802
H	-1.196945	-4.610398	-4.352420
C	-0.610969	0.331464	-4.661585
H	-0.742790	-0.219354	-5.605142
H	-0.352044	1.369025	-4.919768
H	-1.567772	0.343246	-4.124297
C	0.366231	3.134538	1.325313
H	0.370186	2.618438	0.353116
C	0.774895	1.569793	4.779968
H	0.660056	1.877871	5.821256
C	1.804761	-0.357532	-4.623952
H	2.656044	-0.744792	-4.046661
H	2.076825	0.641789	-4.995824
H	1.670449	-1.016988	-5.495199
C	2.690649	0.718071	0.377212
H	3.365669	0.252739	1.112252
H	2.786550	1.806891	0.492288
C	1.445601	-4.685433	0.114355
H	1.263244	-5.616068	-0.444851
H	1.643952	-4.954311	1.162927
H	2.353526	-4.221465	-0.298997
C	-1.015353	-4.381930	0.652226
H	-1.877726	-3.703756	0.594091
H	-0.827021	-4.599896	1.713564
H	-1.282209	-5.329566	0.160903
C	1.868057	-1.551534	2.886004
H	1.858059	-1.724479	1.800057
C	1.454837	4.224428	1.304899
H	1.459591	4.791424	2.248490
H	1.266567	4.934087	0.485368
H	2.463065	3.805053	1.167681
C	-1.022331	3.773128	1.495575
H	-1.803185	3.005333	1.572323
H	-1.254455	4.407554	0.627767
H	-1.062849	4.404661	2.396331
C	0.977794	-2.628861	3.527216
H	0.985080	-2.548490	4.624222
H	1.347026	-3.631757	3.265241
H	-0.062419	-2.535368	3.187891
C	3.324829	-1.702141	3.362514
H	3.985238	-0.947296	2.910519
H	3.711562	-2.698685	3.100189
H	3.393849	-1.590953	4.455242
B	-1.146475	-0.466457	0.104326
H	-1.578046	-1.428125	-0.450650
I	-1.888491	1.296626	-1.185471

I	-2.156760	-0.485650	2.131385

(13) 5-NHC

69

N	0.125994	-0.205447	0.207493
N	1.524274	-0.289205	1.845585
C	0.185240	-0.263590	1.572774
C	-1.097789	-0.154778	-0.550341
C	2.091696	-0.354581	3.169195
C	-1.647380	1.105839	-0.850443
C	-1.008104	2.402789	-0.376206
H	-0.198292	2.145124	0.321891
C	2.895272	0.759632	5.134413
H	3.113645	1.672400	5.691904
C	-2.845613	-1.288379	-1.738648
H	-3.324521	-2.207458	-2.082217
C	-1.678861	-1.367761	-0.965726
C	2.369507	0.852419	3.838037
C	2.338212	-1.622720	3.728297
C	-1.073377	-2.718645	-0.614801
H	-0.257347	-2.546725	0.102203
C	-2.814431	1.128602	-1.626391
H	-3.268718	2.087547	-1.883563
C	2.863389	-1.658717	5.027744
H	3.056660	-2.622394	5.502636
C	1.396984	-0.195743	-0.356501
H	1.546921	-0.152049	-1.428577
C	-3.406143	-0.054452	-2.068800
H	-4.316298	-0.014838	-2.670929
C	-2.002557	3.281821	0.398829
H	-2.823951	3.630638	-0.245537
H	-1.489717	4.170993	0.795665
H	-2.433921	2.727842	1.243988
C	2.073306	2.208205	3.212074
H	1.879217	2.049292	2.140262
C	3.134942	-0.481378	5.724905
H	3.538918	-0.531466	6.738166
C	-0.382713	3.168659	-1.555846
H	0.363365	2.554794	-2.082189
H	0.115459	4.082824	-1.198996
H	-1.151834	3.463442	-2.285799
C	2.281091	-0.248748	0.677407
H	3.364161	-0.262195	0.698062
C	-0.467612	-3.387939	-1.861712
H	-1.244249	-3.596863	-2.613189
H	0.008769	-4.342519	-1.591481
H	0.292286	-2.746541	-2.332850
C	-2.089678	-3.640681	0.077561
H	-2.504765	-3.158366	0.973272
H	-1.599989	-4.576635	0.386610
H	-2.920931	-3.905077	-0.593592
C	2.011696	-2.909214	2.983475
H	1.817914	-2.649544	1.931435
C	3.264828	3.172664	3.317570
H	3.476145	3.444727	4.362603
H	3.044627	4.103672	2.773910
H	4.178251	2.733217	2.890307
C	0.798635	2.820664	3.820906
H	-0.058659	2.143619	3.704090
H	0.559651	3.774236	3.324939
H	0.937987	3.020427	4.894605
C	0.726493	-3.549220	3.538575
H	0.863898	-3.851042	4.588370
H	0.466189	-4.447137	2.956718
H	-0.116477	-2.846166	3.488908
C	3.184212	-3.901981	2.994355
H	4.104236	-3.442704	2.603603
H	2.943702	-4.775064	2.369442
H	3.394475	-4.271648	4.009196
B	-1.040820	-0.292413	2.580538
H	-0.629887	-0.367249	3.725776
H	-1.697857	0.730013	2.405953
H	-1.747630	-1.253051	2.289871

(14) TS_1

71

N	-2.564780	2.864105	1.893961
N	-1.867570	1.460464	3.397935
C	-1.850179	1.707037	2.052639
C	-2.761828	3.547794	0.633835
C	-1.158955	0.381251	4.054728
C	-3.981072	3.362358	-0.051394
C	-5.105025	2.496710	0.502626
H	-4.658990	1.763210	1.194632
C	-1.149793	-1.810045	5.013503
H	-1.655878	-2.741033	5.271103
C	-1.940729	5.047731	-1.045037
H	-1.163179	5.703295	-1.440866
C	-1.725258	4.381505	0.168951
C	-1.871619	-0.789545	4.379546
C	0.205028	0.573885	4.344599
C	-0.437215	4.604853	0.949006
H	-0.402989	3.876948	1.773350
C	-4.137606	4.054360	-1.260960
H	-5.061336	3.937209	-1.828512
C	0.873922	-0.482482	4.978177
H	1.934771	-0.379447	5.215010
C	-3.001338	3.334759	3.116036
H	-3.567734	4.253225	3.207377
C	-3.130832	4.884845	-1.752488
H	-3.275713	5.410020	-2.698532
C	-5.846519	1.705401	-0.584784
H	-6.452427	2.364855	-1.223955
H	-6.529988	0.983115	-0.116447
H	-5.154319	1.145080	-1.227472
C	-3.360702	-0.935694	4.102417
H	-3.617994	-0.253468	3.275298
C	0.205796	-1.660900	5.305999
H	0.747270	-2.474721	5.792136
C	-6.104571	3.356837	1.302341
H	-5.620230	3.898790	2.126296
H	-6.894318	2.722108	1.730337
H	-6.581390	4.100822	0.645943
C	-2.561057	2.451991	4.062868
H	-2.665249	2.452407	5.140803
C	-0.426824	6.009572	1.579528
H	-0.443279	6.788596	0.802096
H	0.481712	6.151320	2.183575
H	-1.299962	6.165230	2.230300
C	0.815859	4.367575	0.091605
H	0.809292	3.362344	-0.351758
H	1.718820	4.462915	0.712489
H	0.895493	5.102299	-0.723265
C	0.947571	1.860466	4.012667
H	0.243922	2.549698	3.521114
C	-4.178776	-0.514410	5.339677
H	-3.956761	-1.178065	6.189158
H	-5.255371	-0.584292	5.124637
H	-3.960815	0.516489	5.653792
C	-3.755670	-2.349884	3.659047
H	-3.161524	-2.701351	2.804811
H	-4.809468	-2.360969	3.347240
H	-3.649278	-3.078061	4.477526
C	2.103174	1.614431	3.027992
H	2.868812	0.958005	3.467796
H	2.588000	2.566786	2.765531
H	1.743769	1.144041	2.102349
C	1.440210	2.559189	5.292064
H	0.608881	2.763390	5.982820
H	1.923523	3.515462	5.041743
H	2.176418	1.939459	5.825040
B	-1.061273	0.914589	0.962649
H	-0.348531	0.040034	1.356589

H	-2.728711	0.791067	-0.357281
I	-3.577036	-4.075852	-0.059025
H	-0.772768	1.521517	-0.030123
I	-2.859759	-0.890251	-0.051301

(15) Int_1

69

N	0.620228	-0.998933	-1.127522
N	0.585341	-1.090728	1.054754
C	-0.245510	-1.112545	-0.052841
C	0.202834	-1.031975	-2.513719
C	0.122876	-1.238930	2.418728
C	-0.039364	0.191034	-3.167299
C	0.096717	1.528135	-2.455845
H	0.714746	1.389377	-1.554154
C	-0.623898	-0.259886	4.467791
H	-0.858204	0.613583	5.078172
C	-0.364493	-2.301451	-4.462778
H	-0.492456	-3.255860	-4.977073
C	0.055029	-2.291098	-3.124955
C	-0.158607	-0.075064	3.158122
C	-0.028462	-2.544603	2.921417
C	0.323058	-3.598268	-2.392507
H	0.680862	-3.359303	-1.379123
C	-0.457653	0.118075	-4.503813
H	-0.658802	1.040716	-5.050021
C	-0.494743	-2.666773	4.237848
H	-0.627609	-3.660712	4.669423
C	1.905251	-0.882054	-0.703368
H	2.739432	-0.766269	-1.384219
C	-0.620191	-1.111206	-5.143080
H	-0.947280	-1.141587	-6.184293
C	-1.282819	2.036848	-1.999221
H	-1.937441	2.230989	-2.863008
H	-1.170096	2.972774	-1.432553
H	-1.791069	1.305908	-1.352213
C	-0.012310	1.316984	2.563530
H	0.623878	1.254440	1.666398
C	-0.791726	-1.538010	5.000854
H	-1.155599	-1.655284	6.023629
C	0.818843	2.581107	-3.307288
H	1.792824	2.210611	-3.656333
H	1.004258	3.477194	-2.698684
H	0.224473	2.883235	-4.183526
C	1.883032	-0.939918	0.683181
H	2.694959	-0.882429	1.397593
C	1.429282	-4.414149	-3.081655
H	1.125164	-4.727765	-4.091259
H	1.650207	-5.322389	-2.501234
H	2.357082	-3.831004	-3.173932
C	-0.967138	-4.420529	-2.235240
H	-1.744774	-3.846014	-1.711161
H	-0.769690	-5.336720	-1.658693
H	-1.370321	-4.718412	-3.214816
C	0.281368	-3.785258	2.096582
H	0.671184	-3.461643	1.119289
C	0.691204	2.294361	3.515369
H	0.080007	2.518138	4.403230
H	0.884998	3.240090	2.989862
H	1.660088	1.896815	3.848295
C	-1.383352	1.862057	2.124158
H	-1.877298	1.188295	1.407655
H	-1.261239	2.842666	1.641080
H	-2.055542	1.983032	2.987813
C	-0.992866	-4.603931	1.827888
H	-1.426195	-4.983814	2.765370
H	-0.764407	-5.468094	1.186452
H	-1.758791	-3.995831	1.324719
C	1.372519	-4.644009	2.756960
H	2.290733	-4.062762	2.925842
H	1.622013	-5.502083	2.115144
H	1.038469	-5.037862	3.728256
B	-1.750772	-1.249765	-0.082246
H	-2.310607	-1.260001	-1.139490
H	-2.341898	-1.354640	0.952641
I	3.137592	2.156161	0.146681

(16) TS_2

69

N	0.885537	-1.547969	-0.574525
N	-0.249338	-1.542196	1.304638
C	-0.395379	-1.508711	-0.065834
C	1.258559	-1.770883	-1.967401
C	-1.315164	-1.809370	2.265276
C	1.804305	-0.703660	-2.704671
C	1.895585	0.707505	-2.161829
H	1.255314	0.792365	-1.269488
C	-2.943866	-1.056653	3.852759
H	-3.457625	-0.247632	4.373451
C	1.608319	-3.301345	-3.782869
H	1.533290	-4.299607	-4.216043
C	1.133921	-3.081667	-2.483174
C	-1.945600	-0.736073	2.920502
C	-1.626707	-3.161197	2.521967
C	0.569310	-4.245014	-1.681045
H	-0.067897	-3.832614	-0.886094
C	2.266294	-0.990325	-3.998402
H	2.693395	-0.184125	-4.596313
C	-2.634540	-3.418875	3.461892
H	-2.907495	-4.452952	3.680616
C	1.791632	-1.537997	0.452276
H	2.860481	-1.557885	0.275432
C	2.178296	-2.272404	-4.530941
H	2.544321	-2.471871	-5.540090
C	1.370967	1.743645	-3.168053
H	2.037412	1.846626	-4.038113
H	1.297669	2.718689	-2.667040
H	0.366915	1.476807	-3.528066
C	-1.551831	0.703913	2.676622
H	-1.001122	0.771287	1.724739
C	-3.288722	-2.379595	4.120198
H	-4.071546	-2.603033	4.847741
C	3.330399	1.053160	-1.728377
H	3.721944	0.338552	-0.988336
H	3.339742	2.052414	-1.269589
H	4.015533	1.053948	-2.590515
C	1.079188	-1.531516	1.631014
H	1.418657	-1.547231	2.660024
C	1.703487	-5.037648	-1.004228
H	2.364631	-5.487444	-1.760320
H	1.291073	-5.849540	-0.385674
H	2.319331	-4.395671	-0.357473
C	-0.325300	-5.169402	-2.520378
H	-1.122070	-4.604663	-3.024633
H	-0.796137	-5.922726	-1.873238
H	0.248197	-5.711703	-3.285808
C	-0.932917	-4.328444	1.836527
H	-0.141297	-3.932144	1.184145
C	-0.594610	1.195534	3.777725
H	-1.096706	1.216766	4.757722
H	-0.249210	2.209091	3.528173
H	0.292269	0.549721	3.864070
C	-2.760415	1.640614	2.548162
H	-3.485917	1.262188	1.812938
H	-2.408479	2.622405	2.201921
H	-3.279892	1.779269	3.509108
C	-1.917916	-5.108085	0.949391
H	-2.735732	-5.535671	1.547628
H	-1.404184	-5.938033	0.442595
H	-2.368600	-4.459949	0.182880
C	-0.243106	-5.253692	2.853201
H	0.470048	-4.697393	3.478450
H	0.306027	-6.050523	2.329643

H	-0.973816	-5.734391	3.520476
B	-1.694918	-1.332351	-0.852449
H	-1.635006	-1.277616	-2.044926
H	-2.724648	-1.274661	-0.248755
I	0.136538	2.936515	0.260816

(17) Int_2

69

N	0.508481	-0.686169	-1.236595
N	0.540405	-1.108056	0.886352
C	-0.310196	-0.899200	-0.162855
C	0.073404	-0.514582	-2.605041
C	0.142231	-1.514020	2.215891
C	0.081937	0.779790	-3.159018
C	0.490217	2.006594	-2.356503
H	0.416363	1.747960	-1.288814
C	-0.389985	-0.969614	4.487356
H	-0.534652	-0.239019	5.284264
C	-0.644438	-1.487309	-4.675928
H	-0.933658	-2.353044	-5.273877
C	-0.288725	-1.666440	-3.333009
C	-0.024625	-0.528435	3.207747
C	-0.028800	-2.891154	2.455414
C	-0.259491	-3.059186	-2.720373
H	-0.252611	-2.946667	-1.627248
C	-0.278759	0.897598	-4.509365
H	-0.286302	1.883430	-4.977063
C	-0.400804	-3.274359	3.751404
H	-0.553957	-4.332183	3.973803
C	1.842606	-0.767709	-0.862878
H	2.645090	-0.642357	-1.579014
C	-0.635457	-0.220969	-5.260139
H	-0.915980	-0.104669	-6.309086
C	-0.445553	3.201472	-2.591225
H	-0.363079	3.590562	-3.617440
H	-0.180181	4.019733	-1.905710
H	-1.490579	2.924176	-2.399158
C	0.221221	0.946507	2.925493
H	0.102173	1.103811	1.842105
C	-0.579743	-2.325170	4.756293
H	-0.871611	-2.643800	5.759049
C	1.949194	2.396298	-2.661404
H	2.648412	1.573098	-2.455640
H	2.250704	3.259153	-2.048441
H	2.062029	2.674547	-3.720635
C	1.863378	-1.031947	0.473118
H	2.686211	-1.187902	1.159911
C	1.030429	-3.799134	-3.120178
H	1.071449	-3.952894	-4.209430
H	1.072563	-4.785691	-2.634034
H	1.927192	-3.234470	-2.824734
C	-1.506448	-3.885893	-3.065293
H	-2.423332	-3.349647	-2.783519
H	-1.484648	-4.838990	-2.516814
H	-1.558756	-4.124262	-4.138166
C	0.168343	-3.944793	1.374077
H	0.508795	-3.437824	0.458776
C	1.661815	1.333982	3.312753
H	1.822842	1.199103	4.393601
H	1.852365	2.389667	3.067731
H	2.406364	0.722339	2.782808
C	-0.793913	1.865157	3.618304
H	-1.822897	1.578870	3.361774
H	-0.641363	2.902060	3.284894
H	-0.682382	1.851072	4.713250
C	-1.152626	-4.656487	1.035598
H	-1.540904	-5.207035	1.905792
H	-0.996014	-5.380240	0.221270
H	-1.918131	-3.935579	0.716887
C	1.266244	-4.949626	1.763114
H	2.216142	-4.439176	1.980610
H	1.438016	-5.661117	0.941656
H	0.982866	-5.529231	2.654473
B	-1.893060	-0.957839	-0.145499
H	-2.338500	-1.317554	-1.207585
H	-2.304168	-1.550205	0.820907
I	-2.636185	1.245493	0.114016

(18) TS_3

71

N	-0.581550	-1.516679	2.645821
N	0.519943	-1.732006	0.766865
C	-0.298871	-0.876389	1.461123
C	-1.233930	-0.915727	3.799633
C	1.291759	-1.409159	-0.425490
C	-2.506811	-1.382505	4.181623
C	-3.279452	-2.418264	3.391133
H	-2.746667	-2.636931	2.453622
C	1.570854	-1.392838	-2.801998
H	1.206292	-1.630762	-3.802713
C	-1.133133	0.572009	5.681851
H	-0.611076	1.327330	6.271297
C	-0.523098	0.067721	4.525778
C	0.787437	-1.747820	-1.693565
C	2.547202	-0.795893	-0.227473
C	0.863853	0.566013	4.143429
H	1.100643	0.198450	3.136211
C	-3.063780	-0.837737	5.348871
H	-4.049909	-1.176962	5.669449
C	3.285102	-0.470256	-1.372095
H	4.259068	0.010048	-1.260708
C	0.012816	-2.753707	2.664113
H	-0.088064	-3.426095	3.507376
C	-2.387001	0.123618	6.094406
H	-2.839598	0.531427	7.000335
C	-4.670773	-1.904858	2.987835
H	-5.328120	-1.774172	3.861353
H	-5.135393	-2.632462	2.307361
H	-4.603443	-0.942823	2.459524
C	-0.515041	-2.493666	-1.891477
H	-1.012142	-2.622611	-0.918544
C	2.798326	-0.753832	-2.647725
H	3.387789	-0.485094	-3.526639
C	-3.387590	-3.744239	4.163081
H	-2.397882	-4.127344	4.455525
H	-3.866329	-4.498265	3.522105
H	-3.987204	-3.626978	5.079430
C	0.696374	-2.891706	1.481908
H	1.295911	-3.709655	1.100502
C	1.931549	-0.001442	5.095185
H	1.768940	0.350537	6.124976
H	2.935480	0.321864	4.780608
H	1.913279	-1.101187	5.107469
C	0.926839	2.100429	4.074419
H	0.171360	2.499168	3.381967
H	1.917487	2.422244	3.722833
H	0.760225	2.560040	5.059630
C	3.128306	-0.505066	1.148744
H	2.380942	-0.777237	1.907250
C	-0.242923	-3.907484	-2.435519
H	0.196414	-3.869412	-3.444657
H	-1.187324	-4.467814	-2.476464
H	0.447962	-4.462227	-1.782805
C	-1.496664	-1.736918	-2.798674
H	-1.674750	-0.714839	-2.434310
H	-2.458817	-2.268866	-2.807962
H	-1.128102	-1.672889	-3.834217
C	3.443931	0.987781	1.333828
H	4.228666	1.320041	0.638426
H	3.803590	1.176993	2.356117
H	2.554061	1.608915	1.159031
C	4.367884	-1.376669	1.416184
H	4.132473	-2.447045	1.321902

H	4.748509	-1.196912	2.432896
H	5.175429	-1.145795	0.705765
B	-0.970102	0.456346	1.079255
H	-2.722643	-0.749351	0.228136
I	-3.231783	-4.242889	0.097240
H	-1.785848	0.897200	1.827199
H	-2.915927	-1.499432	0.161755
I	-0.406430	1.702845	-0.553192

(19) Int_3

69

N	1.015135	0.284703	-1.675294
N	1.314730	-0.827165	0.182895
C	0.346334	-0.505937	-0.750859
C	0.422894	0.806145	-2.889800
C	1.131522	-1.698002	1.325415
C	-0.120011	2.104488	-2.863304
C	-0.108745	2.956770	-1.603260
H	0.675939	2.577840	-0.928380
C	0.667780	-1.991470	3.650578
H	0.444009	-1.583781	4.637490
C	-0.182804	0.486529	-5.183003
H	-0.211720	-0.123396	-6.087820
C	0.420893	-0.024755	-4.025884
C	0.858210	-1.111923	2.574435
C	1.259496	-3.085537	1.115974
C	1.024706	-1.422613	-4.021892
H	1.525799	-1.578360	-3.054040
C	-0.709789	2.562355	-4.050150
H	-1.146207	3.561709	-4.077994
C	1.072738	-3.911818	2.230710
H	1.161956	-4.993453	2.118842
C	2.311890	0.465037	-1.310135
H	3.004517	1.064526	-1.887781
C	-0.745389	1.762838	-5.193140
H	-1.212440	2.141452	-6.104557
C	-1.452371	2.846658	-0.859427
H	-2.278268	3.232409	-1.477013
H	-1.414119	3.428767	0.072869
H	-1.690003	1.804207	-0.597718
C	0.749318	0.393180	2.766266
H	1.172483	0.896113	1.882486
C	0.769461	-3.371232	3.481213
H	0.619041	-4.034683	4.335254
C	0.246130	4.423540	-1.883317
H	1.187807	4.504880	-2.444064
H	0.380194	4.953213	-0.929709
H	-0.544226	4.940318	-2.449072
C	2.501253	-0.239303	-0.133338
H	3.385217	-0.347673	0.482903
C	2.098255	-1.579709	-5.111340
H	1.666226	-1.483655	-6.118549
H	2.566034	-2.573074	-5.043080
H	2.886548	-0.820165	-5.006994
C	-0.065976	-2.500300	-4.149148
H	-0.811907	-2.413059	-3.345210
H	0.379903	-3.504715	-4.094536
H	-0.596087	-2.415380	-5.109536
C	1.624415	-3.671595	-0.241308
H	1.427988	-2.906056	-1.007727
C	1.573299	0.881344	3.967291
H	1.160637	0.522529	4.922604
H	1.574441	1.980116	3.986281
H	2.619134	0.551369	3.893241
C	-0.719440	0.835298	2.886798
H	-1.306033	0.539601	2.005650
H	-0.772279	1.930082	2.980517
H	-1.195955	0.389203	3.773386
C	0.775513	-4.896059	-0.612441
H	0.980823	-5.750946	0.048700
H	1.006696	-5.212930	-1.640086
H	-0.298305	-4.668949	-0.555885
C	3.127875	-4.002277	-0.293658
H	3.744434	-3.116850	-0.080133
H	3.404584	-4.379943	-1.289529
H	3.380847	-4.774546	0.448219
B	-1.119498	-0.869124	-0.898594
H	-1.710008	-0.434861	-1.838224
I	3.156248	2.971730	0.784298
I	-2.266752	-2.116331	0.401164

(20) TS_4

69

N	0.820839	-1.549038	-0.514546
N	-0.267784	-1.517853	1.392798
C	-0.447255	-1.495641	0.028186
C	1.155060	-1.813076	-1.910244
C	-1.283437	-1.770095	2.411219
C	1.736093	-0.785102	-2.675713
C	1.894910	0.631804	-2.164584
H	1.311375	0.748929	-1.237705
C	-2.822459	-0.989691	4.072230
H	-3.303972	-0.171892	4.609883
C	1.400624	-3.388063	-3.705471
H	1.272035	-4.389112	-4.119273
C	0.962064	-3.125917	-2.401254
C	-1.871484	-0.685878	3.087387
C	-1.578560	-3.117460	2.706724
C	0.366329	-4.252359	-1.569215
H	-0.227626	-3.803326	-0.761202
C	2.161481	-1.114171	-3.972118
H	2.614550	-0.338280	-4.590900
C	-2.541160	-3.358280	3.696321
H	-2.801895	-4.388483	3.946215
C	1.754890	-1.532917	0.488537
H	2.818060	-1.566288	0.282313
C	2.003337	-2.398953	-4.481536
H	2.340137	-2.631728	-5.493691
C	1.330906	1.659518	-3.158429
H	1.936533	1.719376	-4.075736
H	1.319597	2.648259	-2.679492
H	0.296546	1.414507	-3.439728
C	-1.487096	0.749149	2.803713
H	-0.959050	0.798147	1.838083
C	-3.161953	-2.307649	4.369211
H	-3.910109	-2.518996	5.135855
C	3.361050	0.949880	-1.826312
H	3.780269	0.237802	-1.098788
H	3.422624	1.956220	-1.387440
H	3.992672	0.920286	-2.727640
C	1.073108	-1.506010	1.681358
H	1.434976	-1.506814	2.702774
C	1.483254	-5.087564	-0.916012
H	2.103628	-5.571643	-1.685296
H	1.053990	-5.875812	-0.278932
H	2.142700	-4.466606	-0.292220
C	-0.596961	-5.142558	-2.368415
H	-1.378326	-4.545891	-2.860033
H	-1.087160	-5.860204	-1.695277
H	-0.073433	-5.724845	-3.140331
C	-0.900679	-4.295950	2.024736
H	-0.197446	-3.908369	1.273864
C	-0.506162	1.263957	3.872758
H	-0.989127	1.310667	4.861608
H	-0.162521	2.269819	3.591980
H	0.380121	0.617050	3.957709
C	-2.698846	1.683443	2.685518
H	-3.438556	1.291863	1.971936
H	-2.355301	2.659639	2.315469
H	-3.198128	1.837277	3.654745
C	-1.917762	-5.183401	1.288639
H	-2.637486	-5.630415	1.990162
H	-1.403009	-6.006894	0.772170

H	-2.486725	-4.607847	0.544869
C	-0.069040	-5.113529	3.028863
H	0.677377	-4.484560	3.535536
H	0.460357	-5.927197	2.511135
H	-0.709033	-5.565081	3.801285
B	-1.695140	-1.328574	-0.849552
H	-1.531564	-1.190719	-2.021847
I	0.224726	2.874127	0.310300
I	-3.700080	-1.390712	-0.159687

(21) product

69

N	0.873584	-1.447713	-0.810152
N	1.275991	-0.074964	0.822961
C	0.254405	-0.654991	0.120782
C	0.227966	-2.408509	-1.682160
C	1.189348	0.639425	2.084874
C	0.146149	-2.133585	-3.059526
C	0.648792	-0.832964	-3.669573
H	0.788805	-0.108318	-2.852698
C	1.016152	2.678865	3.326717
H	0.907459	3.763469	3.367232
C	-0.768038	-4.572202	-1.970560
H	-1.132036	-5.516473	-1.563081
C	-0.224942	-3.615454	-1.104742
C	1.067644	2.039862	2.079925
C	1.318241	-0.123715	3.265002
C	-0.106404	-3.902462	0.385676
H	-0.007810	-2.941334	0.909344
C	-0.403997	-3.132065	-3.878094
H	-0.485115	-2.957504	-4.952079
C	1.265253	0.569311	4.480886
H	1.347796	0.013434	5.416884
C	2.251609	-1.346869	-0.701895
H	2.916392	-1.908256	-1.346366
C	-0.853052	-4.336976	-3.343186
H	-1.280068	-5.098201	-3.999214
C	-0.366175	-0.217723	-4.644998
H	-0.506529	-0.845591	-5.537517
H	-0.006899	0.764649	-4.984891
H	-1.340347	-0.073006	-4.159016
C	1.057117	2.845472	0.791503
H	0.756779	2.173407	-0.026586
C	1.105259	1.953478	4.513600
H	1.056903	2.472706	5.473008
C	2.006132	-1.046736	-4.365819
H	2.763385	-1.452060	-3.679179
H	2.384544	-0.094758	-4.766675
H	1.905238	-1.752585	-5.204927
C	2.503716	-0.483281	0.318610
H	3.434051	-0.136969	0.751808
C	1.162775	-4.724490	0.678830
H	1.114296	-5.706203	0.184140
H	1.268816	-4.892042	1.761623
H	2.068605	-4.210821	0.323616
C	-1.355980	-4.574969	0.969488
H	-2.259047	-3.990055	0.746442
H	-1.259794	-4.645757	2.062655
H	-1.496143	-5.595896	0.583552
C	1.543639	-1.629984	3.260561
H	1.429218	-1.993641	2.229270
C	2.474611	3.364171	0.481667
H	2.820858	4.049091	1.271203
H	2.481445	3.910947	-0.473166
H	3.201776	2.541418	0.407659
C	0.042062	3.995746	0.813823
H	-0.964149	3.628326	1.057573
H	-0.003848	4.468801	-0.177993
H	0.319366	4.774342	1.540340
C	0.520516	-2.388762	4.119924
H	0.607735	-2.121906	5.183609
H	0.692156	-3.472921	4.035392
H	-0.505402	-2.170967	3.793401
C	2.982014	-1.959716	3.702246
H	3.726502	-1.442218	3.079498
H	3.165063	-3.042424	3.629517
H	3.149562	-1.656654	4.747056
B	-1.332163	-0.496272	0.162195
H	-1.857757	-1.450666	-0.333031
I	-1.849915	1.252862	-1.259300
I	-2.269806	-0.213741	2.198783