

Supporting Information

Reversible Carbon-Boron Bond Formation at Platinum Centers Through σ -BH Complexes

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1. General

All manipulations were carried out using standard Schlenk and glovebox techniques, under an atmosphere of argon and of high purity nitrogen, respectively. All solvents were dried and degassed prior to use. *n*-Pentane was distilled over sodium and stored under Na/K alloy. Dichloromethane- d_2 (CD_2Cl_2) was heated under reflux over calcium hydride, distilled under Argon and stored under 3 Å activated molecular sieves. NMR spectra were recorded on Bruker DRX-500, DRX-400 and DPX-300 spectrometers, and they were referenced to external $SiMe_4$ (δ 0 ppm) using the residual protio solvent peaks as internal standard (1H NMR experiments) or the characteristic resonances of the solvent nuclei (^{13}C NMR experiments). ^{11}B NMR spectra were referenced to an external standard of $BF_3 \cdot Et_2O$. Spectral assignments were made by routine one- and two-dimensional NMR experiments where appropriate. Elemental analysis was carried out with a LECO TruSpec CHN elementary analyser. HBpin and HBcat were purchased from Aldrich or TCI, stored under argon and used as received. Borane HBdab was prepared from $SMe_2 \cdot BH_3$ and 1,2-phenylenediamine as previously described.^[1] Complex $[Pt(I^tBu^iPr)(I^iBu^iPr)][BAr^F]$, **1**, was obtained accordingly to published procedures.^[2]

2. Synthesis and spectroscopic and analytical data for complexes **2a-c**.

General procedure: Complex **1** (80 mg, 0.057 mmol) was dissolved in 2 mL of dry CH₂Cl₂ and mixed via cannula with a solution of the corresponding borane (0.063 mmol) in 0.5 mL of CH₂Cl₂. The mixture was stirred at rt for 35 min (**2a**), 10 min (**2b**) or 15 h (**2c**) and the solvent was removed under reduced pressure. Complexes **2a** and **2c** were washed with pentane (2 x 5 mL) and dried under vacuum. Compounds **2a** and **2c** can be crystallized by slow diffusion of a concentrated solution of **2a** or **2c** in CH₂Cl₂ into pentane (Yields: **2a**: 76%; **2c**: 81%). Complex **2b** proved to be extremely sensitive to trace amounts of water present in the solvents used during the attempts of purification, leading to hydride Pt(II) complex [Pt(H)(I^tBu'Pr)₂][BAR^F]^[3] (together with HOBcat) and could not be isolated in pure form. This complex can be prepared and spectroscopically characterized *in situ*. Alternatively, it can be prepared in higher spectroscopic purity using the following method: complex **1** (80 mg, 0.057 mmol) was suspended in 3 mL of dry pentane in a vial inside the glove-box. Then HOBcat (0.063 mmol) was added, the vial was closed and the suspension was stirred for 24 h at rt. The solvent was decanted and the off-white solid dried under vacuum. Under these reaction conditions the amounts of boron by-products resulting from hydrolysis of complex **2b** are considerably lower, but still present.

Complex 2a: ¹H-NMR (300 MHz, CD₂Cl₂, 25 °C): δ = 7.74 (br, 8H, H_{ortho}-BAR^F), 7.58 (br, 4H, H_{para}-BAR^F), 7.19 (br, 2H, =CH), 7.06 (d, 2H, J_{H,H} = 1.4 Hz, =CH), 5.96 (sept, 2H, J_{H,H} = 6.8 Hz, CH(CH₃)₂), 1.90 (s, 18H, ^tBu), 1.50 (d, 12H, J_{H,H} = 6.8 Hz, CH(CH₃)₂), 0.96 (s, 12H, CH₃-Bpin). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C): δ = 177.5 (Pt=C), 162.4 (q, J_{C,B} = 50 Hz, C_{ipso}-BAR^F), 135.2 (br, C_{ortho}-BAR^F), 129.3 (br q, J_{C,F} = 31 Hz, C_{meta}-BAR^F), 125.0 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 120.5 (br, =CH), 117.9 (br, C_{para}-BAR^F), 116.1 (s+d, J_{Pt,C} = 32 Hz, =CH), 83.8 (s+d, J_{Pt,C} = 47 Hz, C_q-Bpin), 59.3 (C_q-^tBu), 54.5 (CH(CH₃)₂), 32.2 (^tBu), 24.9 (CH₃-Bpin), 23.4 (CH(CH₃)₂). ¹¹B{¹H}(128 MHz, CD₂Cl₂, 25 °C): δ = 12.7 (br s+d, J_{Pt,B} = 1483 Hz, Pt-Bpin), -6.6 (s, BAR^F). **Elemental analysis calcd (%) for C₅₈H₆₀B₂F₂₄N₄O₂Pt:** C, 45.90; H, 3.98; N, 3.69; **Found:** C, 45.7; H, 4.1; N, 3.78.

Complex 2b: ¹H-NMR (400 MHz, CD₂Cl₂, 25 °C): δ = 7.74 (br, 8H, H_{ortho}-BAR^F), 7.57 (br, 4H, H_{para}-BAR^F), 7.24 and 7.14 (d, 2H each, J_{H,H} = 1.9 Hz, =CH), 7.00 and 6.92 (m, 2H each, CH-Bcat), 5.96 (sept, 2H, J_{H,H} = 6.7 Hz, CH(CH₃)₂), 1.87 (s, 18H, ^tBu), 1.53 (d, 12H, J_{H,H} = 6.7 Hz, CH(CH₃)₂). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C): δ = 173.5 (Pt=C), 162.2 (q, J_{C,B} = 50 Hz, C_{ipso}-BAR^F), 149.0 (C_q-Bcat), 135.3 (br, C_{ortho}-BAR^F), 129.2 (br q, J_{C,F} = 30 Hz, C_{meta}-BAR^F), 125.0 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 122.5 (CH-Bcat), 121.2 (br, =CH), 117.9 (br, C_{para}-BAR^F), 116.6 (br, =CH), 111.9 (CH-Bcat), 59.4 (C_q-^tBu), 55.1 (CH(CH₃)₂), 32.0 (^tBu), 23.3 (CH(CH₃)₂). ¹¹B{¹H}(128 MHz, CD₂Cl₂, 25 °C): δ = 14.7 (br s+d, J_{Pt,B} = 1695 Hz, Pt-Bcat), -6.6 (s, BAR^F).

Complex 2c: ¹H-NMR (300 MHz, CD₂Cl₂, 25 °C): δ = 7.75 (br, 8H, H_{ortho}-BAR^F), 7.58 (br, 4H, H_{para}-BAR^F), 7.25 and 7.05 (d, 2H each, J_{H,H} = 1.8 Hz, =CH), 6.86 and 6.77 (m, 2H each, CH-Bdab), 5.66 (br, 2H, NH), 5.36 (br, 2H, CH(CH₃)₂), 1.93 (s, 18H, ^tBu), 1.26 (d, 12H, J_{H,H} = 6.8 Hz, CH(CH₃)₂). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C): δ = 179.8 (Pt=C), 162.2 (q, J_{C,B} = 50 Hz, C_{ipso}-BAR^F), 136.3 (C_q-Bdab),

135.2 (br, C_{ortho}-BAR^F), 129.3 (br q, J_{C,F} = 34 Hz, C_{meta}-BAR^F), 125.0 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 120.6 (br, =CH), 119.4 (CH-Bdab), 117.9 (br, C_{para}-BAR^F), 116.1 (br, =CH), 110.4 (CH-Bdab), 59.3 (C_q-^tBu), 55.1 (CH(CH₃)₂), 32.8 (^tBu), 23.0 (CH(CH₃)₂). ¹¹B{¹H}(128 MHz, CD₂Cl₂, 25 °C): δ = 8.8 (br s+d, J_{Pt,B} = 1390 Hz, Pt-Bdab), -6.6 (s, BAR^F). **Elemental analysis calcd (%) for C₅₈H₅₄B₂F₂₄N₆Pt:** C, 46.20; H, 3.61; N, 5.57; **Found:** C, 46.1; H, 3.7; N, 5.7.

3. Synthesis and spectroscopic data for complexes 3a-c.

General procedure: Complex **1** (70 mg, 0.050 mmol) was dissolved in 0.4 mL of dry CD₂Cl₂ in a screw-cap NMR tube and cooled to -78 °C. Then, a borane solution (0.060 mmol in 0.2 mL of CD₂Cl₂) was transferred via cannula into the NMR tube, and the mixture was shaken at -78 °C. The sample was analyzed by NMR in a pre-cooled (-30 °C) NMR apparatus.

Complex 3a: ¹H-NMR (400 MHz, CD₂Cl₂, -30 °C): δ = 7.74 (br, 8H, H_{ortho}-BAR^F), 7.57 (br, 4H, H_{para}-BAR^F), 7.25, 7.07, 7.04 and 7.02 (br, 1H each, =CH), 5.00 (br, 1H, CH(CH₃)₂), 4.70 (sept, 1H, J_{H,H} = 6.0 Hz, CH(CH₃)₂), 2.28 (d+d, 1H, J_{H,H} = 12.0 Hz, J_{Pt,H} = 60.0 Hz, Pt-CH_aCH_b), 2.10 (d+d, 1H, J_{H,H} = 12.0 Hz, J_{Pt,H} ~ 85 Hz, Pt-CH_aCH_b), 1.66 (s, 9H, ^tBu), 1.57-1.43 (m, 12H, CH(CH₃)₂), 1.39 (s, 3H, CH₃) and 1.30 (br, 3H, CH₃), 1.15 and 1.08 (s, 6H each, CH₃-Bpin), -3.93 (s+d, 1H, ¹J_{Pt,H} = 357.0 Hz, H-Bpin). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, -30 °C): δ = 167.0 and 164.9 (Pt=C), 161.7 (q, J_{C,B} = 50 Hz, C_{ipso}-BAR^F), 134.7 (br, C_{ortho}-BAR^F), 128.7 (br q, J_{C,F} = 34 Hz, C_{meta}-BAR^F), 124.5 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 120.7 (=CH), 117.5 (br, C_{para}-BAR^F), 117.1, 116.5 and 116.0 (=CH), 85.4 (C_q-Bpin), 65.5 and 58.4 (C_q-^tBu), 53.8 and 53.3 (CH(CH₃)₂), 36.9 (Pt-CH₂), 33.1 (Pt-CH₂-C(CH₃)), 31.1 (^tBu), 28.1 (CH₃), 24.7 (2 x CH₃-Bpin), 24.6, 24.3 and 23.7 (CH₃), 23.0 (2 x CH₃-Bpin), 21.5 (CH₃). ¹¹B{¹H}(128 MHz, CD₂Cl₂, -30 °C): δ = 21.8 (br, Pt-H-Bpin), -6.8 (s, BAR^F).

Complex 3b: ¹H-NMR (400 MHz, CD₂Cl₂, -30 °C): δ = 7.76 (br, 8H, H_{ortho}-BAR^F), 7.57 (br, 4H, H_{para}-BAR^F), 7.34, 7.21, 7.17 and 7.14 (br, 1H each, =CH), 7.09 and 7.06 (br, 2H each, HBcat), 4.76 (br, 2H, CH(CH₃)₂), 2.48 (d+d, 1H, J_{H,H} = 12.0 Hz, J_{Pt,H} = 57.6 Hz, Pt-CH_aCH_b), 2.32 (d+d, 1H, J_{H,H} = 12.0 Hz, J_{Pt,H} = 88.3 Hz, Pt-CH_aCH_b), 1.72 (s, 9H, ^tBu), 1.66 (d, 3H, J_{H,H} = 6.0 Hz, CH(CH₃)₂), 1.55 (s, 3H, CH₃), 1.41 (br, 6H, CH(CH₃)₂), 1.35 (br, 6H, CH₃ + CH(CH₃)₂), -3.28 (s+d, 1H, ¹J_{Pt,H} = 327.5 Hz, H-Bpin). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, -30 °C): δ = 166.3 and 163.0 (Pt=C), 161.7 (q, J_{C,B} = 50 Hz, C_{ipso}-BAR^F), 148.6 (C_q-Bcat), 134.7 (br, C_{ortho}-BAR^F), 128.7 (br q, J_{C,F} = 34 Hz, C_{meta}-BAR^F), 124.5 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 123.1 (CH-Bcat), 121.0, 117.8, 117.2 and 116.6 (=CH), 117.5 (br, C_{para}-BAR^F), 112.2 (CH-Bcat), 65.8 (s+d, J_{Pt,C} = 21 Hz, C_q-^tBu), 58.7 (C_q-^tBu), 54.2 and 53.4 (CH(CH₃)₂), 39.3 (s+d, J_{Pt,C} = 650 Hz, Pt-CH₂), 33.1 (Pt-CH₂-C(CH₃)), 31.3 (^tBu), 28.2 (s+d, J_{Pt,C} = 50 Hz, Pt-CH₂-C(CH₃)), 24.7, 24.2, 22.6 and 21.8 (CH(CH₃)₂). ¹¹B{¹H}(128 MHz, CD₂Cl₂, -30 °C): δ = 21.3 (br, Pt-H-Bcat), -6.7 (s, BAR^F).

Complex 3c: ¹H-NMR (400 MHz, CD₂Cl₂, -30 °C): δ = 7.75 (br, 8H, H_{ortho}-BAR^F), 7.57 (br, 4H, H_{para}-BAR^F), 7.25, 7.13, 7.09 and 6.96 (br, 1H each, =CH), 7.01 and 6.93 (br, 2H each, HBdab), 6.45 (br, 2H, NH), 4.84 and 4.67 (br, 1H each, CH(CH₃)₂), 2.31 (d+d, 1H, J_{H,H} = 12.0 Hz, J_{Pt,H} ~ 87 Hz, Pt-CH_aCH_b),

2.22 (d+d, 1H, $J_{H,H} = 12.0$ Hz, $J_{Pt,H} \sim 68$ Hz, Pt-CH_aCH_b), 1.79 (s, 9H, ^tBu), 1.55-1.53 (m, 6H, CH₃ + CH(CH₃)₂), 1.42-1.39 (m, 6H, CH₃ + CH(CH₃)₂), 1.28 (d, 3H, $J_{H,H} = 6.0$ Hz, CH(CH₃)₂), 0.63 (d, 3H, $J_{H,H} = 6.0$ Hz, CH(CH₃)₂), -2.32 (s+d, 1H, $^1J_{Pt,H} = 339.2$ Hz, H-Bdab). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, -30 °C): $\delta = 167.6$ and 164.6 (Pt=C), 161.7 (q, $J_{C,B} = 50$ Hz, C_{ipso}-BAr^F), 135.8 (C_q-Bdab), 134.6 (br, C_{ortho}-BAr^F), 128.7 (br q, $J_{C,F} = 34$ Hz, C_{meta}-BAr^F), 124.5 (q, $J_{C,F} = 272$ Hz, CF₃-BAr^F), 120.6 (=CH), 120.2 (CH-Bdab), 117.6 (=CH), 117.5 (br, C_{para}-BAr^F), 116.7 and 116.0 (=CH), 111.2 (CH-Bdab), 65.8 and 58.6 (C_q-^tBu), 53.3 and 52.9 (CH(CH₃)₂), 34.2 (Pt-CH₂), 32.8 (Pt-CH₂-C(CH₃)), 31.0 (^tBu), 28.4 , 24.9 , 23.8 , 21.9 and 21.7 (CH₃). ¹¹B{¹H}(128 MHz, CD₂Cl₂, -30 °C): $\delta = 18.6$ (br, Pt-H-Bdab), -6.7 (s, BAr^F).

4. Synthesis and spectroscopic data for complex 4a.

Complex **3a**, as prepared in the previous section, was allowed to stand for 70 min at -5 °C and the NMR data was recorded between -5 to 0 °C.

Complex 4a: ¹H-NMR (400 MHz, CD₂Cl₂, -5 °C): $\delta = 7.74$ (br, 8H, H_{ortho}-BAr^F), 7.58 (br, 4H, H_{para}-BAr^F), 7.15 (br, 2H, =CH), 7.05 and 7.01 (d, 1H each, $J_{H,H} = 1.3$ Hz, =CH), 5.80 (sept, 1H, $J_{H,H} = 6.7$ Hz, CH(CH₃)₂), 5.63 (sept, 1H, $J_{H,H} = 6.6$ Hz, CH(CH₃)₂), 2.44 (br, 2H, CH₂-Bpin), 1.83 (s, 9H, ^tBu), 1.66 (s, 6H, CH₃), 1.45 (d, 6H, $J_{H,H} = 6.6$ Hz, CH(CH₃)₂), 1.40 (d, 6H, d, 6H, $J_{H,H} = 6.7$ Hz, CH(CH₃)₂), 1.04 (s, 12H, CH₃-Bpin), -27.11 (s+d, 1H, $^1J_{Pt,H} = 2167.0$ Hz, Pt-H). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 0 °C): $\delta = 170.9$ and 169.9 (Pt=C), 161.9 (q, $J_{C,B} = 50$ Hz, C_{ipso}-BAr^F), 135.0 (br, C_{ortho}-BAr^F), 129.0 (br q, $J_{C,F} = 32$ Hz, C_{meta}-BAr^F), 124.8 (q, $J_{C,F} = 272$ Hz, CF₃-BAr^F), 120.0 and 119.8 (=CH), 117.8 (br, C_{para}-BAr^F), 116.5 and 115.1 (=CH), 86.1 (C_q-Bpin), 60.1 and 58.5 (C_q-^tBu and C_q(CH₃)₂-CH₂Bpin), 54.7 and 54.2 (CH(CH₃)₂), 32.1 (2 x CH₃), 31.1 (^tBu), 24.3 (CH₃-Bpin), 22.8 and 22.7 (CH(CH₃)₂). The broad signal for the -CH₂-Bpin fragment has been observed by means of an HMQC experiment. ¹¹B{¹H}(128 MHz, CD₂Cl₂, 0 °C): $\delta = 32.9$ (br, -CH₂-Bpin), -6.7 (s, BAr^F).

5. Synthesis and spectroscopic and analytical data for complex 5.

Complex **5** was prepared by addition of ^tBuNC (6.2 μ L, 0.055 mmol), to a solution of complex **4a** synthesized at low temperature as described in the previous section. After stirring for 15 min at rt, the solvent was removed under vacuum and the resulting white solid washed with pentane (2 x 5 mL). Crystals of complex **5** were obtained by slow diffusion of a concentrated solution of **5** in CH₂Cl₂ into hexamethyldisiloxane in 45 % yield.

Complex 5: ¹H-NMR (400 MHz, CD₂Cl₂, 25 °C): $\delta = 7.75$ (br, 8H, H_{ortho}-BAr^F), 7.58 (br, 4H, H_{para}-BAr^F), 7.27 and 7.22 (d, 1H each, $J_{H,H} = 1.8$ Hz, =CH), 7.04 and 7.02 (d, 1H each, $J_{H,H} = 1.9$ Hz, =CH), 5.53 (br, 2H, CH(CH₃)₂), 2.21 (br, 1H, CH₂-Bpin), 1.87 (s, 6H, CH₂-C_q(CH₃)₂), 1.81 (s, 9H, ^tBu), 1.45 (d, 6H, $J_{H,H} = 6.9$ Hz, CH(CH₃)₂), 1.43 (d, 6H, $J_{H,H} = 7.1$ Hz, CH(CH₃)₂), 1.31 (s, 9H, ^tBuNC), 1.19 (s, 12H, CH₃-Bpin), -7.92 (t+d, 1H, $J_{H,H} = 5.2$ Hz, $^1J_{Pt,H} = 1132.5$ Hz, Pt-H) (one of the diastereotopic CH₂-Bpin broad resonances is not observed). ¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C): $\delta = 161.7$ (q, $J_{C,B} = 50$ Hz, C_{ipso}-

BAR^F), 160.7 (br, 2 Pt=C, detected by HMBC), 135.8 (br, C_{ortho}-BAR^F), 128.9 (br q, J_{C,F} = 32 Hz, C_{meta}-BAR^F), 124.6 (q, J_{C,F} = 272 Hz, CF₃-BAR^F), 120.2 and 119.8 (=CH), 117.5 (br, C_{para}-BAR^F), 114.9 and 114.3 (s+d, J_{Pt,C} ~ 28 Hz, =CH), 83.3 (C_q-Bpin), 59.8 (C_q-^tBu), 58.0 (C_q-^tBuNC), 57.8 (C_q(CH₃)₂-CH₂Bpin), 54.0 and 53.9 (CH(CH₃)₂), 30.2 (br, 2 x CH₃ and ^tBu), 29.5 (^tBuNC), 24.5 (CH₃-Bpin), 22.4 (br, CH(CH₃)₂). The signal of the CH₂-B fragment has not been identified. ¹¹B{¹H}(128 MHz, CD₂Cl₂, 25 °C): δ = 32.7 (br, -CH₂-Bpin), -6.6 (s, BAR^F). **Elemental analysis calcd (%) for C₆₃H₆₉B₂F₂₄N₅O₂Pt: C, 47.21; H, 4.34; N, 4.37; Found: C, 47.4; H, 4.3; N, 4.5.**

6. NMR spectra.

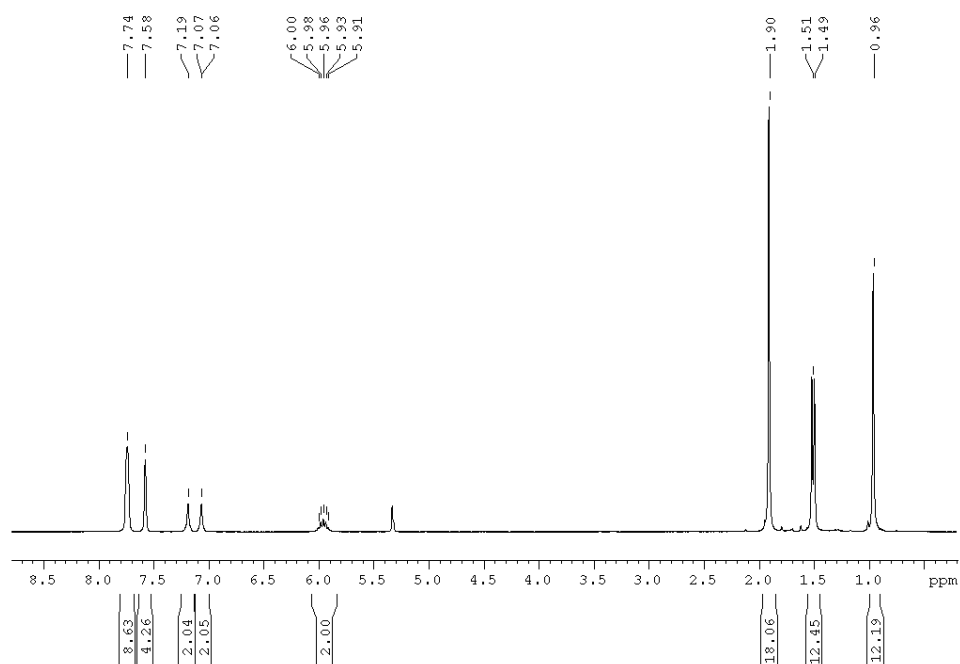


Figure S1. ¹H NMR (300 MHz) of complex **2a** in CD₂Cl₂.

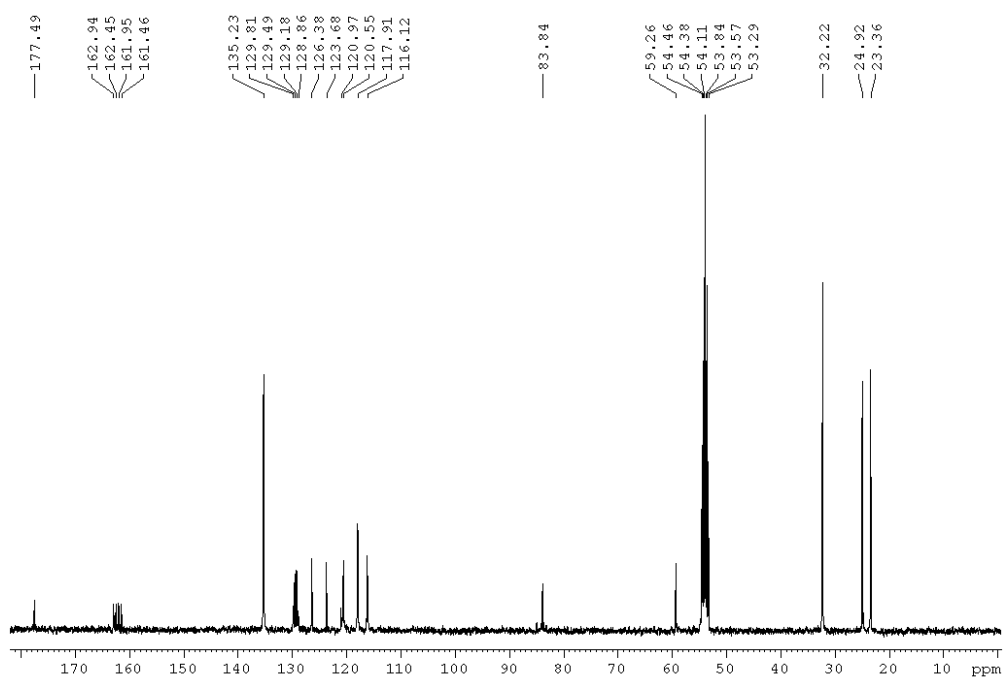


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **2a** in CD_2Cl_2 .

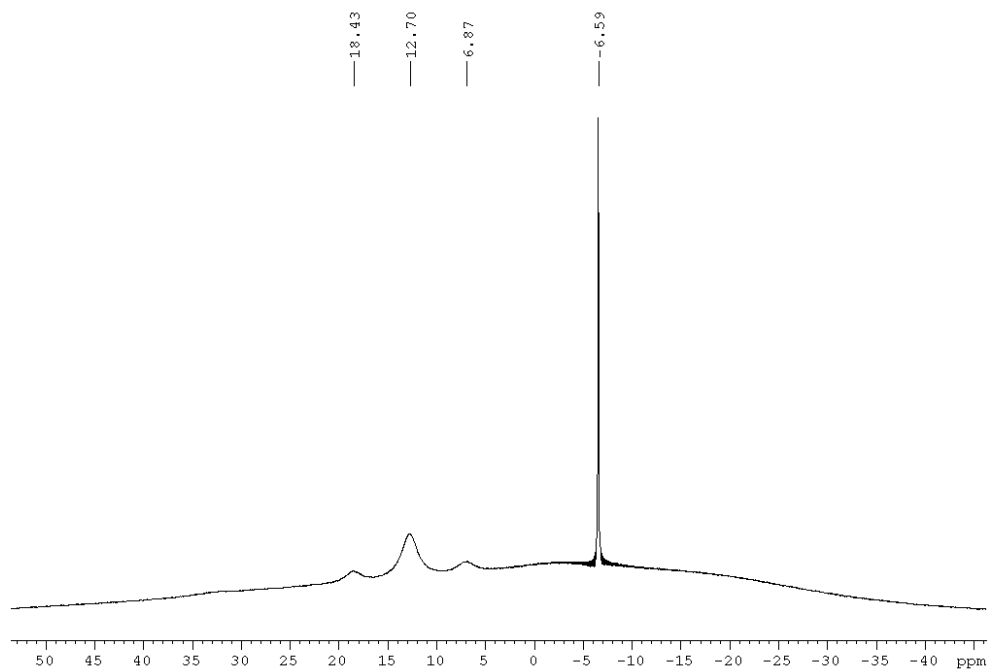


Figure S3. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **2a** in CD_2Cl_2 .

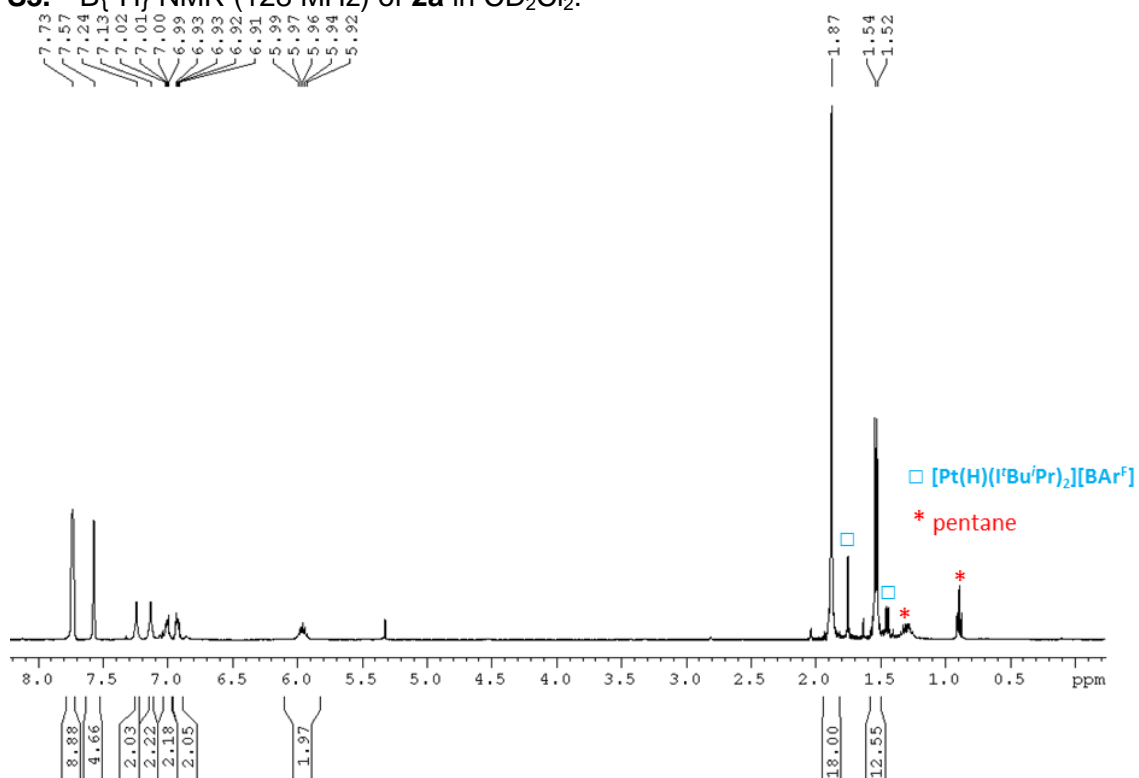


Figure S4. ^1H NMR (400 MHz) of complex **2b** in CD_2Cl_2 .

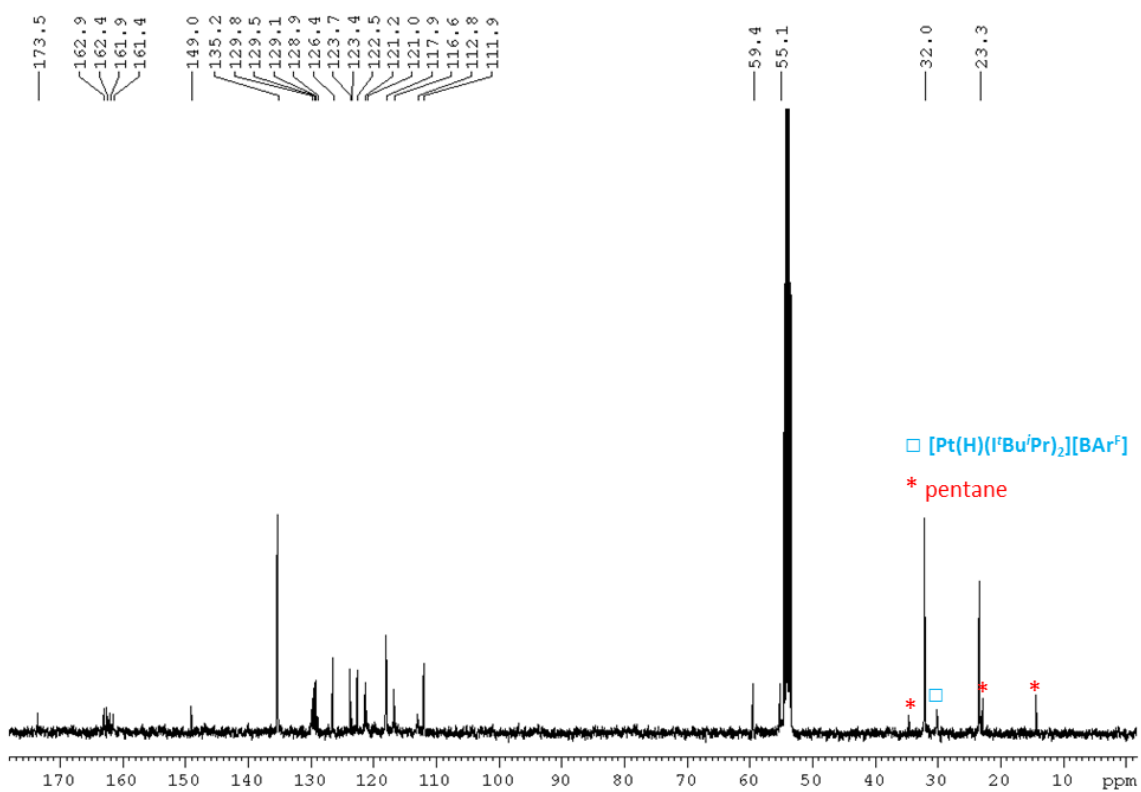


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **2b** in CD_2Cl_2 .

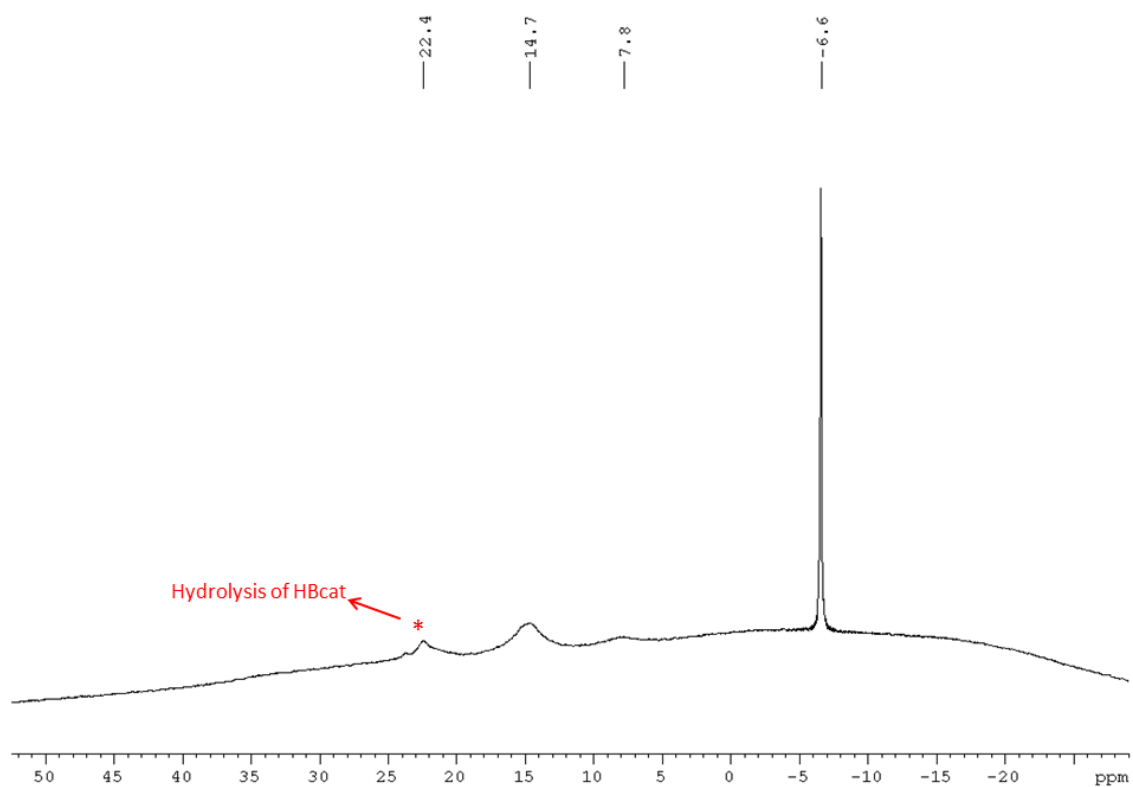


Figure S6. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **2b** in CD_2Cl_2 .

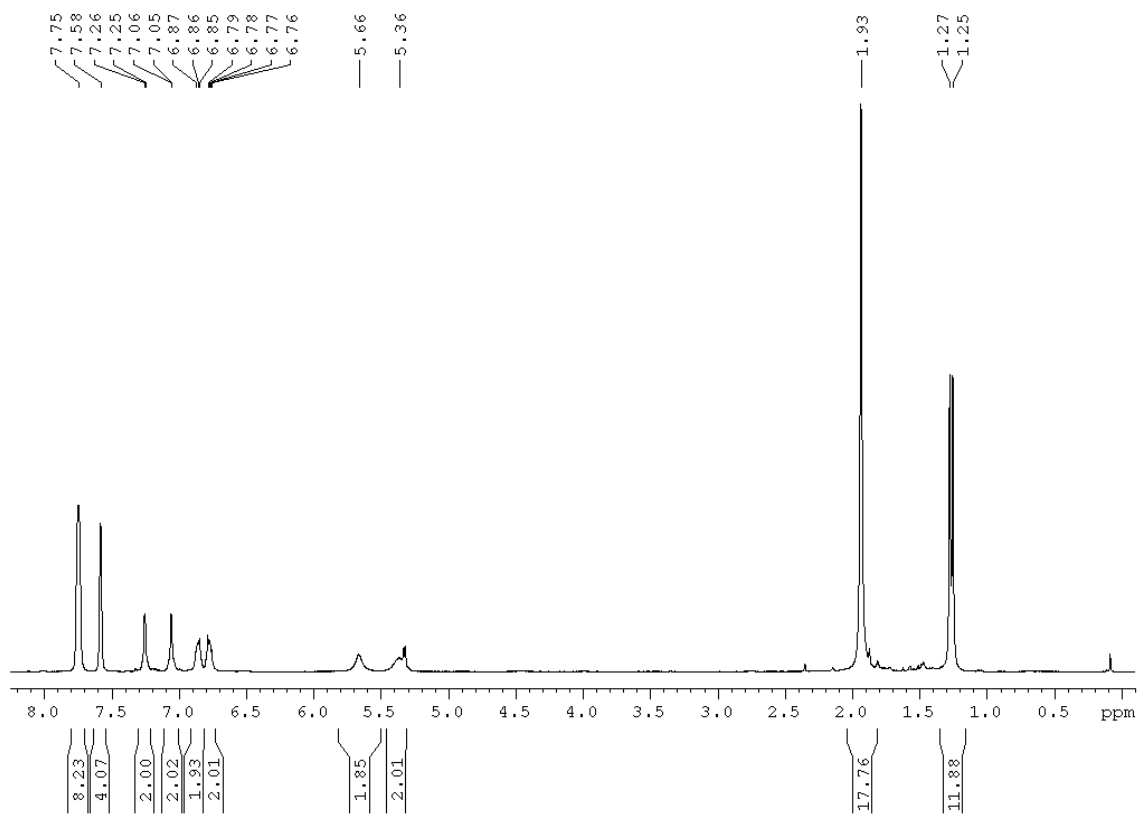
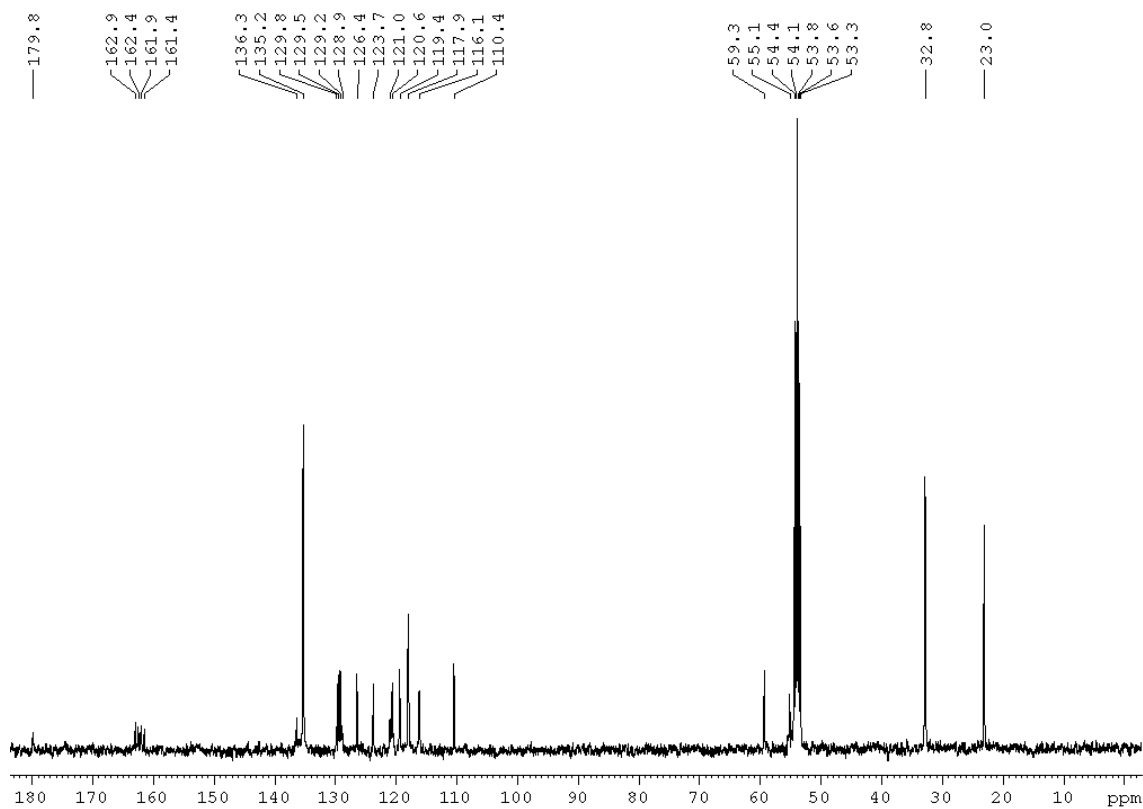


Figure S7. ^1H NMR (400 MHz) of complex **2c** in CD_2Cl_2 .



$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **2c** in CD_2Cl_2 .

Figure S8.

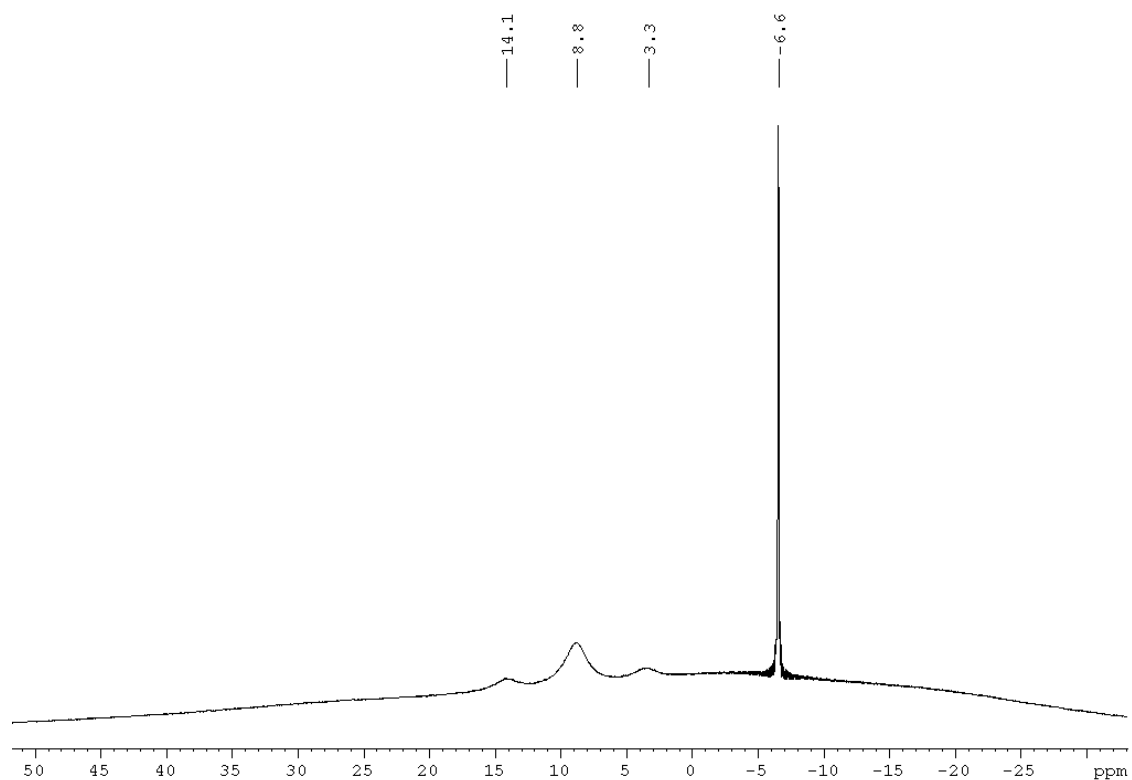


Figure S9. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **2c** in CD_2Cl_2 .

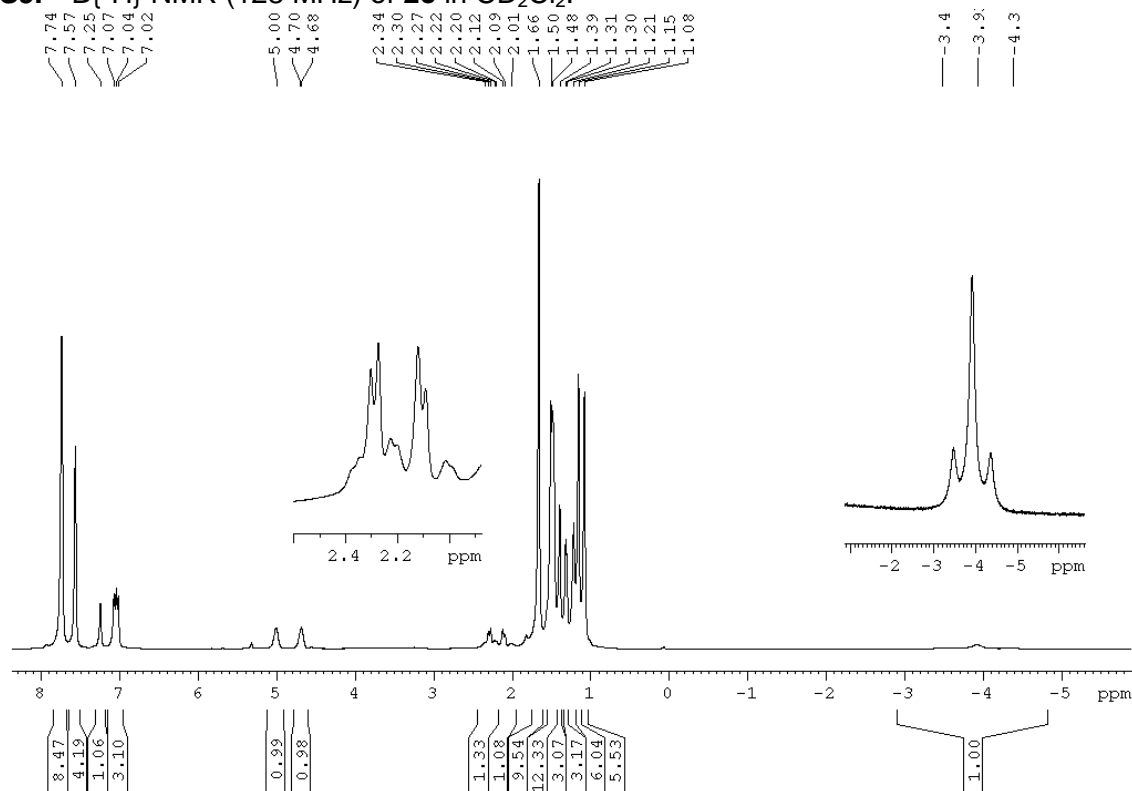


Figure S10. ^1H NMR (400 MHz) of complex **3a** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

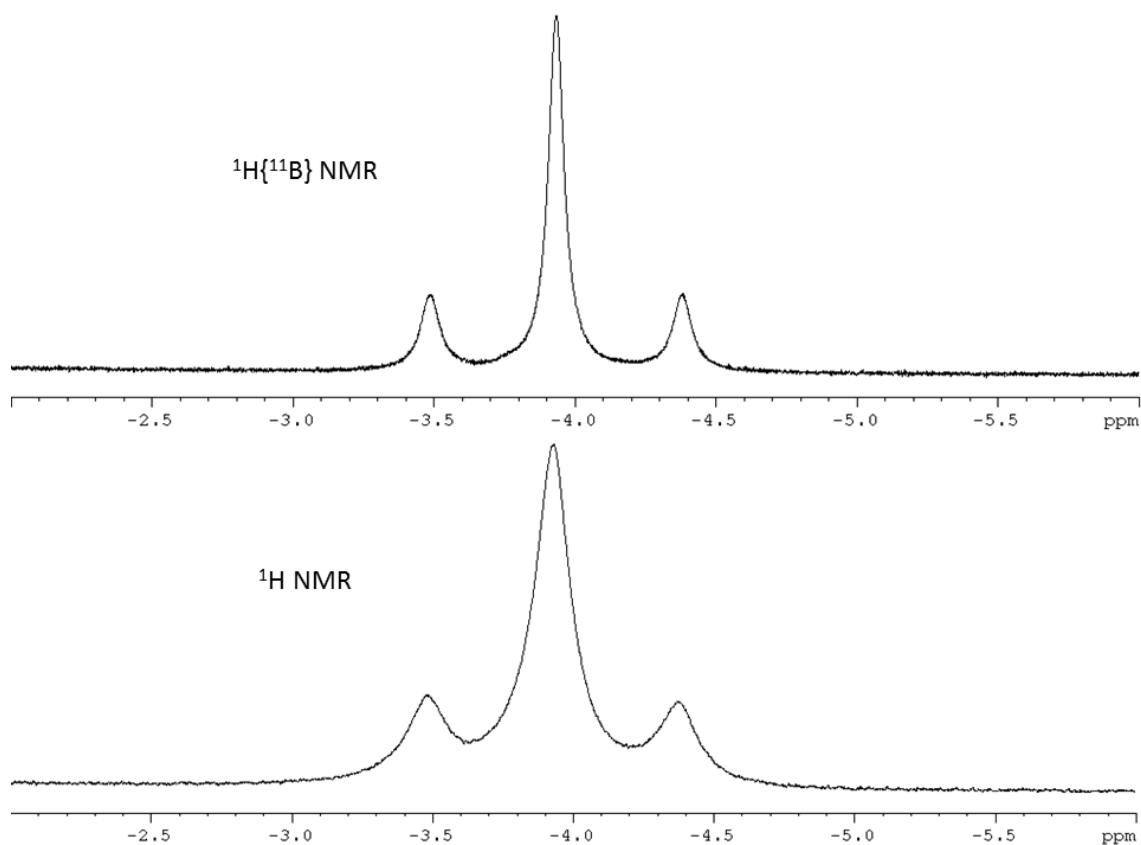


Figure S11. Comparative figure of the ^1H (bottom) and $^1\text{H}\{^{11}\text{B}\}$ (top) NMR (400 MHz) spectra of the hydride resonance of complex **3a** in CD_2Cl_2 at -30°C .

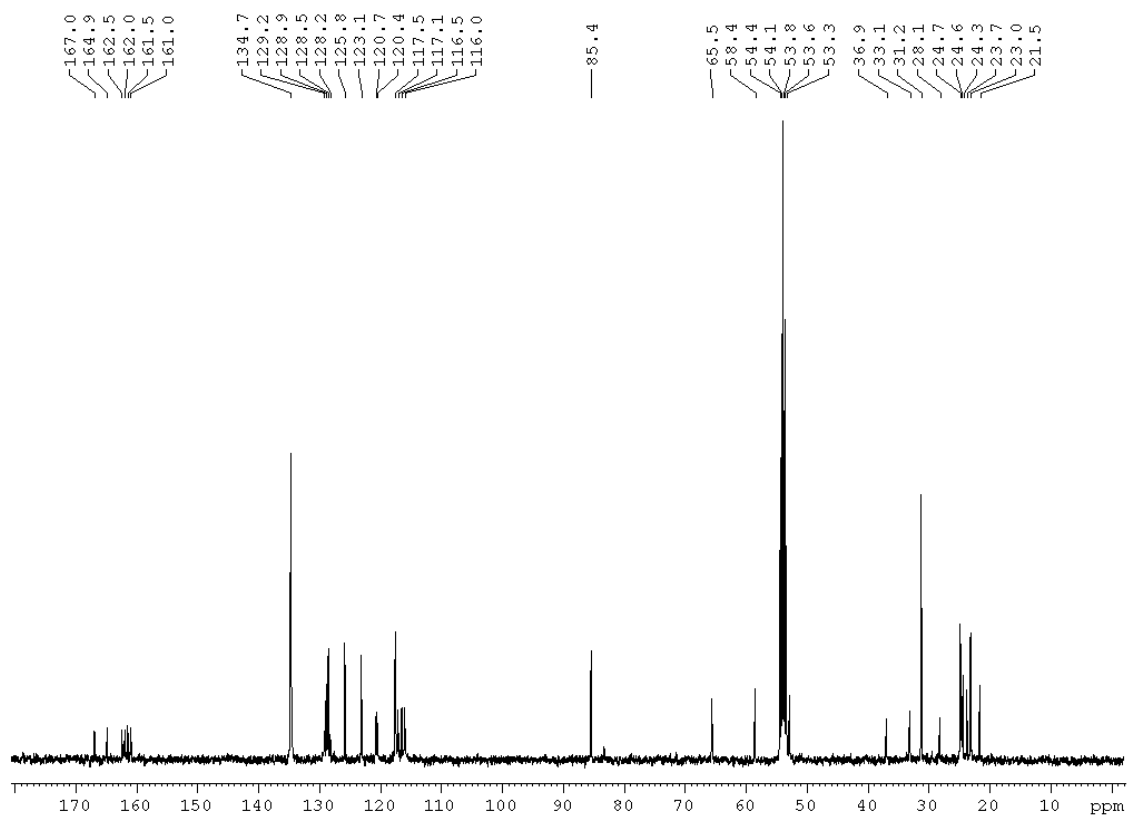


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **3a** in CD_2Cl_2 at -30°C .

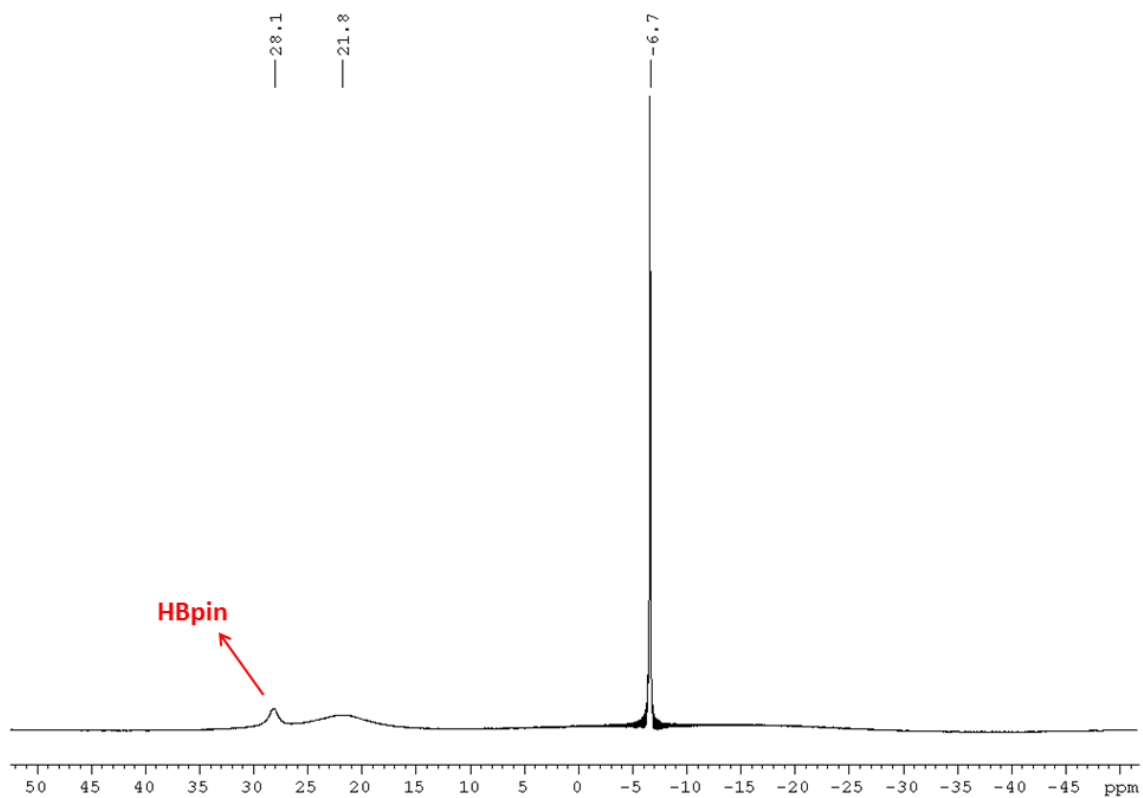


Figure S13. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **3a** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

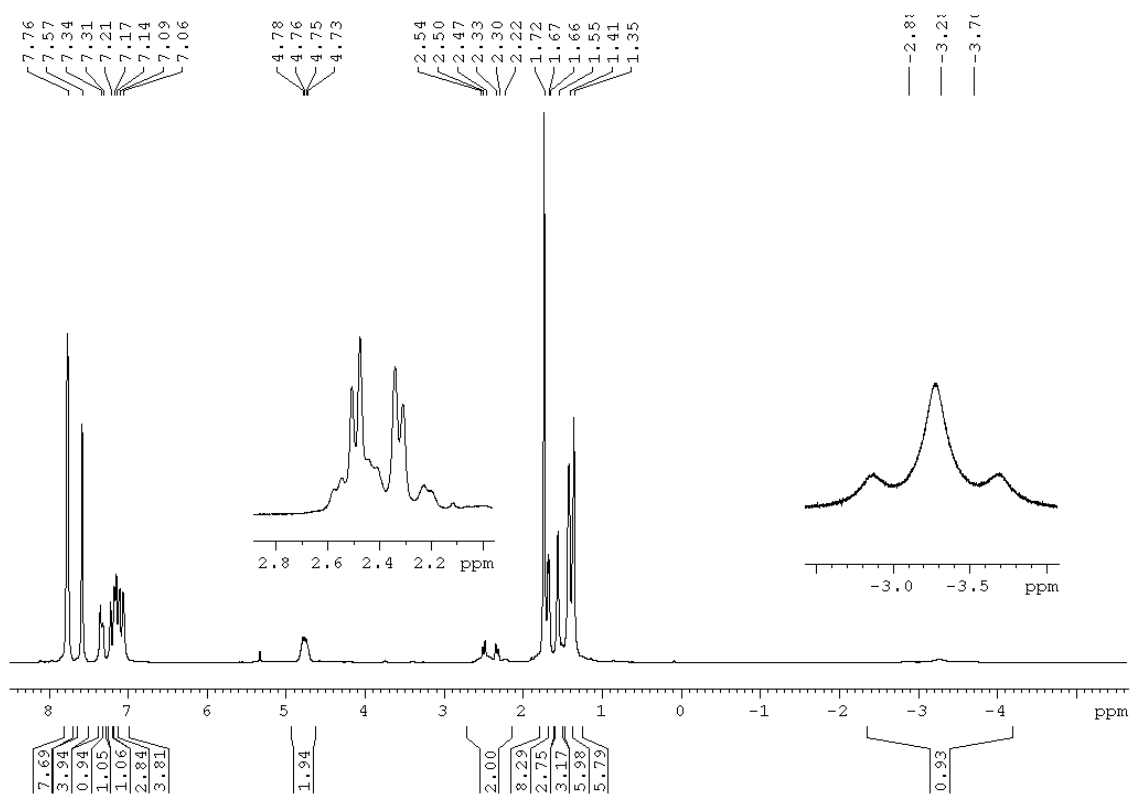


Figure S14. ^1H NMR (400 MHz) of complex **3b** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

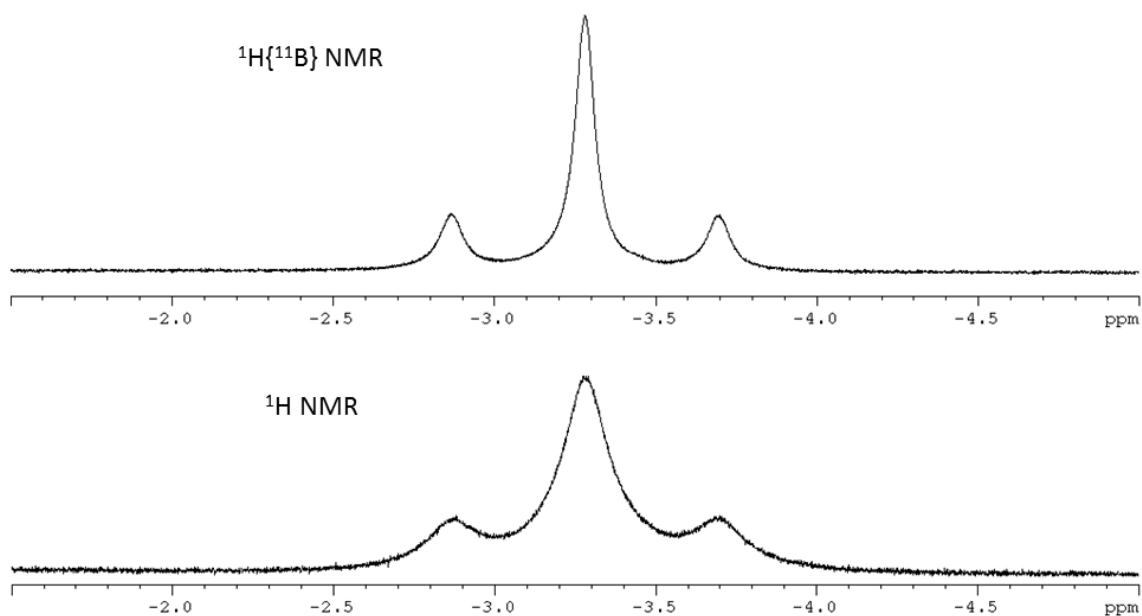


Figure S15. Comparative figure of the ^1H (bottom) and $^1\text{H}\{^{11}\text{B}\}$ (top) NMR (400 MHz) spectra of the hydride resonance of complex **3b** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

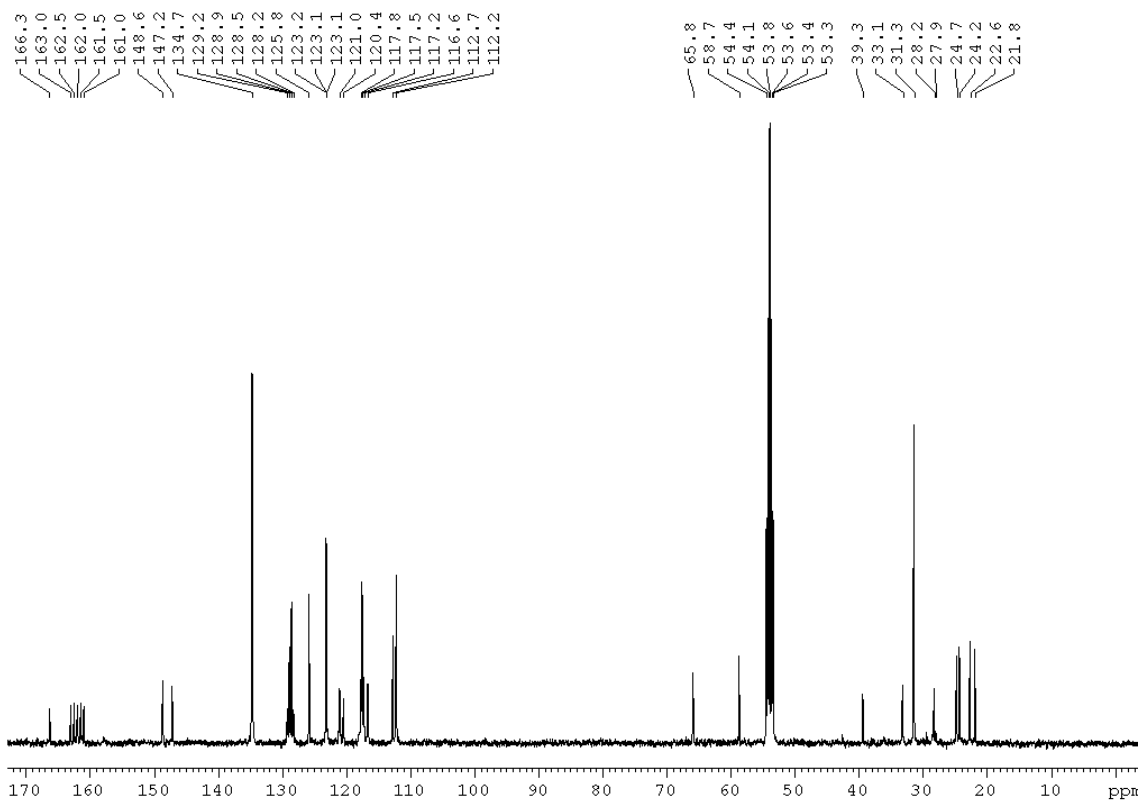


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **3b** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

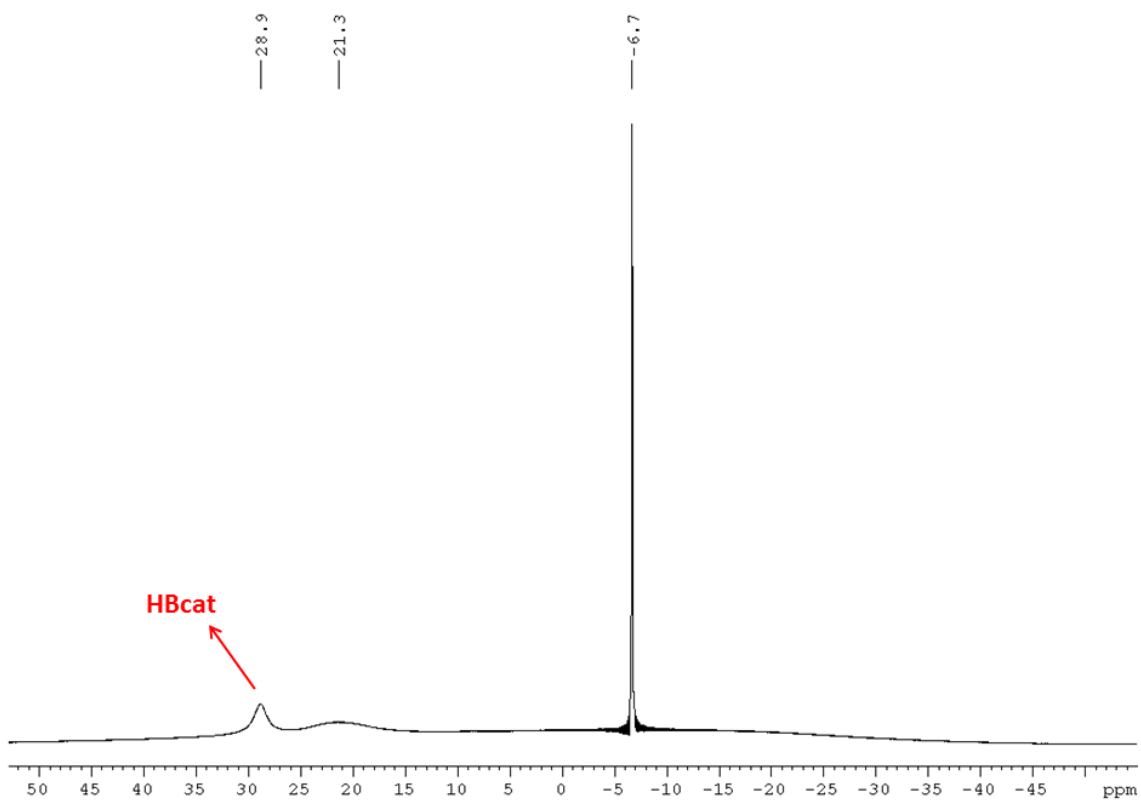


Figure S17. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **3b** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

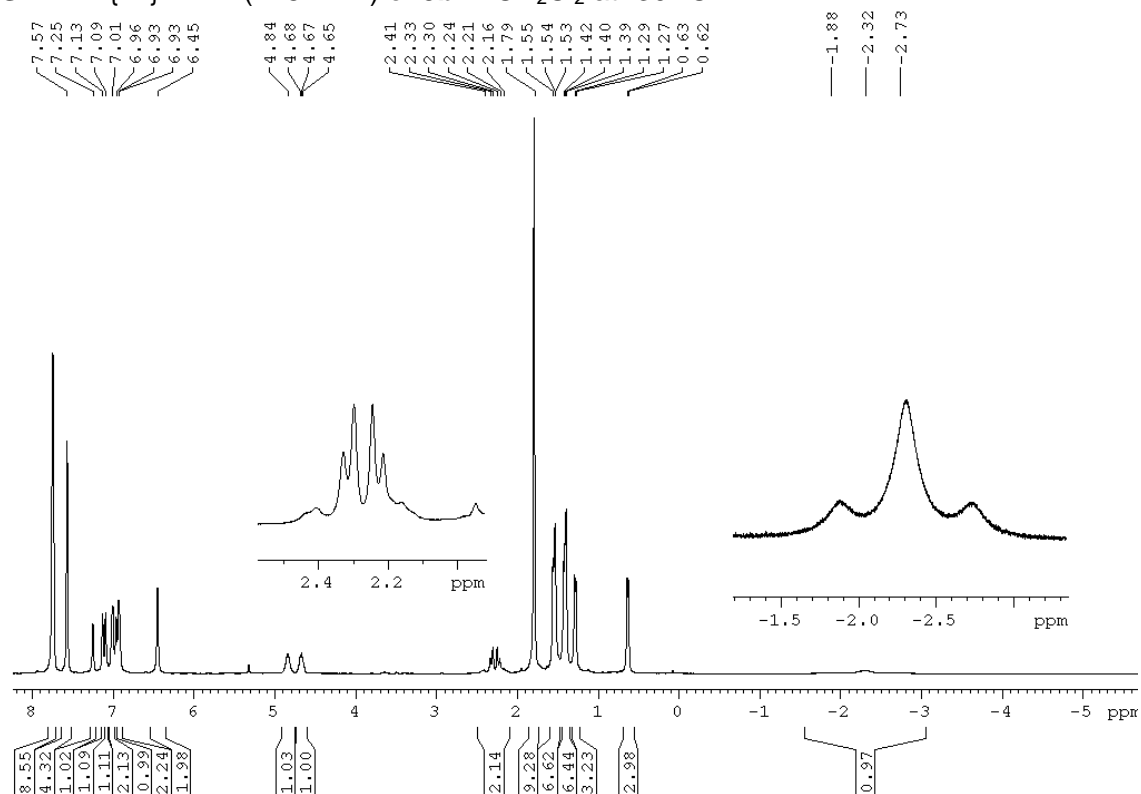


Figure S18. ^1H NMR (400 MHz) of complex **3c** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

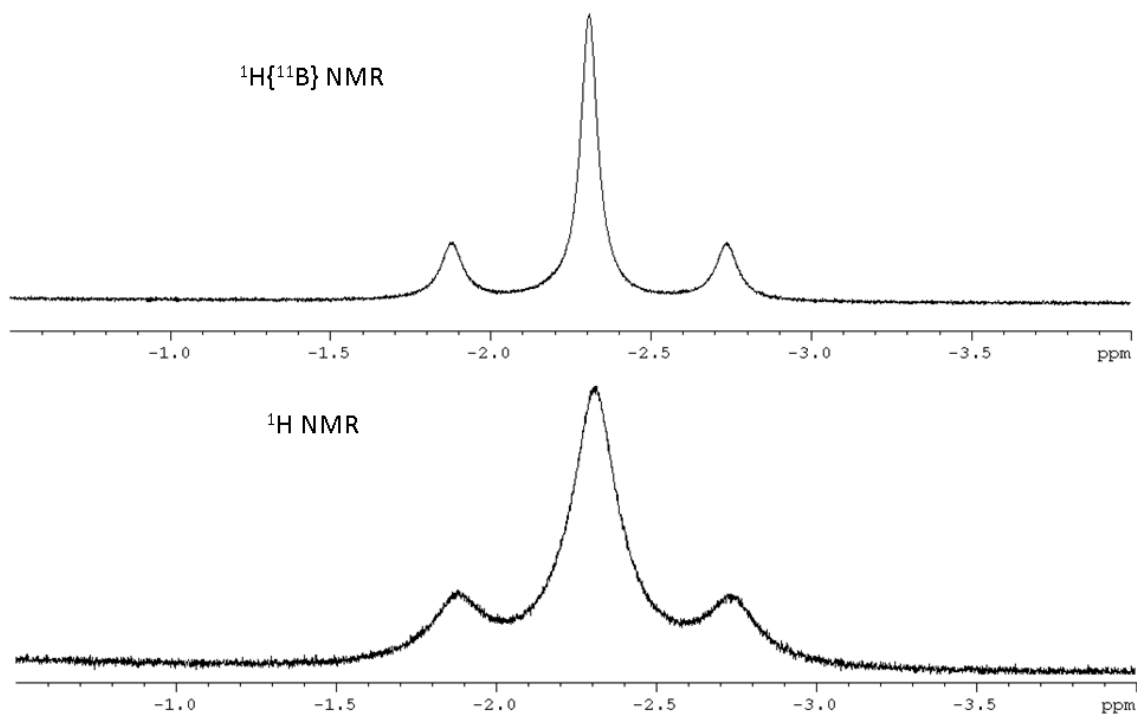


Figure S19. Comparative figure of the ^1H (bottom) and $^1\text{H}\{^{11}\text{B}\}$ (top) NMR (400 MHz) spectra of the hydride resonance of complex **3c** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

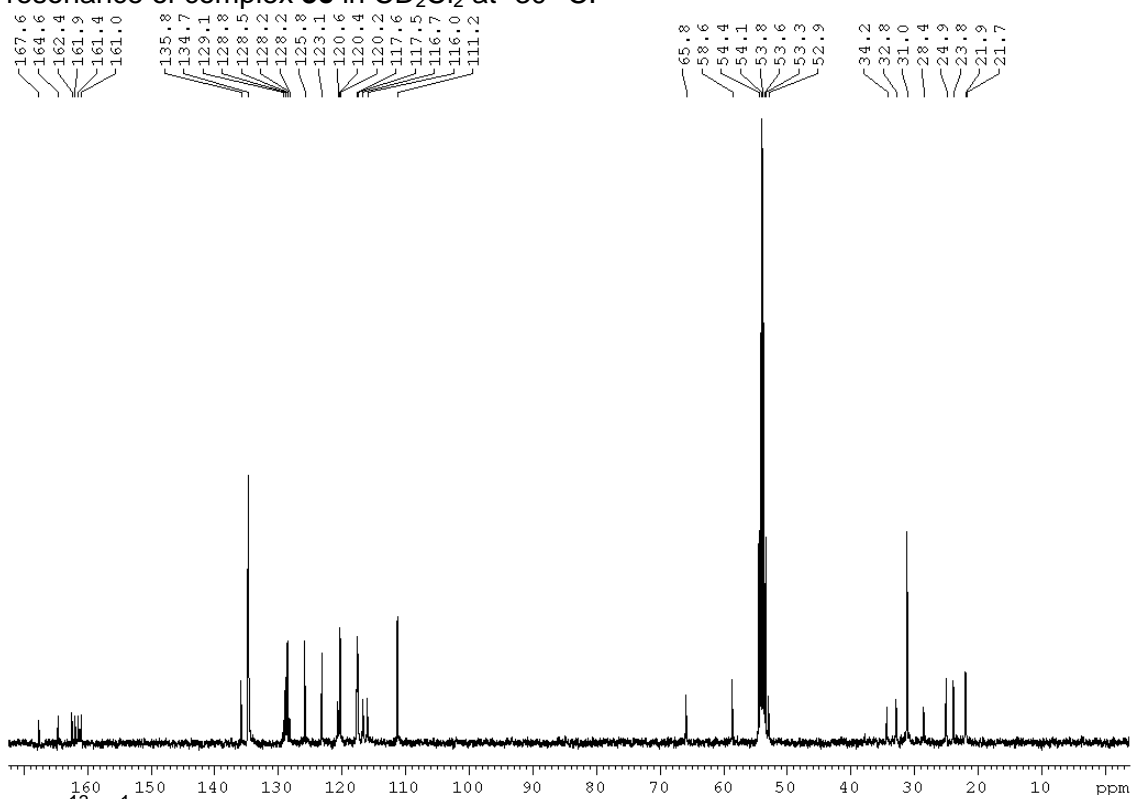


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **3c** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

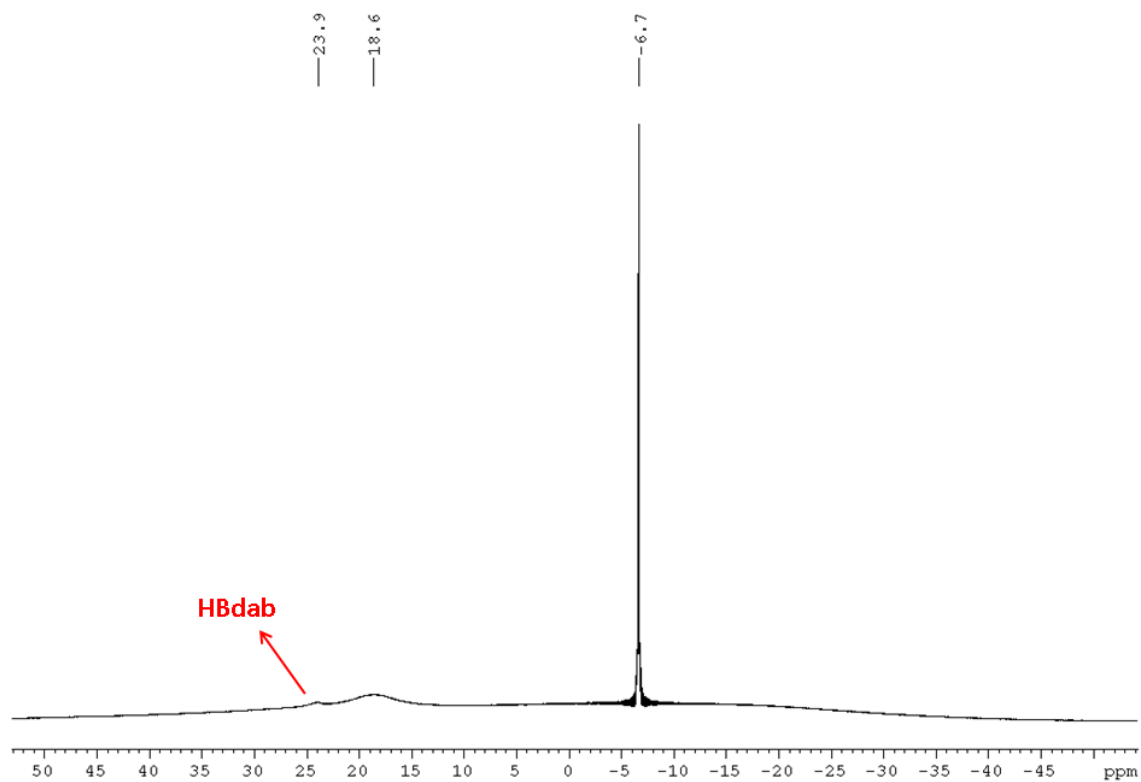


Figure S21. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **3c** in CD_2Cl_2 at $-30\text{ }^\circ\text{C}$.

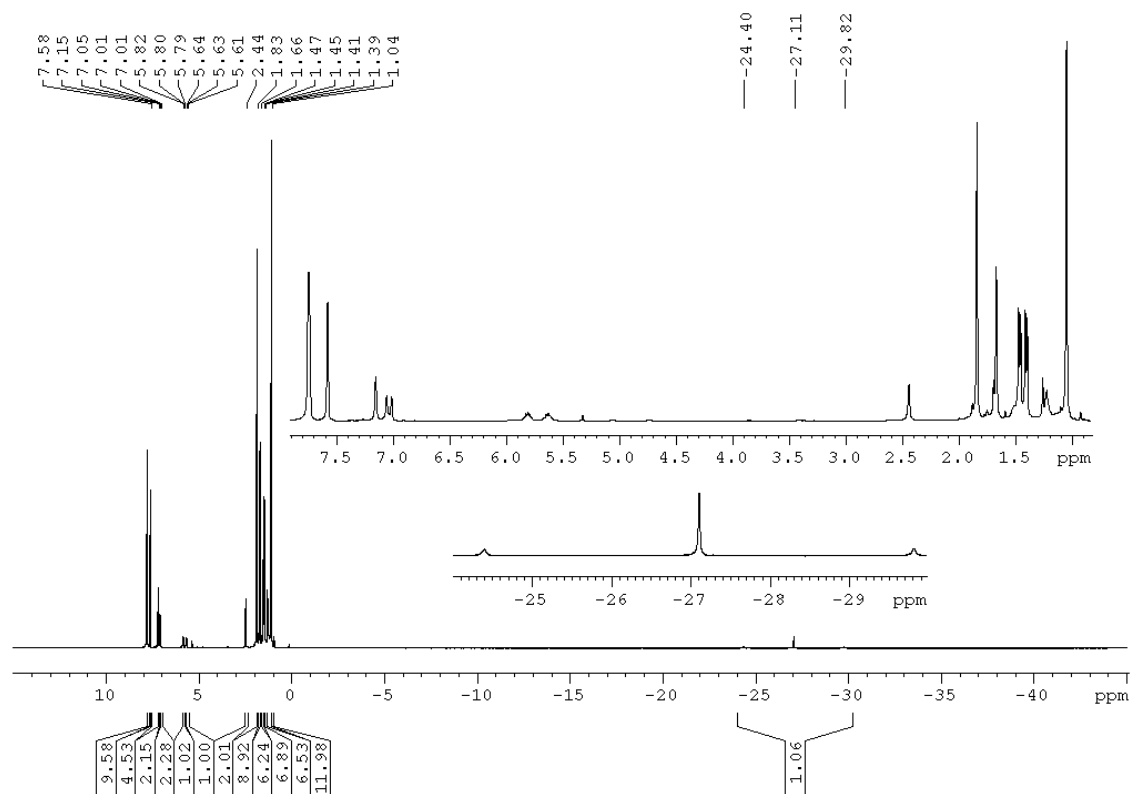


Figure S22. ^1H NMR (400 MHz) of complex **4a** in CD_2Cl_2 at $-5\text{ }^\circ\text{C}$.

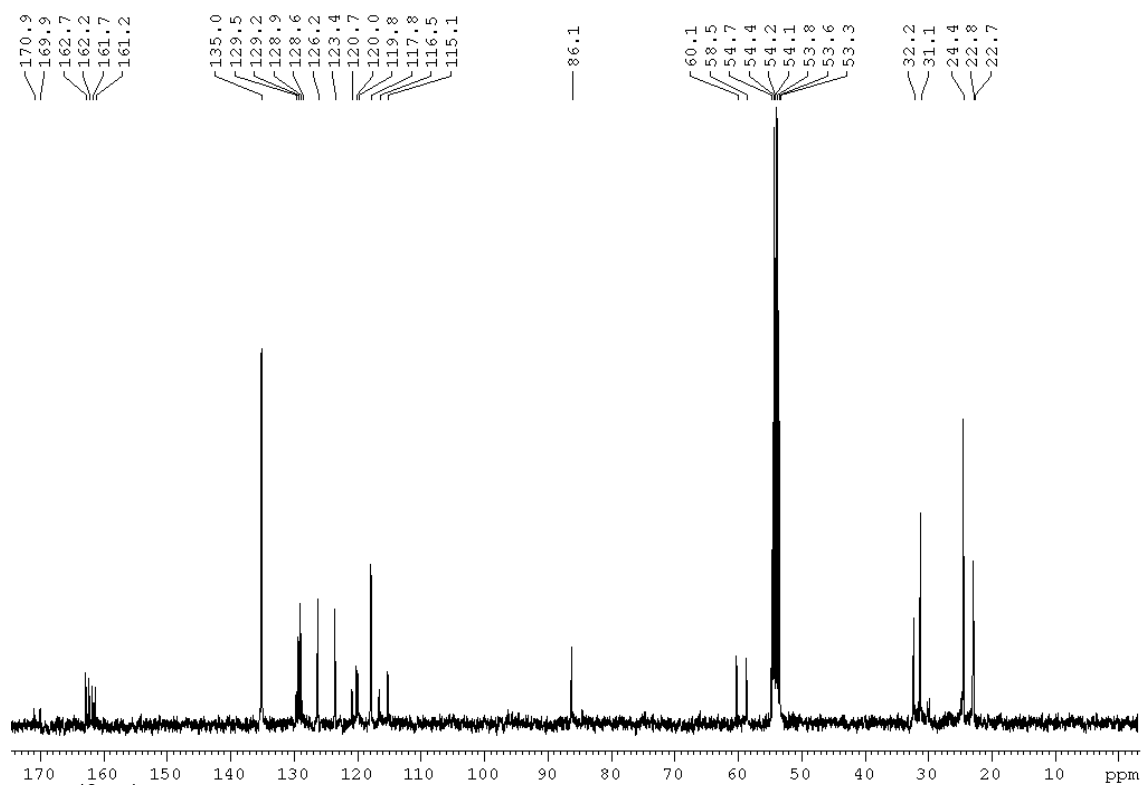


Figure S23. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **4a** in CD_2Cl_2 at $0\text{ }^\circ\text{C}$.

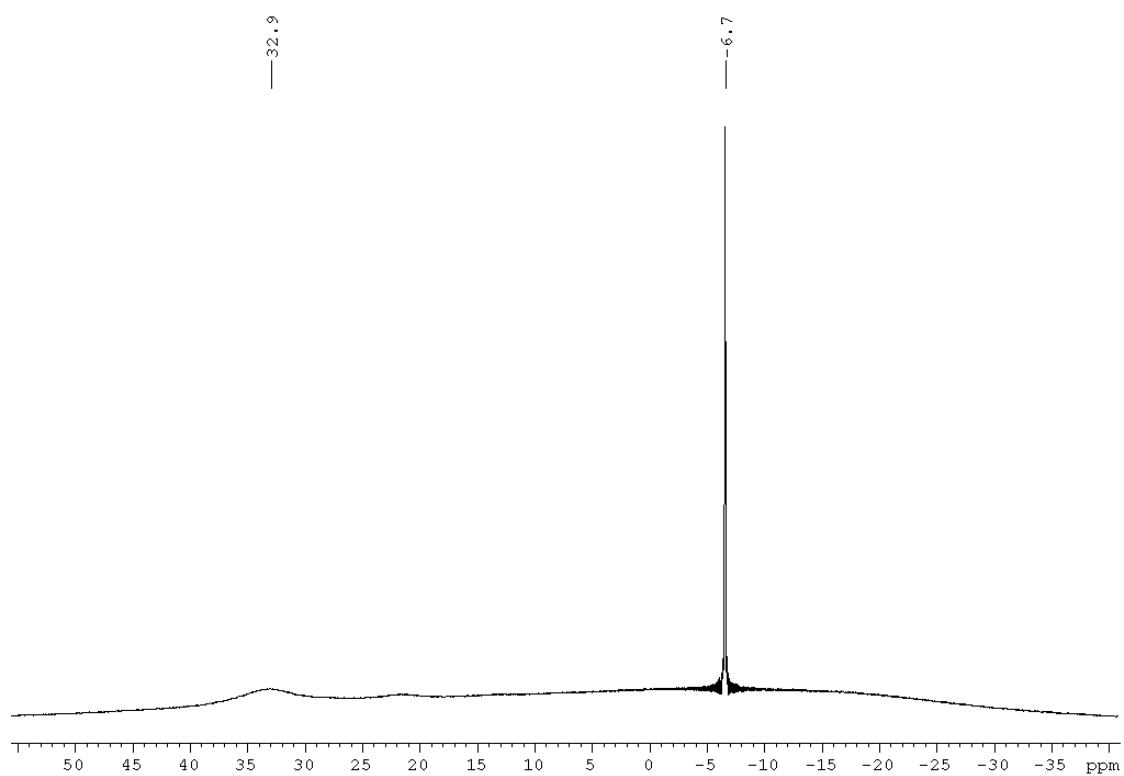


Figure S24. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **4a** in CD_2Cl_2 at $0\text{ }^\circ\text{C}$.

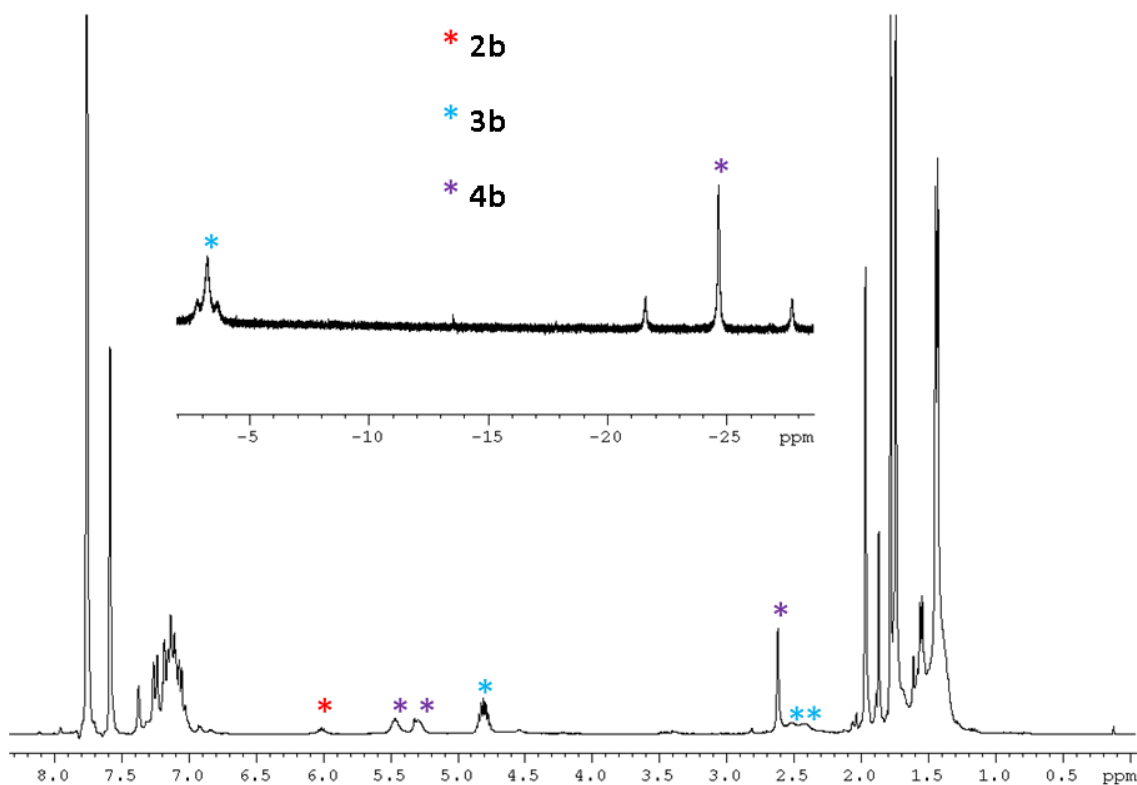


Figure S25. $^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz) of the reaction mixture of complex **1** with HBcat in CD_2Cl_2 at $5\text{ }^\circ\text{C}$ (hydride region in the inset).

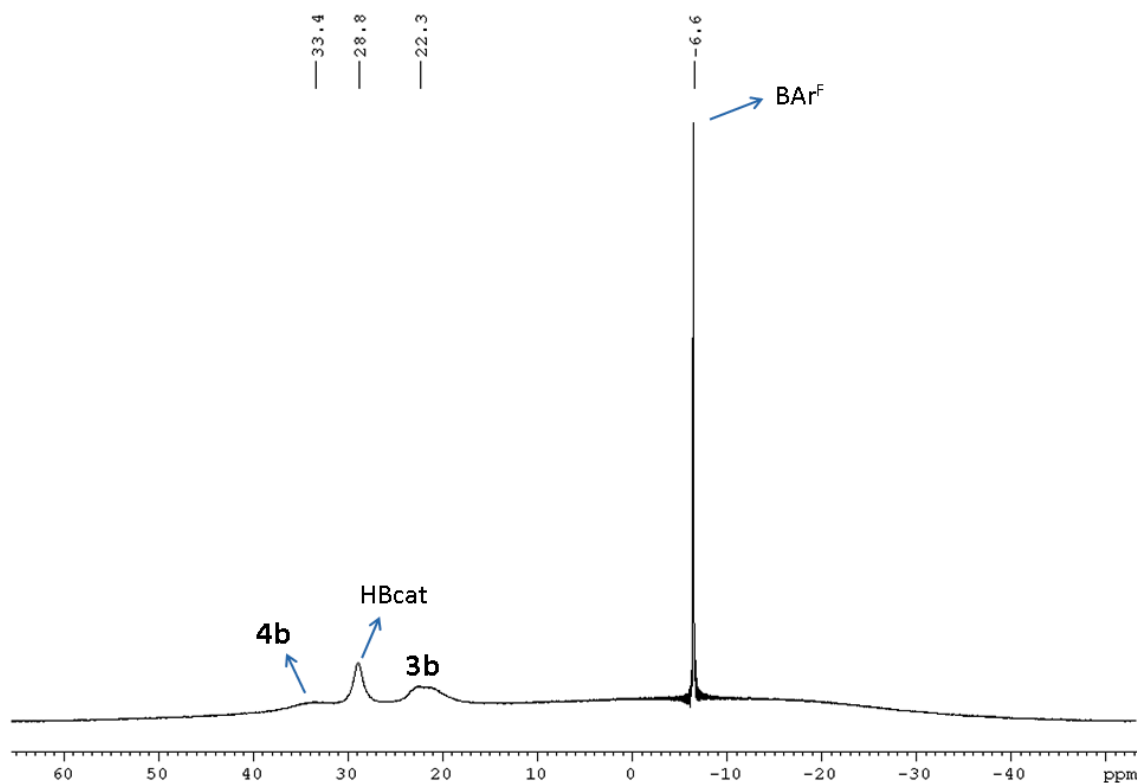


Figure S26. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of the reaction mixture of complex **1** with HBcat in CD_2Cl_2 at $5\text{ }^\circ\text{C}$ (the resonance for complex **2a** is not discernible).

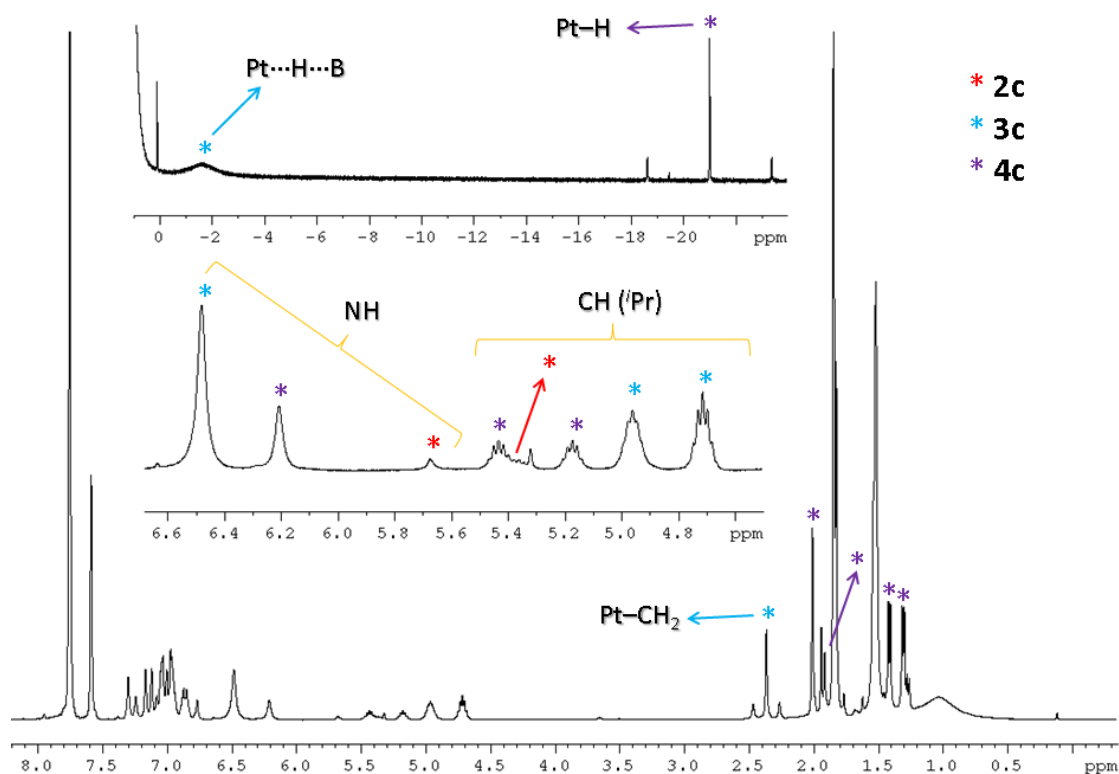


Figure S27. $^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz) of the reaction mixture of complex **1** with HBdab in CD_2Cl_2 at 20°C (inset (top): hydride region; inset (bottom): NH and $\text{CH}(\text{CH}_3)_2$ region).

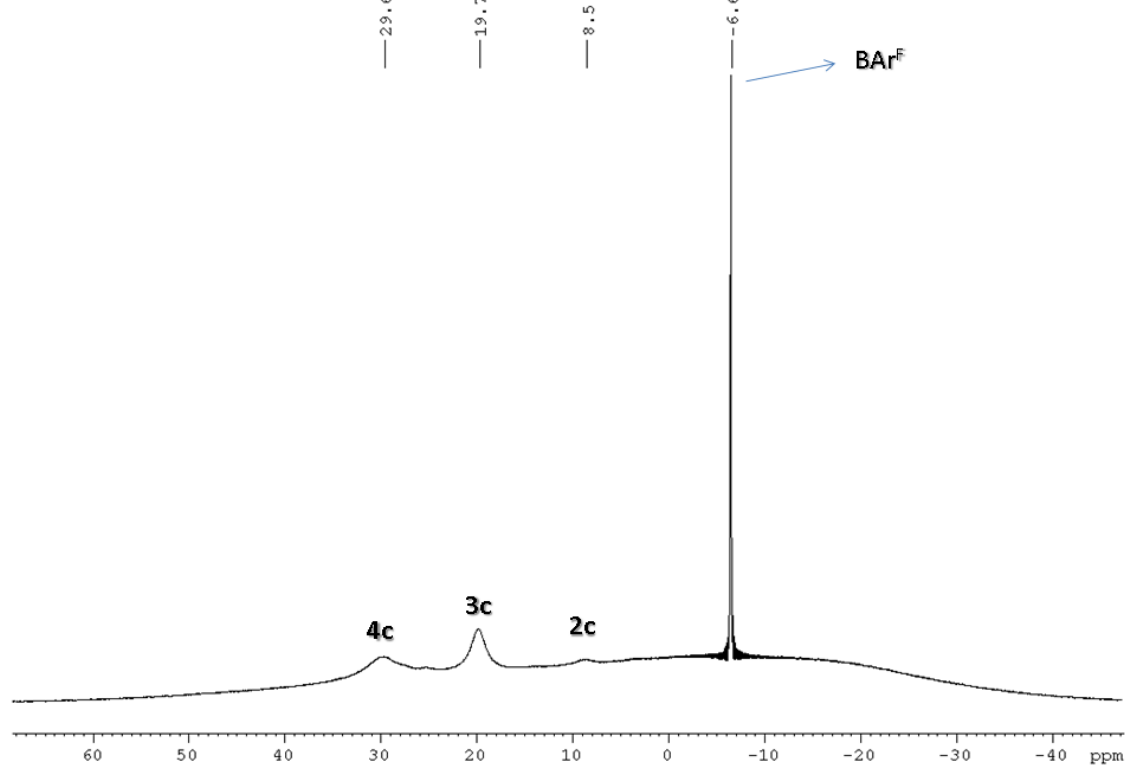


Figure S28. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of the reaction mixture of complex **1** with HBdab in CD_2Cl_2 at 25°C .

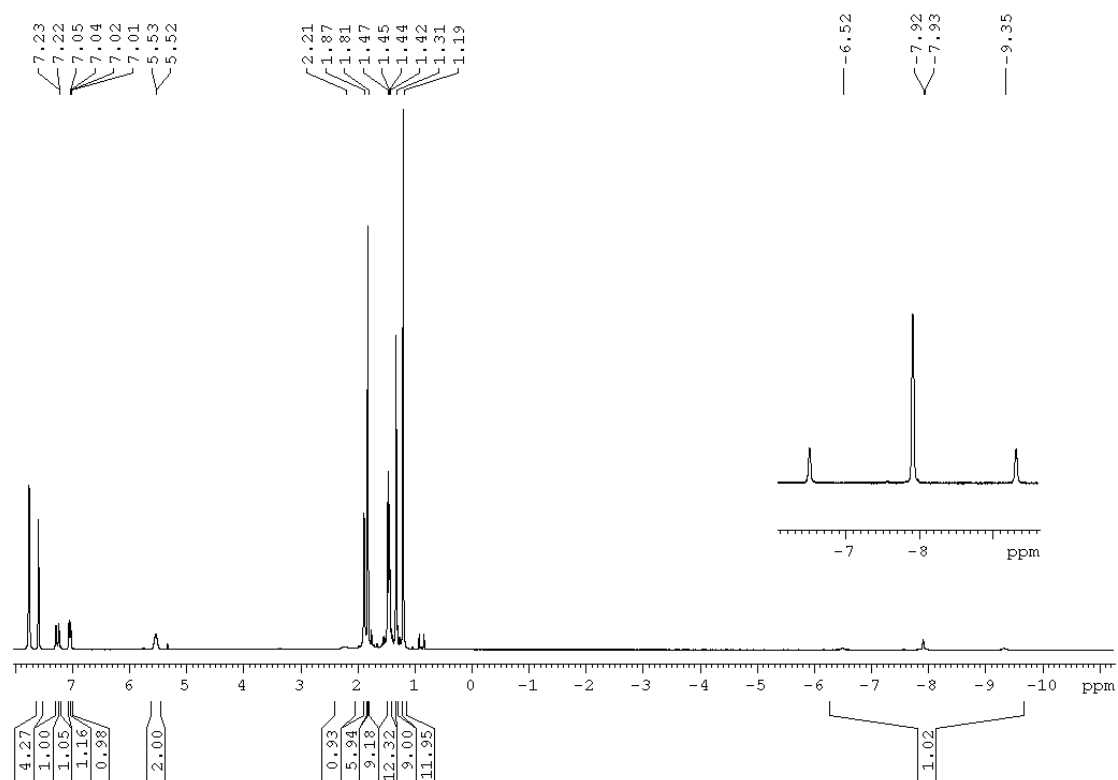


Figure S29. ^1H NMR (400 MHz) of complex **5** in CD_2Cl_2 .

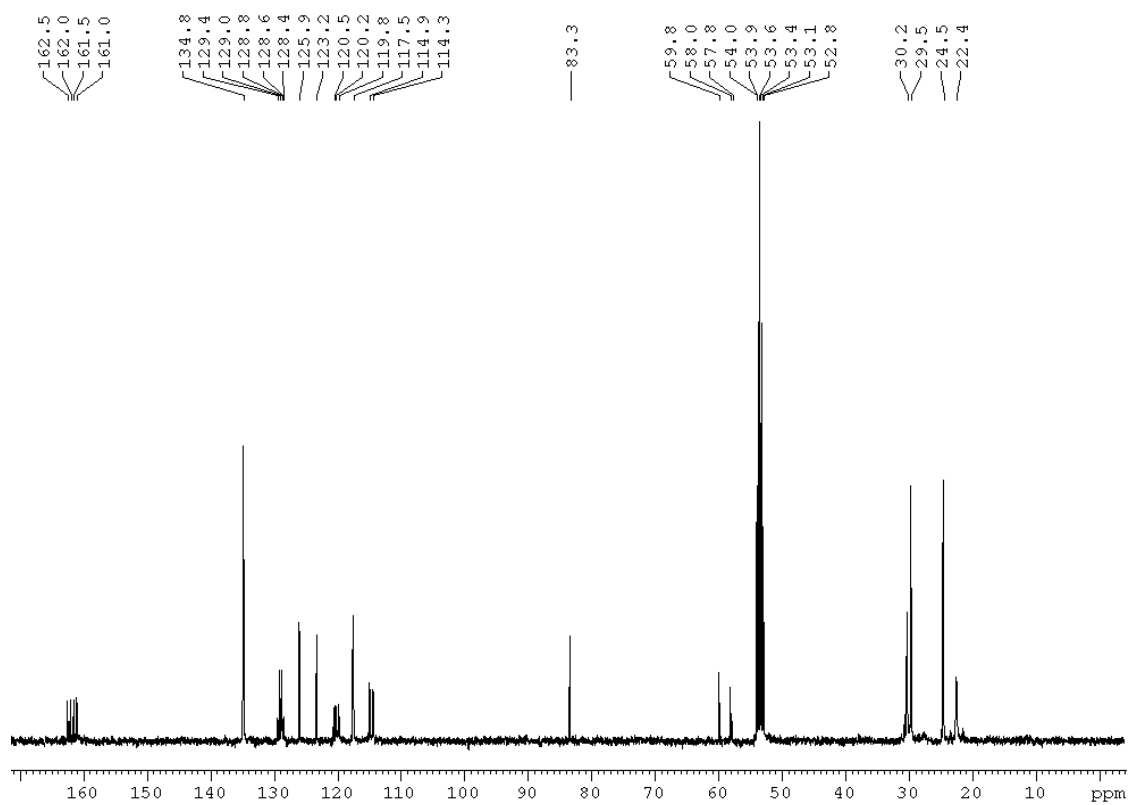


Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz) of **5** in CD_2Cl_2 .

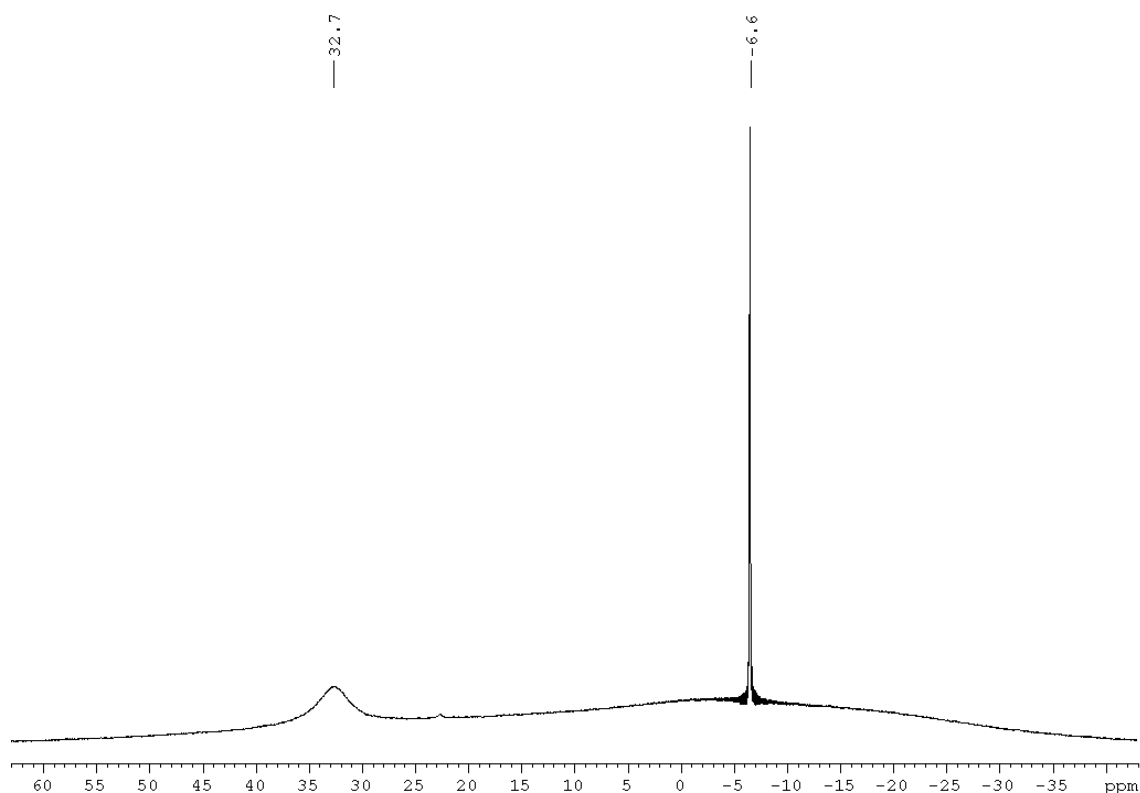


Figure S31. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz) of **5** in CD_2Cl_2 .

7. Computational details

Potential Energy Surface Exploration. Exploration of the potential energy surface of the **1** + HBpin system, with location of intermediates and transition states, was performed using the M06^[4] functional, as implemented in Gaussian 09^[5]. Geometry optimizations were performed in solution (solvent = dichloromethane, DCM, $\epsilon = 8.93$) using the continuum SMD model^[6] and basis sets BS1 (see below). Connections between the transition states and the corresponding minima were checked by displacing in both directions, following the transition vector, the geometry of transition states, with subsequent geometry optimization until a minimum was reached. All energies in solution were corrected by single-point calculations with the larger basis sets BS2 and BS3 (see below). Thermal and entropic corrections were obtained based on vibrational frequencies of the BS1-optimised structures using the quasi-harmonic approximation. Entropic contributions to the Gibbs energies were corrected by employing the approximation described by Grimme where entropic terms for frequencies below a cut-off of 100 cm^{-1} , were calculated using the free-rotor approximation.^[7] A correction of 1.9 kcal mol^{-1} was applied to all Gibbs energies to change the standard state from gas phase (1 bar) to solution (1M). The GoodVibes program developed by Paton and Funes-Ardoiz was employed to introduce these corrections.^[8] All reported energies in the main text correspond to M06/BS3 Gibbs energies in DCM solvent (1M) at 298.15K in kcal mol^{-1} .

Calculations on complex 3c. Geometry optimization and frequency analysis was performed using both M06 and B3LYP-D3^[9] (containing the D3 version of Grimme's dispersion correction)^[10] functionals and basis set BS1' (see below). Relaxed potential energy surface scan calculations were performed using M06-BS1'. QTAIM^[11] analyses were carried out on the optimized structure with Multiwfn software^[12] using different levels of theory that result from combinations of M06 and B3LYP-D3 with BS1' and BS3.

Basis sets. As described above, the following basis set were employed:

- *BS1:* double- ζ 6-31G(d,p)^[13] basis set for the H, C, N, B and O atoms and the scalar relativistic Stuttgart–Dresden SDD pseudopotential and its associated double- ζ basis set for the Pt atom.^[14]
- *BS1':* double- ζ 6-31G(d,p) basis set for the H, C, N, B and O atoms and the scalar relativistic Stuttgart–Dresden SDD pseudopotential and its associated double- ζ basis set, complemented with a set of *f* polarization functions,^[15] for the Pt atom.
- *BS2:* triple- ζ 6-311G++(d,p)^[13] basis set for the H, C, N, B and O atoms and the scalar relativistic Stuttgart–Dresden SDD pseudopotential and its associated double- ζ basis set for the Pt atom.
- *BS3:* triple- ζ def2TZVP basis set for the H, C, N, B and O atoms and quadruple- ζ def2QZVP basis set for the Pt atom.^[16] The scalar relativistic Stuttgart–Dresden SDD pseudopotential and its associated basis set for Pt was used in the energy profile calculations.

Localized Molecular Orbital Analyses. A localized orbital analysis was performed to pinpoint bonding interactions and electron rearrangements along the most favorable reaction path.^[17] Orbital localization of canonical Density Functional Theory molecular orbitals was performed with the CP2K code.^[18] The PBE exchange-correlation functional was used.^[19] The Quickstep algorithm was used to solve the electronic structure problem,^[20] employing a double zeta plus polarization gaussian basis set ^[21] to represent the valence orbitals and plane waves for the electron density (up to a 400 Ry cutoff). Goedecker-Teter-Hutter type pseudopotentials were used for valence-core interactions.^[22] Models were treated as isolated in a cubic box of 20 Å edge.^[23]

8. Optimized structure of complex 3c

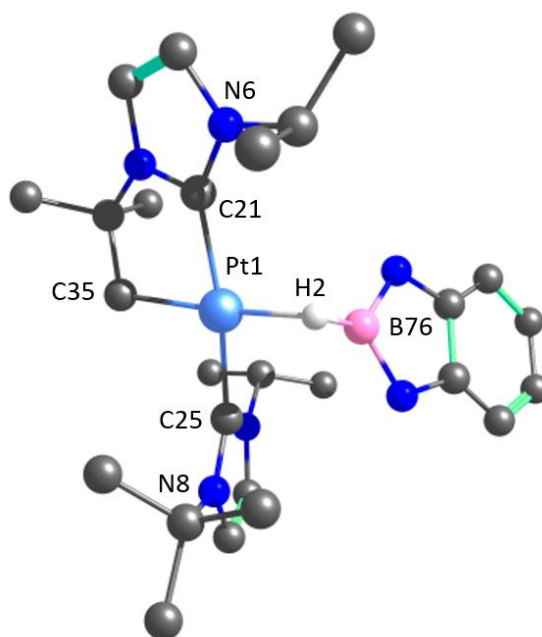


Figure S32. Optimized geometry of complex **3c** using M06/BS1'.

Parameter	Experimental (Crystal structure)	M06	B3LYP-D3
Pt1-H2	1.69(3) Å	1.869 Å	1.786 Å
Pt1-B76	2.313(3) Å	2.443 Å	2.349 Å
Pt1-H2-B76	105(2)°	101.6°	99.5°
C21-Pt1-C25	168.5(1)°	170.3°	169.6°
C35-Pt1-H2	169(1)°	170.1°	167.9°
C35-Pt1-H2-B76	-167(4)°	-157.5°	-158.3°
N6-C21-C25-N8	82.3(4)°	66.8°	66.6°

Table S1. Comparison of experimental (single-crystal X-Ray diffraction) and calculated geometrical parameters of **3c**.

9. Optimized structures of σ -BH complexes

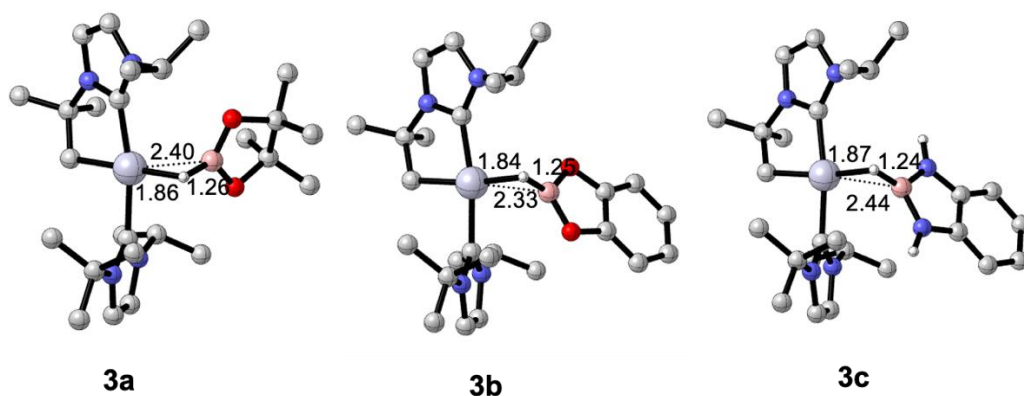


Figure S33. M06/BS1 optimized geometries of σ -BH complexes **3a-c**. The optimized values of the Pt-H-B angles are: 98.7° (**3a**), 95.5° (**3b**) and 101.6° (**3c**). Hydrogen atoms of C-H bonds have been omitted for clarity.

10. QTAIM analysis of complex **3c**.

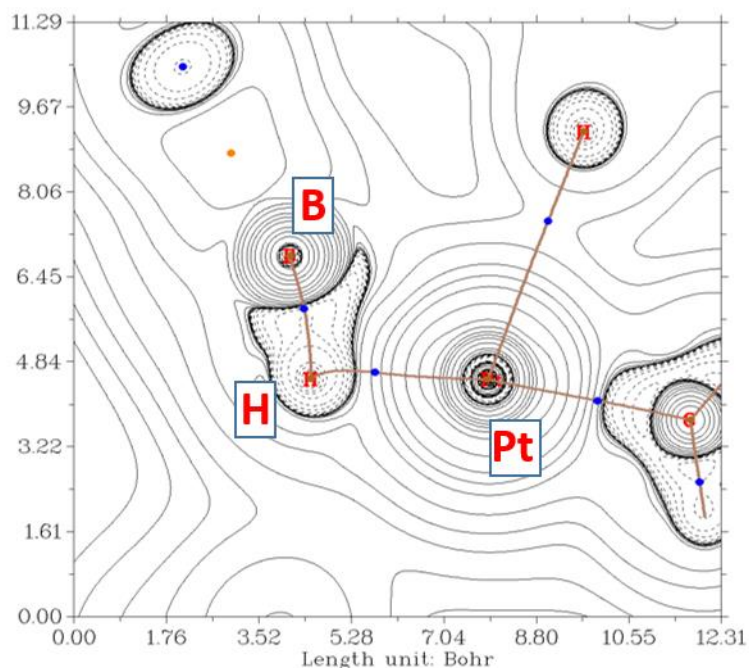


Figure S34. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** using B3LYP-D3/BS1'.

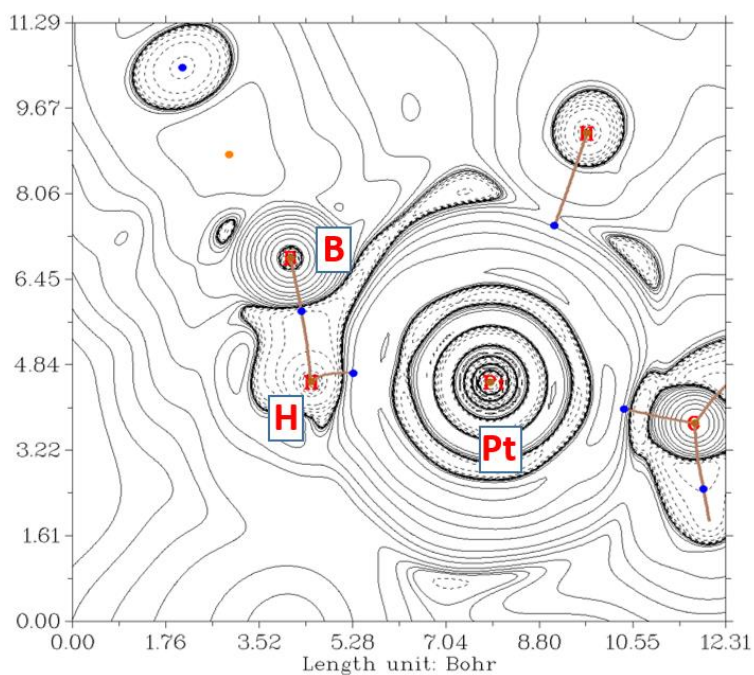


Figure S35. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** using B3LYP-D3/BS3.

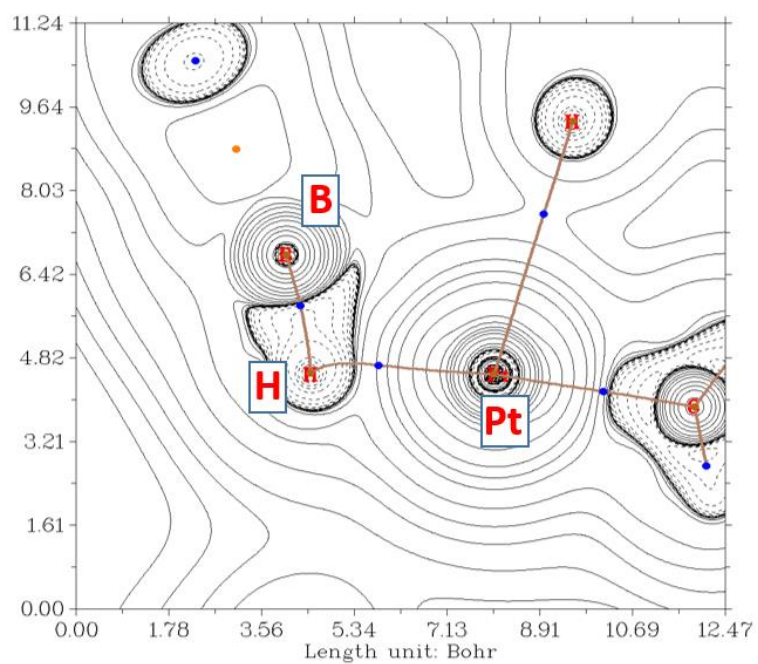


Figure S36. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** using M06/BS1'.

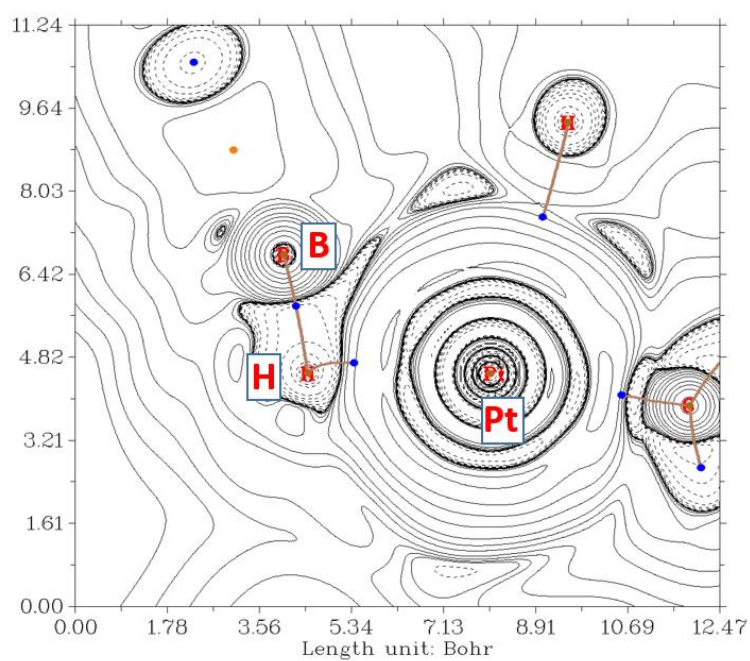


Figure S37. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** using M06/BS3.

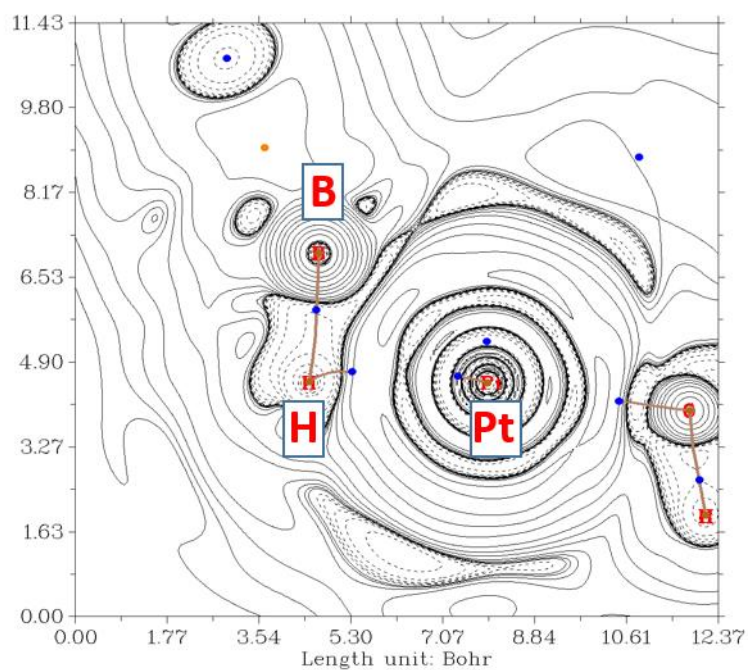


Figure S38. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** (Pt-H-B = 85°) using B3LYP-D3-BS3.

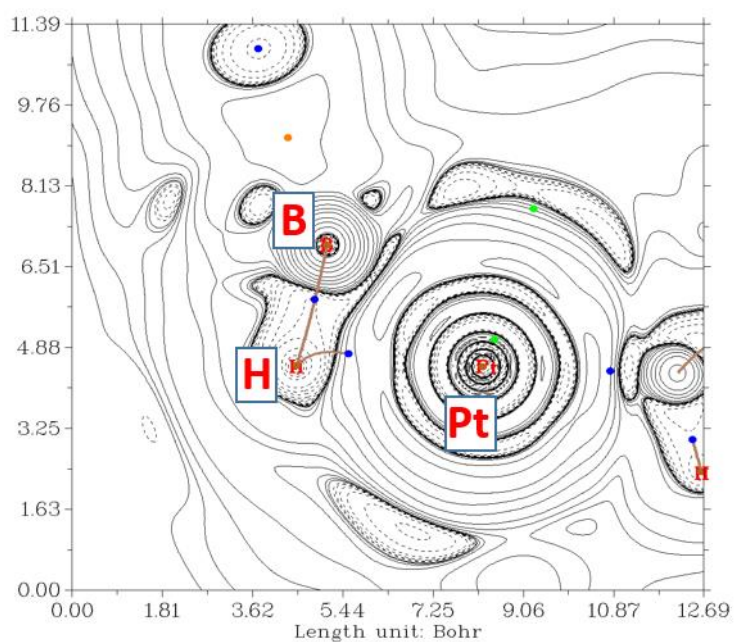
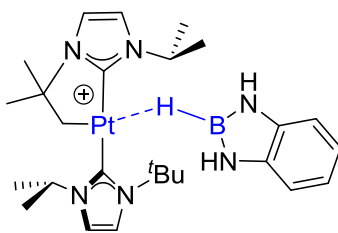


Figure S39. Plot of the Laplacian of the electronic density ($\nabla^2\rho$) of complex **3c** (Pt-H-B = 75°) using B3LYP-D3/BS3.

11. Relaxed potential energy scan calculations on **3c**



Pt-H-B Angle	Energy/Hartrees	Energy/kcal mol ⁻¹
67.8	Borane dissociation	
77.8	-1487.860763	6.1
85.7	-1487.866453	2.5
95.7	-1487.870384	0.1
105.7 ^a	-1487.870457	0.0
115.7	-1487.868728	1.1
125.7	-1487.866094	2.7
135.7	-1487.863436	4.4
144.4	-1487.862064	5.3
154.4	-1487.860288	6.4
164.4	-1487.858551	7.5
174.4	-1487.857641	8.0

^a The energy difference between the optimized minimum (Pt-H-B = 101.6°) and this structure is 0.14 kcal mol⁻¹.

Table S4. Energy values of complex **3c** at fixed values of the Pt-H-B angle using M06/BS1'.

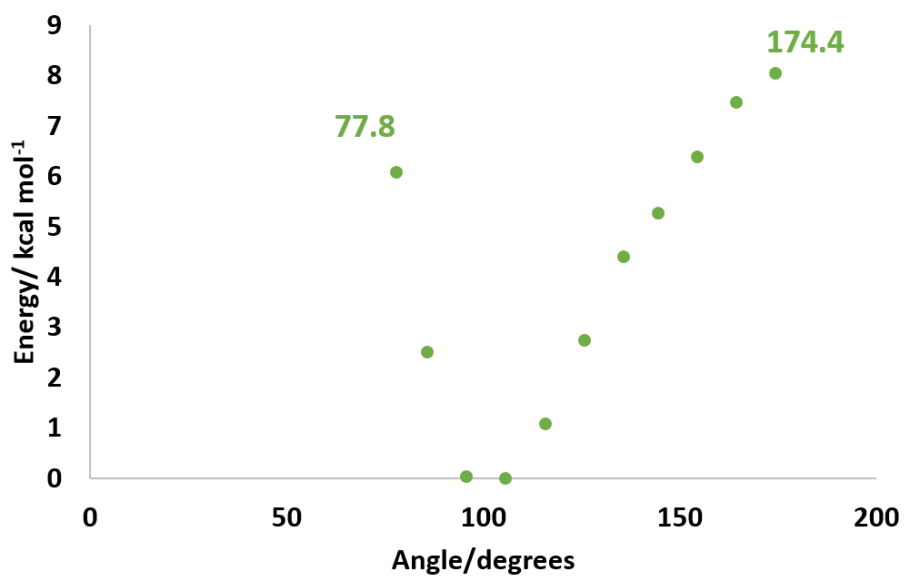
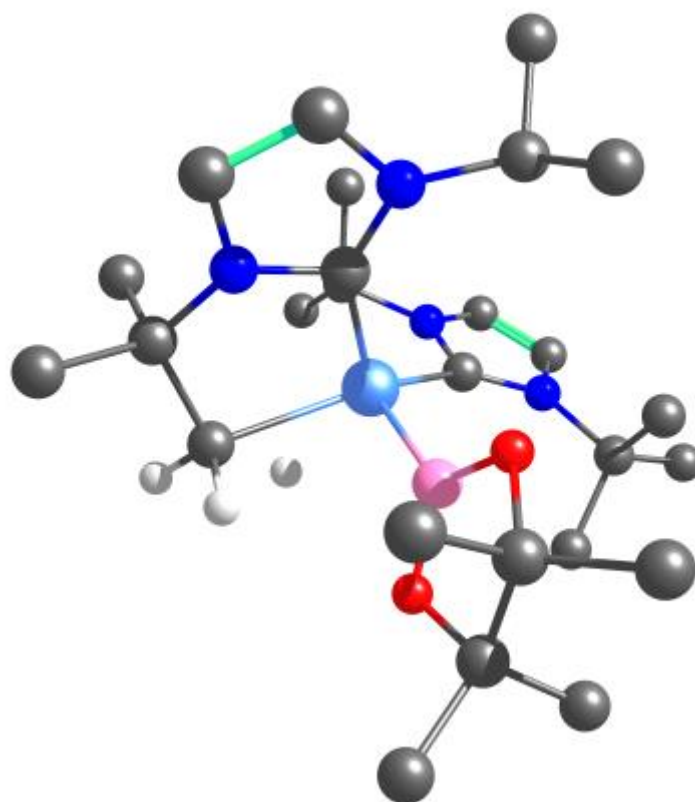


Figure S40. Plot of the energy required for the modification of the angle between the Pt, H and B atoms in complex **3c**.

12. High energy transition states*

- *NHC ligands in a cis geometry*



* Gibbs energies shown were obtained using M06/BS3

Figure S41. Transition state connecting **Int1** and **2a**. This transition state is located 52.3 kcal mol⁻¹ above the reagents. Most of the H atoms have been omitted for clarity.

- *NHC ligands in a trans geometry*

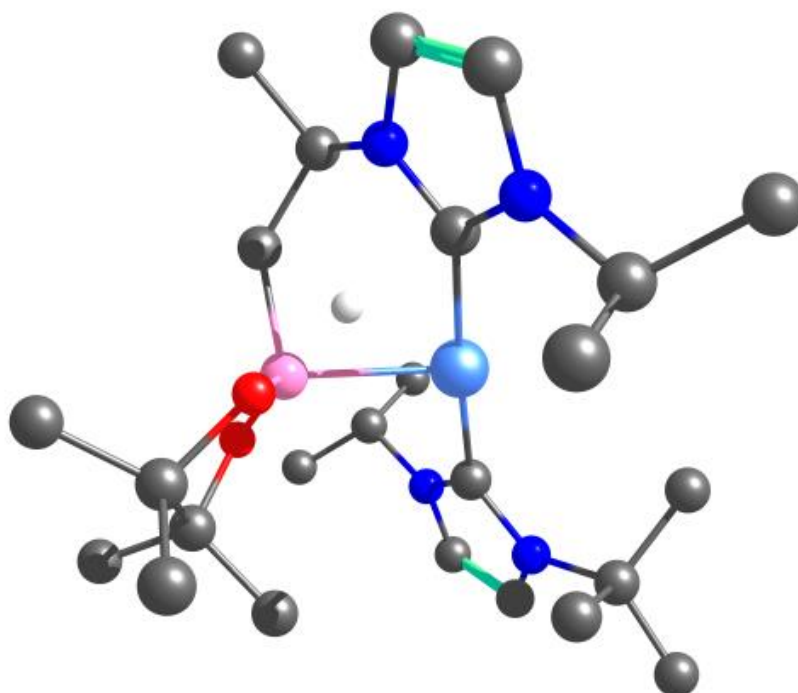


Figure S42. Transition state **TS D**, which connects **Int5** (See Figure S48) and **2a**. This transition state is located 39.9 kcal mol⁻¹ above the reagents. Most of the H atoms have been omitted for clarity.

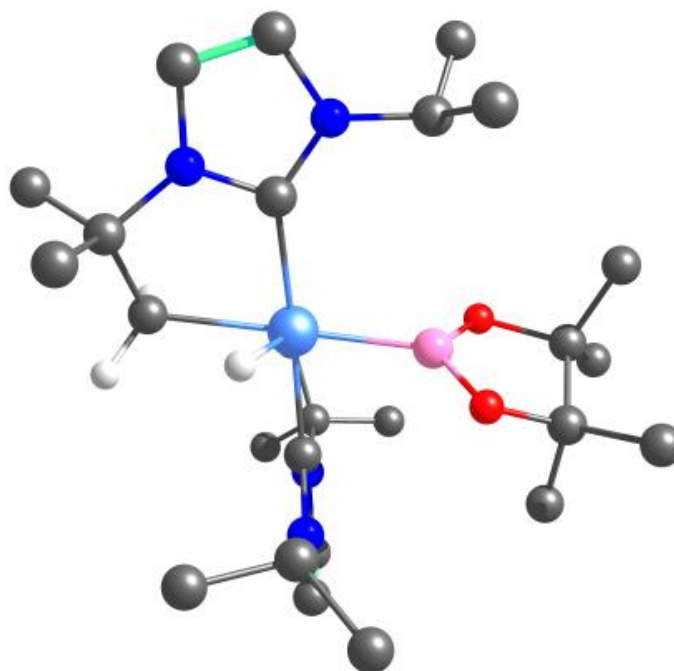


Figure S43. Transition state **TS E**, which connects **3a** and **2a**. This transition state is located 34.0 kcal mol⁻¹ above the reagents. Most of the H atoms have been omitted for clarity.

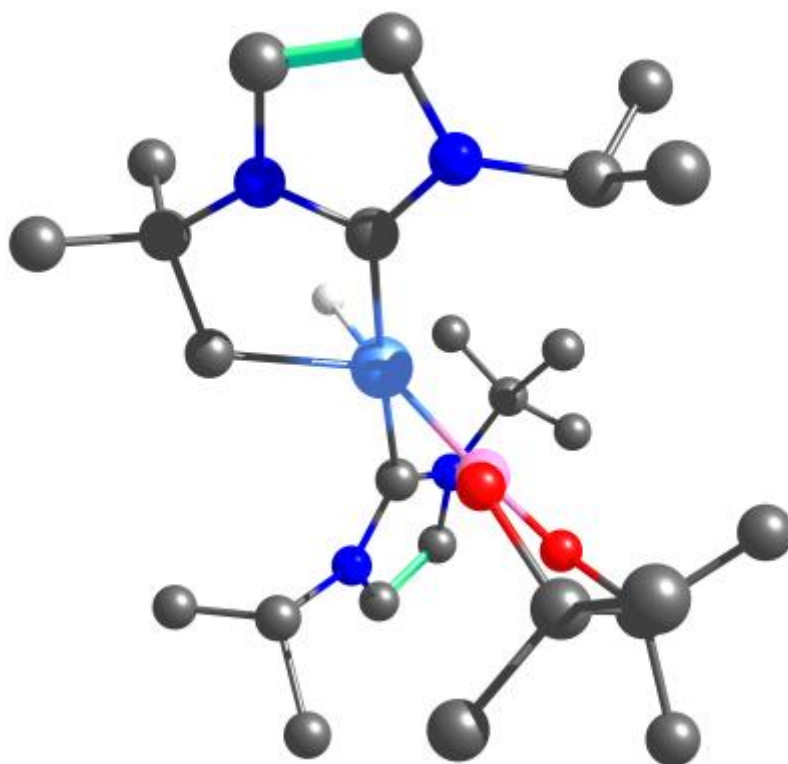


Figure S44. Transition state connecting **2a** and the Pt(IV) species $[\text{Pt}(\text{I}^t\text{Bu}^i\text{Pr})(\text{H})(\text{Bpin})(\text{I}^t\text{Bu}^i\text{Pr})][\text{BAr}^{\text{F}}]$. This transition state is located $38.3 \text{ kcal mol}^{-1}$ above the reagents. Most of the H atoms have been omitted for clarity.

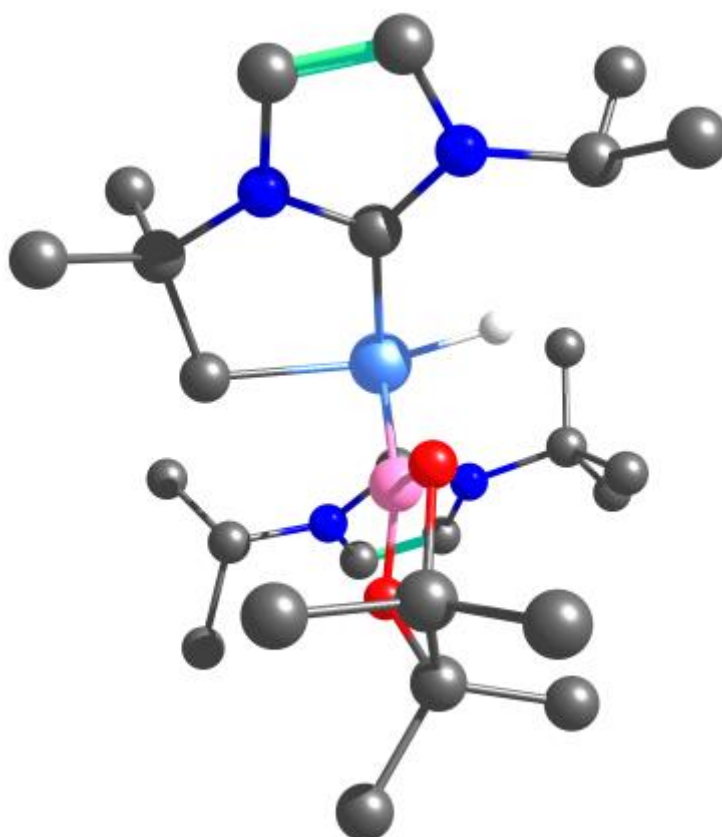
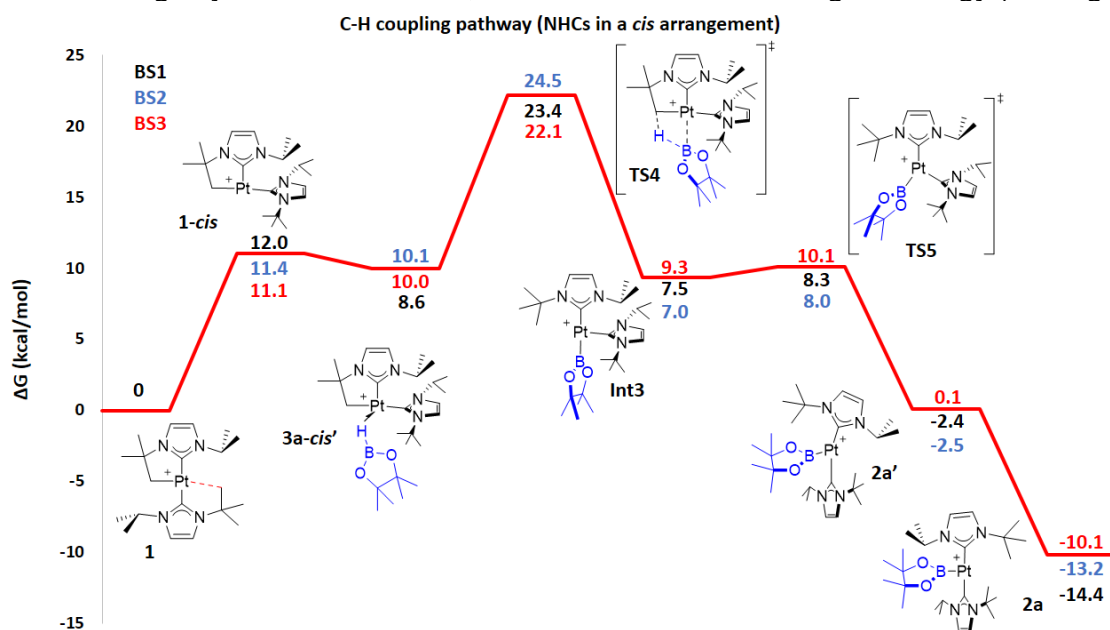
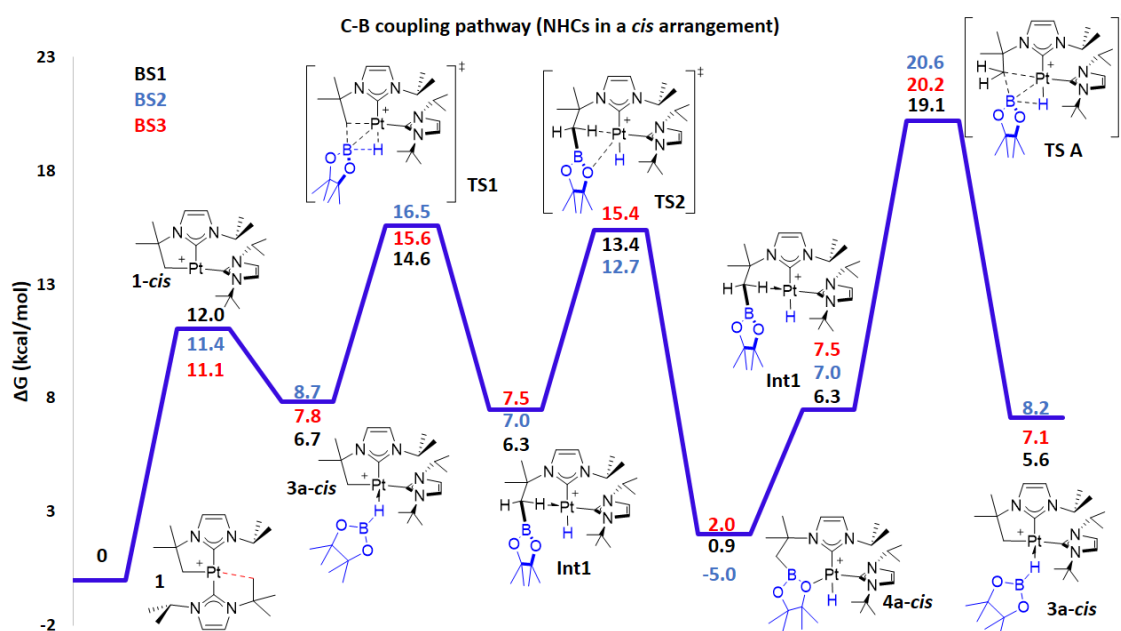


Figure S45. Transition state connecting **3a** and a **Int5** (See Figure S48). This transition state is located $33.5 \text{ kcal mol}^{-1}$ above the reagents. Most of the H atoms have been omitted for clarity.

13. Calculated energy profiles



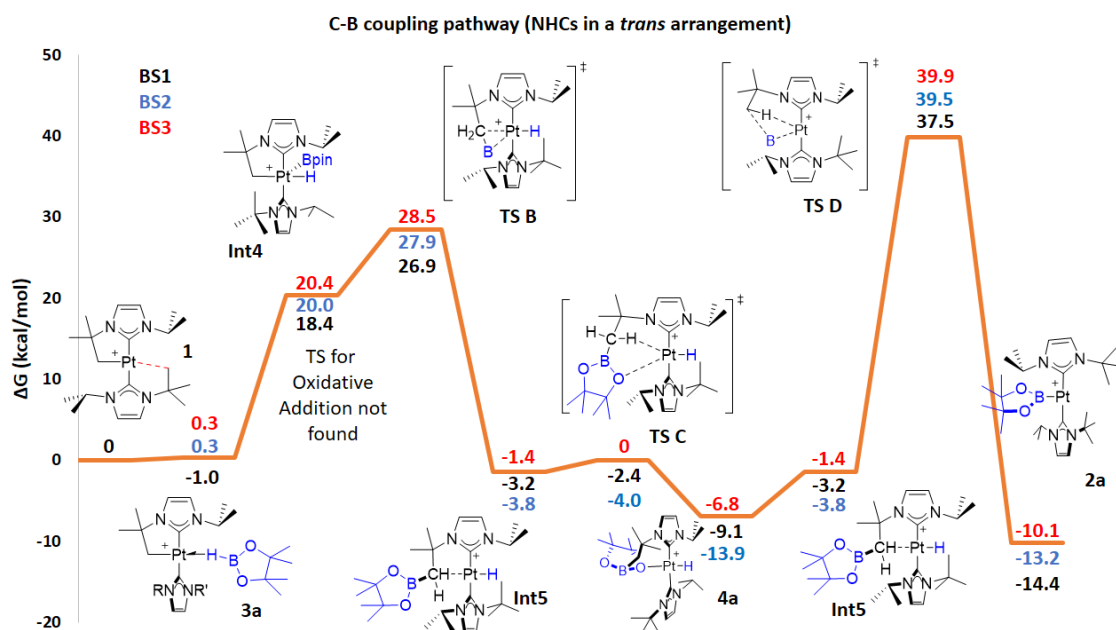


Figure S48. Gibbs energy profile for the C–B coupling pathway in which the NHC ligands adopt a *trans* geometry. Given that transition state **TS D** connects **Int5** and **2a**, **TS C** was shown just once for clarity.

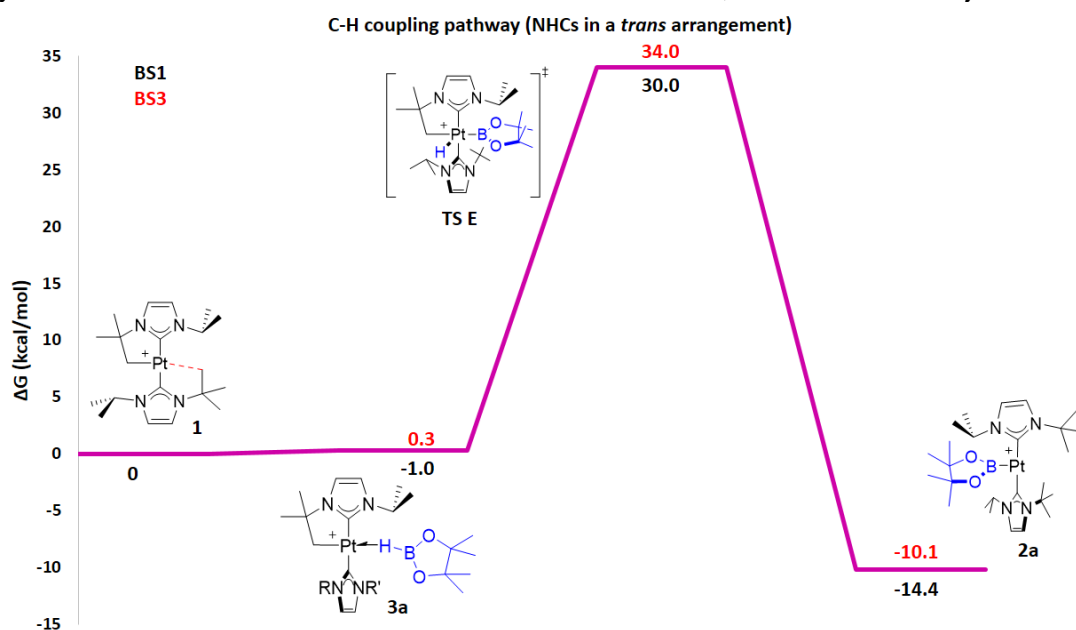


Figure S49. Gibbs energy profile for the C–H coupling pathway in which the NHC ligands adopt a *trans* geometry.

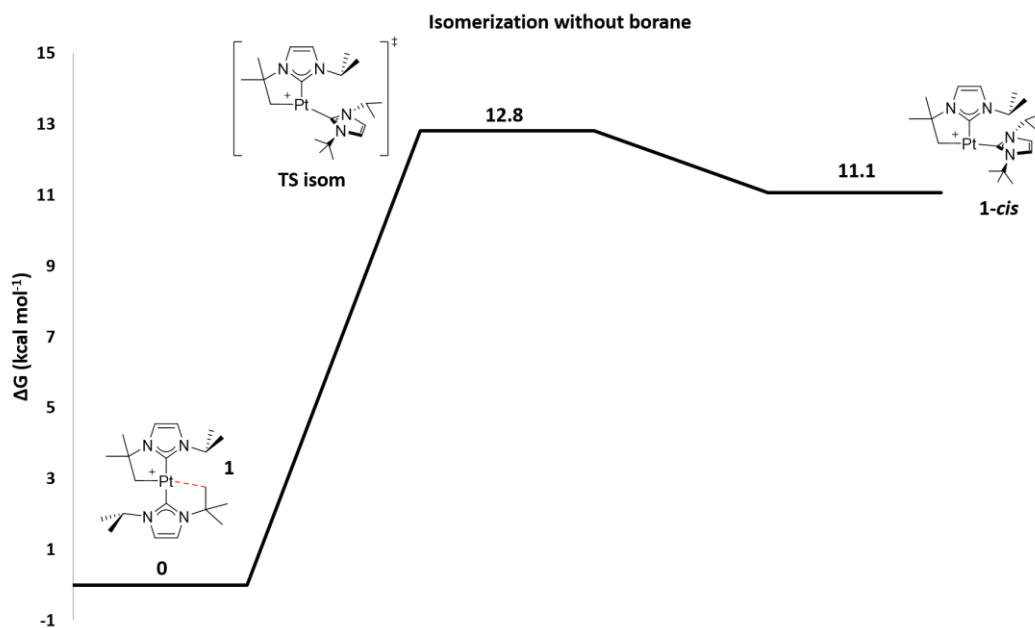


Figure S50 Gibbs energy profile (BS3) for the *trans-cis* isomerization of **1**.

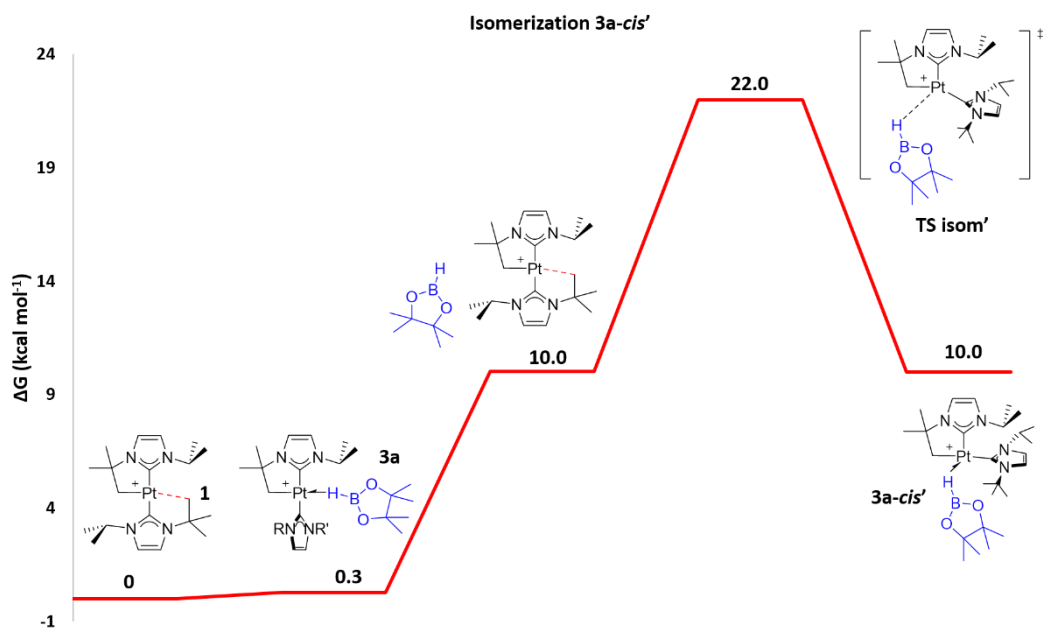


Figure S51. Gibbs energy profile (BS3) for the *trans-cis* isomerization of **3a-cis'**.

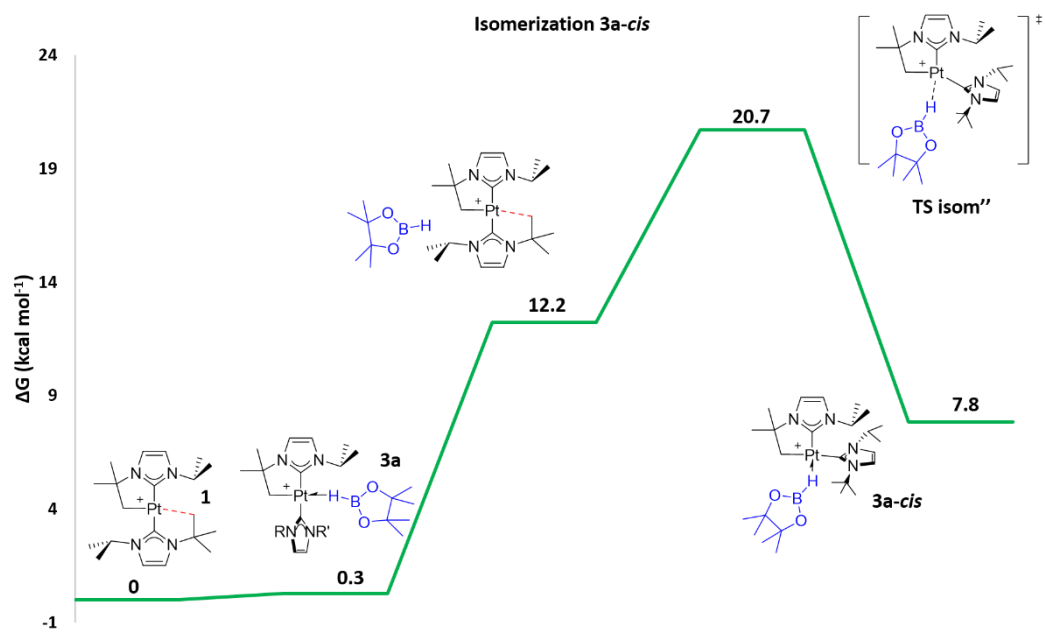
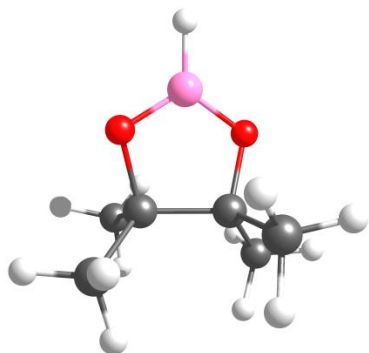


Figure S52. Gibbs energy profile (BS3) for the *trans-cis* isomerization of **3a-cis**.

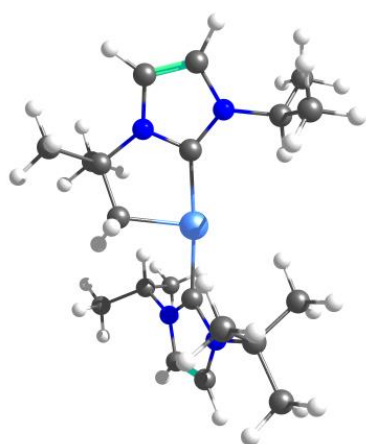
14. Cartesian coordinates of the optimized structures

HBpin



C	0.777721000	-0.189378000	-0.054471000
C	-0.777747000	-0.189315000	0.054489000
O	-1.063268000	1.187221000	0.420848000
O	1.063324000	1.187096000	-0.420980000
B	0.000084000	1.926450000	-0.000057000
H	0.000160000	3.114744000	-0.000034000
C	-1.474437000	-0.433491000	-1.273876000
H	-1.387564000	-1.479440000	-1.589449000
H	-2.539323000	-0.199875000	-1.162353000
H	-1.069398000	0.206380000	-2.066855000
C	-1.344265000	-1.105214000	1.116939000
H	-2.437848000	-1.030698000	1.122134000
H	-1.080856000	-2.149110000	0.905194000
H	-0.982580000	-0.849163000	2.117549000
C	1.344185000	-1.105389000	-1.116849000
H	2.437782000	-1.031085000	-1.121906000
H	1.080542000	-2.149224000	-0.905106000
H	0.982678000	-0.849291000	-2.117511000
C	1.474420000	-0.433435000	1.273915000
H	1.387204000	-1.479265000	1.589792000
H	2.539379000	-0.200231000	1.162240000
H	1.069689000	0.206803000	2.066757000

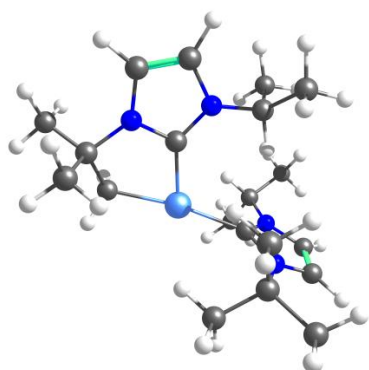
1



C	2.108998000	-0.088593000	0.043149000
C	4.348469000	0.005913000	0.045725000
H	5.326336000	0.414478000	0.259663000
C	3.992859000	-1.124060000	-0.619052000
H	4.598896000	-1.889813000	-1.083204000
C	1.668810000	-2.167797000	-1.123066000
C	2.135168000	-2.689694000	-2.473883000
H	2.303290000	-1.867963000	-3.179590000
H	1.369103000	-3.353489000	-2.891127000
H	3.061124000	-3.270588000	-2.380251000
C	0.330807000	-1.430819000	-1.277858000
H	-0.505406000	-2.139208000	-1.229406000
H	0.290960000	-0.894343000	-2.237777000
C	3.074689000	1.928084000	1.137851000
H	2.052503000	1.945789000	1.542202000
C	4.065617000	2.015592000	2.281332000
H	3.968249000	1.165294000	2.964991000
H	3.885928000	2.934890000	2.848543000
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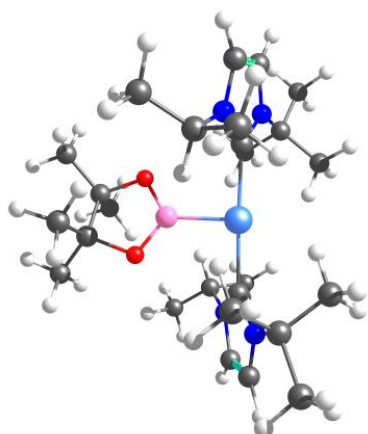
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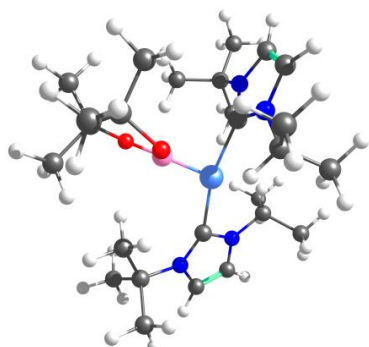


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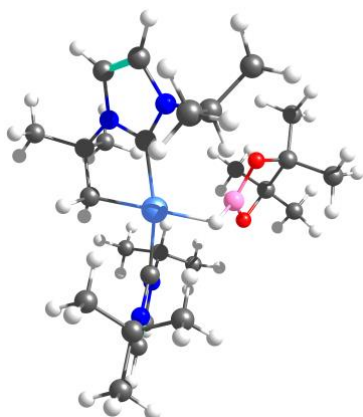
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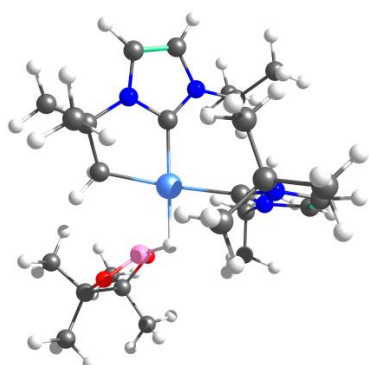
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H	0.255660000	-0.500891000	1.461382000
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O	0.482720000	-2.525518000	0.398995000
O	2.318353000	-1.253463000	0.908687000
C	1.643608000	-3.260596000	-0.094962000
C	2.809036000	-2.609268000	0.707405000
C	1.734209000	-2.994916000	-1.588266000
C	1.438076000	-4.734120000	0.169339000
C	4.129318000	-2.552413000	-0.026738000
C	3.002119000	-3.206729000	2.090475000
H	2.556177000	-3.560706000	-2.041008000
H	0.801640000	-3.312578000	-2.068977000
H	1.888701000	-1.929402000	-1.801541000
H	0.610759000	-5.111587000	-0.442706000
H	2.339675000	-5.296883000	-0.102891000
H	1.206131000	-4.933494000	1.219754000
H	4.899273000	-2.126084000	0.626509000
H	4.450999000	-3.563867000	-0.304907000
H	4.070038000	-1.942576000	-0.933602000
H	3.464714000	-4.198682000	2.035090000
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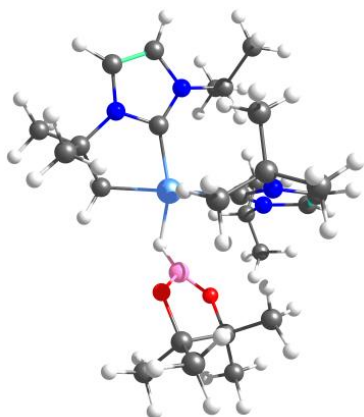


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N	1.204483000	-2.526850000	-0.353293000
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C	3.078218000	2.534125000	-1.610245000
C	2.249173000	3.475409000	-1.091672000
C	1.161529000	-1.449046000	0.465788000
C	2.098644000	-3.470242000	0.113199000
C	2.624714000	-2.970140000	1.254145000
H	4.013452000	2.634207000	-2.143696000
H	2.325043000	4.553640000	-1.073729000
H	2.277320000	-4.409045000	-0.392401000
H	3.354483000	-3.403303000	1.920166000
C	0.346058000	-2.708780000	-1.540207000
C	1.151017000	-3.237342000	-2.712335000
H	1.442086000	-4.284217000	-2.559106000

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H	-1.492630000	-3.710669000	-2.048045000
H	-0.455979000	-4.621330000	-0.928586000
H	-1.388945000	-3.218245000	-0.344979000
C	3.017425000	0.031446000	-1.919511000
C	-0.034807000	3.298501000	0.127331000
C	-1.049858000	2.154139000	-0.001898000
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C	4.430278000	-0.240715000	-1.444808000
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H	4.492652000	-0.220673000	-0.350479000
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B	-2.302761000	-0.355890000	0.422363000
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C	-4.582786000	-2.324184000	-0.127630000
C	-4.822002000	-0.677293000	-1.975224000
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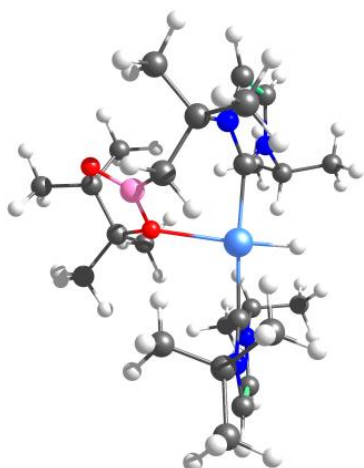
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C	-4.339438000	-1.515388000	0.390841000
C	0.283774000	1.312977000	0.133153000
C	1.043093000	3.438581000	0.018119000
C	0.937509000	3.115790000	1.325494000
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H	-5.022437000	-2.339950000	0.541709000
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H	1.161185000	3.708758000	2.198409000
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C	-0.412419000	3.222106000	-2.716293000
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H	-1.397191000	3.004975000	-2.289587000
C	2.024350000	2.620985000	-2.720783000
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C	-3.194344000	1.888391000	-0.058587000
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C	-1.116963000	-2.501732000	-1.134187000
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H	-2.633585000	-3.734506000	1.754142000
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H	2.077237000	1.833686000	3.579611000
H	0.665082000	2.835618000	4.014222000
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C	0.600897000	-0.333954000	2.669072000
H	0.359093000	-0.787521000	3.637486000
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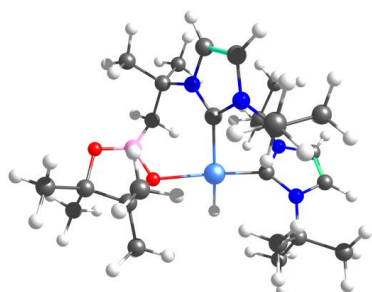
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H	-1.949077000	-3.223623000	1.205446000
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C	4.424174000	0.592766000	-0.631633000
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C	4.550348000	-0.550955000	0.078186000
H	5.428681000	-1.144259000	0.279035000
C	2.981017000	-2.122297000	1.339796000
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H	1.170525000	-2.511381000	0.191322000
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C	2.527259000	2.157092000	-1.205787000
H	1.443527000	1.975990000	-1.237531000

C	3.044652000	2.334385000	-2.620473000
H	4.110297000	2.594661000	-2.633598000
H	2.501799000	3.152503000	-3.106638000
H	2.903192000	1.425710000	-3.216708000
C	2.813854000	3.363754000	-0.331179000
H	2.427225000	3.222034000	0.685431000
H	2.341206000	4.256763000	-0.758323000
H	3.893925000	3.549609000	-0.266739000
C	-4.148125000	-1.870154000	1.344428000
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O	-0.526520000	-1.157489000	-1.018088000
O	-2.480894000	-2.236399000	-1.463230000
C	-0.652112000	-1.151236000	-2.478318000
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C	0.254494000	-2.256134000	-2.987823000
C	-0.207818000	0.187936000	-3.016475000
C	-2.510204000	-2.276715000	-3.874352000
C	-3.047445000	-0.214394000	-2.584003000
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H	-0.734232000	1.023545000	-2.542261000
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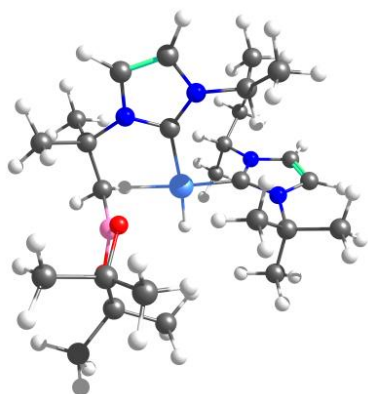


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C	-0.257239000	1.180613000	0.800384000

C	0.049828000	2.568952000	2.566122000
C	-0.860854000	3.143771000	1.753223000
C	2.102706000	-0.211863000	-0.644579000
C	4.051868000	0.866167000	-0.988020000
C	4.344786000	-0.376499000	-0.553842000
H	0.470681000	2.899544000	3.505638000
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H	4.695456000	1.692043000	-1.256449000
H	5.306251000	-0.832723000	-0.380800000
C	1.968843000	2.169603000	-1.492058000
C	2.291926000	3.338795000	-0.579979000
H	3.360517000	3.587737000	-0.612071000
H	1.737390000	4.227170000	-0.903931000
H	2.015626000	3.121538000	0.460184000
C	2.289867000	2.447782000	-2.948106000
H	1.695739000	3.299771000	-3.298349000
H	3.348399000	2.700546000	-3.088707000
H	2.052559000	1.580781000	-3.575729000
C	1.339078000	0.420576000	2.592302000
C	-2.055104000	2.657730000	-0.380120000
C	-2.299839000	1.521199000	-1.377258000
H	-1.376914000	1.305000000	-1.935679000
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C	0.859779000	0.017654000	3.974715000
H	0.896082000	0.859939000	4.677680000
H	-0.167687000	-0.363495000	3.948197000
H	1.509603000	-0.770622000	4.372209000
C	2.746824000	0.986503000	2.613706000
H	3.068674000	1.303394000	1.614122000
H	2.817334000	1.850845000	3.287321000
H	3.448063000	0.224183000	2.975837000
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H	-1.286783000	4.701141000	-0.443686000
H	-0.614421000	3.621583000	-1.692147000
H	-2.274782000	4.229759000	-1.836853000
C	-3.372462000	2.998427000	0.317145000
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H	-3.311140000	3.921918000	0.902123000
C	3.116623000	-2.514743000	0.007082000
C	4.462467000	-2.910903000	0.608097000
H	5.276800000	-2.892324000	-0.124661000
H	4.731207000	-2.278591000	1.463568000
H	4.380460000	-3.942140000	0.967875000
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H	2.281540000	-2.358368000	2.006783000
H	2.023488000	-3.912272000	1.196986000
H	1.303599000	-0.452277000	1.933802000
H	1.047253000	-2.506649000	0.721428000
H	0.905303000	1.921962000	-1.402737000
H	0.393477000	-1.707514000	-1.574547000
B	-2.866028000	0.186215000	-0.791310000
O	-4.141911000	-0.091410000	-0.431031000

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C	-4.231989000	-1.520279000	-0.164448000
C	-2.764465000	-1.901463000	0.194454000
C	-4.726083000	-2.165960000	-1.447654000
C	-5.222823000	-1.744016000	0.954730000
C	-2.339769000	-3.286266000	-0.230462000
C	-2.404395000	-1.651401000	1.646559000
H	-4.911927000	-3.236890000	-1.310832000
H	-5.669799000	-1.691328000	-1.737238000
H	-4.013047000	-2.036889000	-2.270305000
H	-6.226569000	-1.463495000	0.616839000
H	-5.245527000	-2.803654000	1.237224000
H	-4.982821000	-1.149249000	1.841156000
H	-1.309804000	-3.478844000	0.092164000
H	-2.986370000	-4.034906000	0.243205000
H	-2.387815000	-3.418434000	-1.315536000
H	-2.878096000	-2.391354000	2.301033000
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Int1

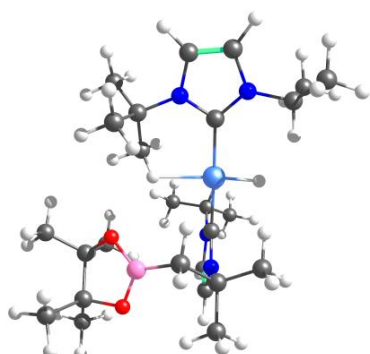


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C	-0.324147000	-1.555164000	0.698073000
C	-0.529652000	-2.889642000	2.502159000
C	0.479809000	-3.383595000	1.748128000
C	-1.952568000	0.945230000	-0.407218000
C	-4.138333000	1.457458000	-0.362388000
C	-3.489822000	2.362331000	0.401063000
H	-0.940441000	-3.233591000	3.441109000
H	1.113614000	-4.244016000	1.905104000
H	-5.188481000	1.357562000	-0.595425000
H	-3.879180000	3.197463000	0.961688000
C	-3.460161000	-0.470470000	-1.850626000
C	-4.824363000	-1.090767000	-1.623666000
H	-5.632303000	-0.398484000	-1.891140000
H	-4.924833000	-1.969156000	-2.269499000
H	-4.968421000	-1.411085000	-0.585748000
C	-3.336446000	0.109935000	-3.248673000
H	-3.511501000	-0.672360000	-3.995797000

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C	-2.171614000	-0.986608000	2.303950000
C	1.497781000	-2.796112000	-0.502683000
C	1.696413000	-1.492575000	-1.286677000
H	0.758238000	-1.250133000	-1.898887000
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C	-2.059515000	-0.636635000	3.775014000
H	-2.166729000	-1.521998000	4.413830000
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C	-3.446146000	-1.742743000	1.979052000
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H	-3.508079000	-2.672153000	2.560180000
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H	3.543801000	-3.353706000	-0.849311000
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O	2.849508000	-0.143149000	0.662358000
C	3.918441000	1.496004000	-0.642786000
C	4.018995000	0.722951000	0.709566000
C	3.043413000	2.734519000	-0.565706000
C	5.246941000	1.834227000	-1.282670000
C	3.943101000	1.588475000	1.946660000
C	5.229682000	-0.193676000	0.784942000
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H	2.089910000	2.520373000	-0.071406000
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H	5.841792000	2.477391000	-0.622339000
H	5.829043000	0.937779000	-1.514977000
H	4.008381000	0.960178000	2.842429000
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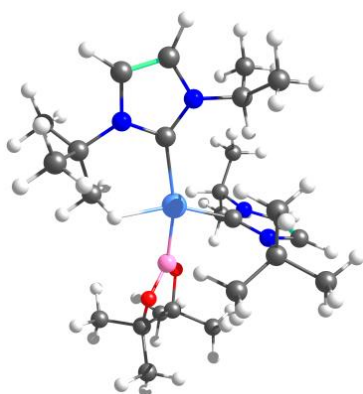
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N	1.537593000	-1.965253000	-0.722826000
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N	-4.025188000	0.522980000	-0.550204000
C	0.568549000	-1.681015000	0.193993000
C	2.203033000	-2.889179000	1.167680000
C	2.549994000	-2.702338000	-0.127014000
C	-2.763921000	0.737084000	-0.103684000
C	-4.781477000	1.676305000	-0.446968000
C	-3.973105000	2.634507000	0.060543000
H	2.712072000	-3.409185000	1.967160000
H	3.429095000	-3.031335000	-0.659014000
H	-5.822328000	1.715138000	-0.735475000
H	-4.173774000	3.673151000	0.280190000
C	-4.568294000	-0.769552000	-1.014598000
C	-5.342399000	-1.437195000	0.106801000
H	-6.201928000	-0.822759000	0.405040000
H	-5.721425000	-2.409622000	-0.226982000
H	-4.708426000	-1.597614000	0.986711000
C	-5.405471000	-0.582562000	-2.265215000
H	-5.687052000	-1.564759000	-2.659031000
H	-6.334423000	-0.037537000	-2.057908000
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C	1.518450000	-1.564468000	-2.175924000
C	1.505534000	-0.030053000	-2.267484000
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H	1.919965000	-1.654754000	3.836947000
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H	-0.641338000	-1.781649000	-2.419253000

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C	2.756031000	-2.123704000	-2.867426000
H	2.709607000	-1.833638000	-3.922639000
H	3.686541000	-1.723909000	-2.453599000
H	2.777996000	-3.219335000	-2.828399000
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C	-1.944156000	3.734742000	1.863922000
H	-2.627302000	4.516523000	1.515739000
H	-2.423764000	3.188141000	2.684547000
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H	-1.694288000	4.282588000	-0.832150000
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H	-0.903272000	1.195392000	2.093890000
H	0.350098000	2.374260000	1.677316000
H	-0.757107000	-1.869917000	2.348648000
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H	-3.687859000	-1.372823000	-1.263270000
H	-1.860814000	-1.735345000	-0.477283000
B	2.582330000	0.658646000	-1.354686000
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O	2.273575000	1.619542000	-0.426215000
C	4.592394000	1.271285000	-0.494063000
C	3.438032000	1.767399000	0.426528000
C	5.161118000	2.359994000	-1.389251000
C	5.710346000	0.544591000	0.220235000
C	3.546822000	3.210200000	0.867219000
C	3.208669000	0.865447000	1.630382000
H	5.769783000	3.072337000	-0.820561000
H	5.802231000	1.894902000	-2.146489000
H	4.369550000	2.913053000	-1.908776000
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H	5.350523000	-0.358832000	0.722850000
H	2.697034000	3.466093000	1.511799000
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H	3.548093000	3.899344000	0.017056000
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Int3

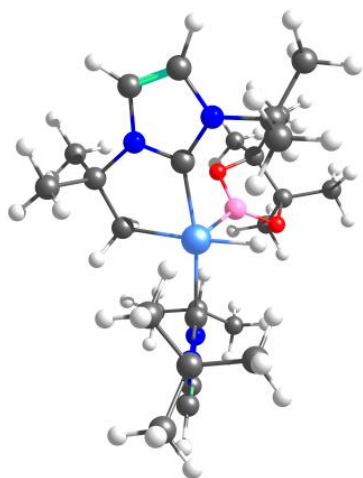


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C	2.477811000	0.582352000	-0.091959000
C	4.731134000	0.384904000	-0.055029000
C	4.443791000	1.705447000	-0.020182000
C	-0.421725000	-1.438979000	-0.041166000
C	-1.162942000	-3.407761000	-0.831272000
C	-1.135404000	-3.494925000	0.515327000
H	5.681531000	-0.130530000	-0.054218000
H	5.097706000	2.564968000	0.024060000
H	-1.450510000	-4.135094000	-1.577207000
H	-1.405947000	-4.320899000	1.153184000
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H	0.470073000	-3.398389000	-3.274593000
H	0.740322000	-1.921525000	-4.218787000
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H	-1.801098000	-1.415345000	-4.306136000
H	-2.056821000	-2.963355000	-3.495178000
H	-2.734676000	-1.465828000	-2.793593000
C	3.422763000	-1.748887000	-0.210168000
C	2.355065000	3.116361000	0.019285000
C	0.872187000	2.889642000	-0.226044000
H	0.671553000	2.473560000	-1.227065000
H	0.321560000	3.835751000	-0.175815000
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H	3.755197000	-2.021676000	1.924007000
H	3.921454000	-3.496124000	0.944089000
C	4.013010000	-2.209484000	-1.532313000
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H	2.172079000	3.031905000	2.178587000
H	3.624245000	3.889980000	1.610876000
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C	-0.978158000	-3.172543000	3.287808000
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H	1.282293000	-1.744044000	3.743351000
H	2.344568000	-1.959887000	-0.187182000

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O	-2.669341000	0.333354000	-1.035564000
O	-2.400006000	1.522333000	0.892738000
C	-4.002403000	0.593435000	-0.532168000
C	-3.756134000	1.777247000	0.445162000
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C	-4.922222000	0.904463000	-1.691361000
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H	-5.720551000	1.902445000	1.329716000
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Int4

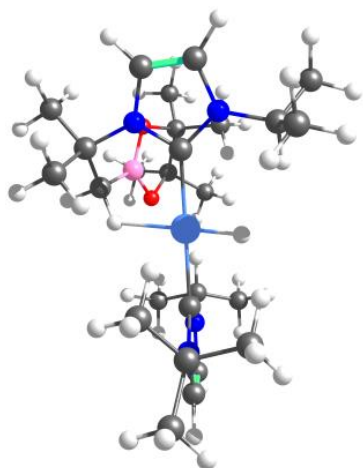


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H	2.963764000	-3.157966000	2.567855000
C	0.508077000	-1.605341000	2.660685000
C	-0.273346000	-2.871271000	2.993314000
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H	-0.963113000	-2.672607000	3.821883000
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H	-1.430981000	-0.661448000	2.523283000
C	2.312644000	-2.042644000	-1.919476000
H	1.945515000	-1.038723000	-2.174209000
C	3.745809000	-2.191204000	-2.388832000
H	4.423934000	-1.506982000	-1.866739000

H	3.792127000	-1.965596000	-3.459246000
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H	-0.766917000	2.422411000	0.754273000
C	-2.130913000	3.001037000	2.306584000
H	-3.140560000	3.413876000	2.426439000
H	-1.425348000	3.707300000	2.759428000
H	-2.075731000	2.055758000	2.858429000
C	-1.913667000	4.098004000	0.047904000
H	-1.672976000	3.939647000	-1.009553000
H	-1.229213000	4.850981000	0.452433000
H	-2.928396000	4.509008000	0.116384000
C	1.298782000	-1.130359000	3.871247000
H	1.939562000	-1.917271000	4.289952000
H	0.597782000	-0.820879000	4.655097000
H	1.926208000	-0.268435000	3.612116000
N	-3.406302000	-0.072848000	-0.585403000
N	-2.646301000	1.769918000	0.244663000
N	2.224483000	-2.121223000	-0.444800000
N	1.465484000	-1.954910000	1.572221000
Pt	-0.393607000	-0.411451000	-0.047208000
H	-0.246656000	-0.350337000	-1.686214000
B	0.997294000	1.051050000	-0.285447000
O	0.983361000	2.012427000	-1.248237000
O	2.059891000	1.128631000	0.568605000
C	2.092170000	2.919039000	-0.948486000
C	3.015185000	2.032729000	-0.058412000
C	1.518573000	4.112612000	-0.208510000
C	2.707772000	3.366364000	-2.255075000
C	3.769377000	2.771797000	1.022544000
C	3.966178000	1.160086000	-0.859067000
H	2.293635000	4.863968000	-0.019225000
H	0.741859000	4.575564000	-0.826167000
H	1.074346000	3.824588000	0.752542000
H	1.995868000	3.993056000	-2.804022000

H	3.607178000	3.965463000	-2.065743000
H	2.979340000	2.520960000	-2.893963000
H	4.396304000	2.066692000	1.580289000
H	4.428638000	3.528472000	0.579940000
H	3.098811000	3.263860000	1.733147000
H	4.775719000	1.750362000	-1.303131000
H	4.410899000	0.416154000	-0.186481000
H	3.443578000	0.625909000	-1.663037000

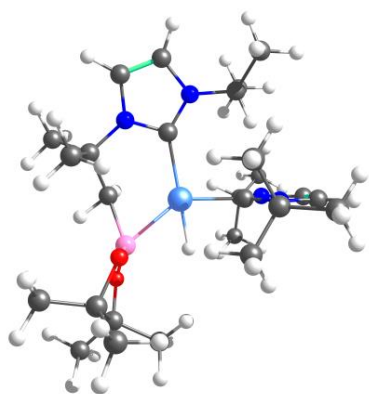
Int5



C	0.707348000	-1.787326000	0.002065000
C	2.113123000	-3.500305000	-0.385121000
H	2.588153000	-4.289203000	-0.950816000
C	2.305998000	-3.099137000	0.893740000
H	2.990949000	-3.470794000	1.640666000
C	1.293391000	-1.290166000	2.396054000
C	0.092062000	-1.848168000	3.149701000
H	-0.827456000	-1.740464000	2.560264000
H	-0.038335000	-1.309996000	4.096301000
H	0.238557000	-2.911619000	3.375528000
C	1.100455000	0.194238000	2.065737000
H	1.117072000	0.753239000	3.014832000
H	0.045553000	0.407021000	1.741897000
C	0.580018000	-2.832809000	-2.279151000
H	0.108005000	-1.867315000	-2.498487000
C	1.676939000	-3.089190000	-3.293695000
H	2.459645000	-2.323342000	-3.245237000
H	1.245784000	-3.071618000	-4.300084000
H	2.140790000	-4.073471000	-3.155488000
C	-0.470784000	-3.928489000	-2.274618000
H	-0.017702000	-4.893395000	-2.011598000
H	-0.923105000	-4.025876000	-3.267928000
H	-1.265827000	-3.713270000	-1.550218000
C	-2.347423000	0.999923000	-0.084165000
C	-3.444655000	2.956177000	-0.320376000
H	-3.559494000	4.015723000	-0.503267000
C	-4.361551000	2.008317000	-0.025590000
H	-5.429098000	2.102133000	0.095876000
C	-4.380472000	-0.503428000	0.355139000
C	-3.641857000	-1.313064000	1.411669000
H	-2.648381000	-1.624899000	1.066168000
H	-4.221742000	-2.216017000	1.636041000
H	-3.530046000	-0.737884000	2.339861000

C	-4.447490000	-1.252133000	-0.970425000
H	-4.981219000	-0.658906000	-1.723379000
H	-4.986252000	-2.197341000	-0.833114000
H	-3.446606000	-1.481699000	-1.353760000
C	-5.795916000	-0.239821000	0.855280000
H	-5.800777000	0.362651000	1.771729000
H	-6.260510000	-1.204493000	1.085590000
H	-6.423724000	0.247458000	0.100947000
C	-0.950599000	3.016197000	-0.637073000
H	-0.190497000	2.225054000	-0.631171000
C	-0.638708000	4.006057000	0.468265000
H	-1.378746000	4.815883000	0.502912000
H	0.345341000	4.457193000	0.298787000
H	-0.619277000	3.512193000	1.447292000
C	-1.001363000	3.658633000	-2.010094000
H	-1.227788000	2.917238000	-2.785381000
H	-0.032122000	4.114522000	-2.242157000
H	-1.757759000	4.452056000	-2.056622000
C	2.546531000	-1.463117000	3.245989000
H	2.663855000	-2.498524000	3.584910000
H	2.444462000	-0.842090000	4.142649000
H	3.451198000	-1.154781000	2.712642000
N	-3.683763000	0.808579000	0.126215000
N	-2.220338000	2.322634000	-0.353645000
N	1.137249000	-2.679573000	-0.921060000
N	1.439737000	-2.046864000	1.118967000
Pt	-0.769047000	-0.357785000	-0.057265000
H	-1.386838000	-0.909301000	-1.351076000
B	2.149295000	0.837643000	1.077339000
O	1.968406000	2.069564000	0.510990000
O	3.320903000	0.239436000	0.706240000
C	3.206154000	2.409814000	-0.166527000
C	3.843546000	1.009073000	-0.407040000
C	4.003866000	3.277447000	0.792490000
C	2.884699000	3.180326000	-1.427496000
C	5.354302000	0.978936000	-0.358576000
C	3.342284000	0.326890000	-1.671640000
H	4.922188000	3.652263000	0.326277000
H	3.392836000	4.140662000	1.081561000
H	4.274062000	2.731695000	1.704422000
H	2.460952000	4.157831000	-1.167758000
H	3.798086000	3.358150000	-2.008900000
H	2.167826000	2.648337000	-2.062113000
H	5.709585000	-0.044120000	-0.527497000
H	5.777078000	1.615421000	-1.145663000
H	5.739186000	1.317853000	0.607946000
H	3.744936000	0.800824000	-2.574326000
H	3.677956000	-0.717759000	-1.658389000
H	2.244340000	0.337091000	-1.729104000

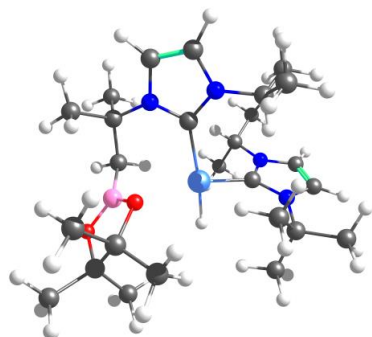
TS1



Pt	0.000484000	0.034583000	-0.430667000
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N	0.400796000	2.936476000	0.030254000
N	1.729100000	-2.041766000	1.072057000
N	2.260287000	-1.842303000	-1.020722000
C	1.102246000	1.778503000	0.054342000
C	2.434659000	3.502591000	0.613255000
C	1.199390000	4.007405000	0.381952000
C	1.418140000	-1.371518000	-0.070365000
C	3.100356000	-2.799975000	-0.486200000
C	2.772926000	-2.921481000	0.819226000
H	3.353618000	3.999077000	0.891983000
H	0.832846000	5.022357000	0.442271000
H	3.849712000	-3.313092000	-1.071233000
H	3.195925000	-3.562155000	1.576222000
C	2.192558000	-1.503043000	-2.459958000
C	3.569418000	-1.536353000	-3.094094000
H	3.944970000	-2.562143000	-3.193555000
H	3.504834000	-1.117249000	-4.103635000
H	4.301113000	-0.951069000	-2.527134000
C	1.233509000	-2.449352000	-3.160691000
H	1.166778000	-2.193528000	-4.224069000
H	1.594929000	-3.483064000	-3.080885000
H	0.227746000	-2.394508000	-2.729435000
C	3.513543000	1.223131000	0.501599000
C	-1.059788000	2.958193000	-0.190990000
C	-1.436284000	1.701247000	-0.991540000
H	-0.993091000	1.733117000	-1.998380000
H	-2.503507000	1.840442000	-1.234256000
C	4.344857000	1.519592000	1.734960000
H	4.881989000	2.471404000	1.641222000
H	3.727750000	1.554772000	2.640278000
H	5.096505000	0.732806000	1.861084000
C	4.330707000	1.305779000	-0.773700000
H	3.714206000	1.092163000	-1.655711000
H	4.765003000	2.307211000	-0.891850000
H	5.153093000	0.581339000	-0.738685000
C	-1.418352000	4.186055000	-1.021333000
H	-1.212558000	5.117282000	-0.481419000
H	-0.866675000	4.198722000	-1.968841000
H	-2.490955000	4.172193000	-1.245741000
C	-1.747275000	3.020182000	1.166746000
H	-2.835762000	3.029393000	1.038932000
H	-1.482383000	2.155628000	1.784587000
H	-1.456294000	3.937682000	1.692796000

C	1.053378000	-1.900588000	2.411383000
C	1.695822000	-2.865112000	3.398863000
H	1.577556000	-3.911010000	3.092482000
H	2.759871000	-2.652481000	3.556481000
H	1.190878000	-2.744065000	4.362988000
C	-0.422013000	-2.251977000	2.267807000
H	-0.881113000	-2.263923000	3.263755000
H	-0.959983000	-1.520005000	1.655532000
H	-0.542995000	-3.248281000	1.822942000
C	1.238535000	-0.478691000	2.922280000
H	2.305250000	-0.241376000	3.028185000
H	0.769062000	-0.386699000	3.908816000
H	3.078347000	0.221529000	0.594931000
H	0.774134000	0.256136000	2.254633000
H	1.796158000	-0.478760000	-2.491539000
H	-0.836907000	-1.282924000	-0.838692000
B	-2.224944000	0.209278000	-0.437531000
O	-3.061740000	-0.347697000	-1.389423000
O	-2.740728000	0.119602000	0.835288000
C	-4.044423000	-1.124747000	-0.667623000
C	-4.095169000	-0.391983000	0.707297000
C	-3.526651000	-2.552423000	-0.566447000
C	-5.342164000	-1.103391000	-1.446507000
C	-4.390741000	-1.282842000	1.893397000
C	-5.022145000	0.812257000	0.712011000
H	-4.271821000	-3.216352000	-0.113026000
H	-3.311222000	-2.922466000	-1.575934000
H	-2.602636000	-2.616152000	0.020759000
H	-5.210695000	-1.639041000	-2.393881000
H	-6.139362000	-1.606591000	-0.885058000
H	-5.665946000	-0.083869000	-1.677396000
H	-4.400091000	-0.685547000	2.812800000
H	-5.378285000	-1.749024000	1.786522000
H	-3.643062000	-2.073970000	2.008869000
H	-6.074741000	0.508263000	0.679506000
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H	-4.829560000	1.478006000	-0.138996000

TS2

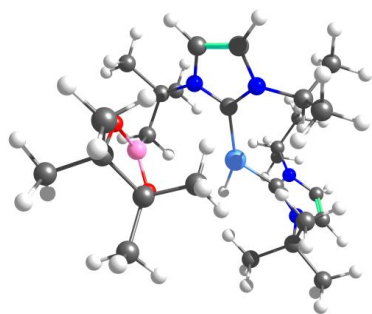


Pt	0.130476000	-0.152728000	-0.546461000
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N	-0.719278000	2.584506000	0.660642000
N	2.568841000	-1.870426000	-0.003502000
N	2.989580000	-0.111042000	-1.216214000
C	0.183303000	1.564582000	0.724256000
C	0.583711000	3.056388000	2.371793000

C	-0.477856000	3.506333000	1.667760000
C	1.993031000	-0.779235000	-0.583023000
C	4.186930000	-0.782252000	-1.051915000
C	3.927310000	-1.870643000	-0.296818000
H	1.089002000	3.471676000	3.232705000
H	-1.072630000	4.398268000	1.799858000
H	5.116584000	-0.431135000	-1.474970000
H	4.604234000	-2.631076000	0.058029000
C	2.804572000	1.090820000	-2.061806000
C	4.064364000	1.932561000	-2.099128000
H	4.860606000	1.450056000	-2.678895000
H	3.837385000	2.883476000	-2.591880000
H	4.448015000	2.152213000	-1.096557000
C	2.364780000	0.678169000	-3.454950000
H	2.208237000	1.568716000	-4.074437000
H	3.137470000	0.061760000	-3.932736000
H	1.429168000	0.108095000	-3.427490000
C	2.127373000	1.079135000	2.248220000
C	-1.763484000	2.834160000	-0.380298000
C	-1.988400000	1.611074000	-1.277332000
H	-1.034455000	1.327017000	-1.777554000
H	-2.598039000	1.949351000	-2.127440000
C	1.971756000	0.719394000	3.713203000
H	2.014653000	1.609643000	4.353207000
H	1.019520000	0.207180000	3.895854000
H	2.788021000	0.054813000	4.018605000
C	3.416551000	1.823260000	1.956556000
H	3.479596000	2.087953000	0.893741000
H	3.487481000	2.745578000	2.547256000
H	4.278103000	1.193988000	2.207468000
C	-1.282695000	4.002855000	-1.235340000
H	-1.087764000	4.893263000	-0.626508000
H	-0.361503000	3.739286000	-1.771145000
H	-2.049130000	4.259607000	-1.975623000
C	-3.075962000	3.180913000	0.316683000
H	-3.872644000	3.250771000	-0.433403000
H	-3.348750000	2.405218000	1.043387000
H	-3.033053000	4.143355000	0.837718000
C	1.889484000	-2.985489000	0.754860000
C	2.950830000	-3.835929000	1.442477000
H	3.581283000	-4.379605000	0.729873000
H	3.587585000	-3.239548000	2.107050000
H	2.436689000	-4.583798000	2.055222000
C	1.129133000	-3.855425000	-0.238704000
H	0.682473000	-4.705449000	0.291051000
H	0.328008000	-3.302284000	-0.739117000
H	1.811842000	-4.249036000	-1.002164000
C	0.973820000	-2.417713000	1.830828000
H	1.554035000	-1.875875000	2.588092000
H	0.462884000	-3.250211000	2.329224000
H	2.101194000	0.163697000	1.649918000
H	0.211763000	-1.741840000	1.421827000
H	1.999636000	1.657080000	-1.574118000
H	-0.061422000	-1.397426000	-1.554706000
B	-2.756677000	0.373135000	-0.673732000
O	-3.811650000	-0.217996000	-1.299384000
O	-2.404819000	-0.238075000	0.504596000

C	-4.069467000	-1.472410000	-0.612855000
C	-3.448676000	-1.219545000	0.795299000
C	-3.355716000	-2.557952000	-1.401593000
C	-5.559794000	-1.730448000	-0.607646000
C	-2.825624000	-2.433612000	1.444058000
C	-4.400990000	-0.534012000	1.761028000
H	-3.553042000	-3.550572000	-0.981079000
H	-3.723678000	-2.545812000	-2.433570000
H	-2.270168000	-2.397628000	-1.425274000
H	-5.905843000	-1.906902000	-1.632434000
H	-5.790861000	-2.624919000	-0.015974000
H	-6.123805000	-0.886397000	-0.200406000
H	-2.407455000	-2.161135000	2.420376000
H	-3.588262000	-3.205329000	1.608254000
H	-2.026027000	-2.864757000	0.832425000
H	-5.172962000	-1.225144000	2.118300000
H	-3.832920000	-0.182191000	2.629823000
H	-4.896503000	0.329799000	1.301797000

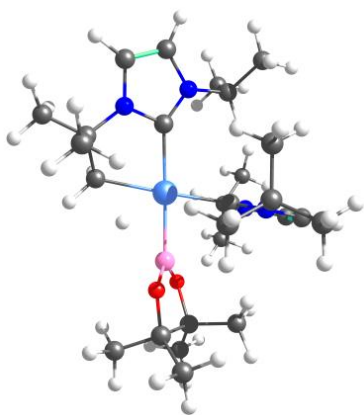
TS3



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N	1.539686000	-2.101220000	0.410797000
N	-3.002339000	1.805544000	-0.144549000
N	-3.788100000	-0.187488000	-0.529565000
C	0.482620000	-1.311382000	0.747594000
C	1.621027000	-1.900837000	2.601269000
C	2.249642000	-2.462643000	1.541958000
C	-2.640839000	0.528124000	-0.446360000
C	-4.869339000	0.619933000	-0.232188000
C	-4.383171000	1.856836000	0.005683000
H	1.842530000	-1.945609000	3.658845000
H	3.136367000	-3.076626000	1.509987000
H	-5.884056000	0.249234000	-0.215734000
H	-4.908651000	2.763720000	0.259087000
C	-3.876046000	-1.637112000	-0.806120000
C	-3.990406000	-2.401441000	0.499568000
H	-4.912644000	-2.131298000	1.030347000
H	-4.014640000	-3.479028000	0.303486000
H	-3.137031000	-2.190238000	1.155961000
C	-5.020935000	-1.929331000	-1.755218000
H	-4.987433000	-2.984968000	-2.044274000
H	-5.995580000	-1.750801000	-1.284227000
H	-4.955697000	-1.322123000	-2.664720000
C	-0.451068000	-0.512546000	2.939826000
C	1.867722000	-2.522014000	-0.993672000
C	2.015888000	-1.264009000	-1.860959000

H	1.017605000	-0.841108000	-2.092083000
H	2.414646000	-1.575195000	-2.838290000
C	0.204494000	0.607528000	3.725511000
H	0.952365000	0.216219000	4.426764000
H	0.694527000	1.329377000	3.060803000
H	-0.552567000	1.139799000	4.312290000
C	-1.155165000	-1.516809000	3.833887000
H	-1.582996000	-2.337540000	3.246967000
H	-0.465354000	-1.944565000	4.572142000
H	-1.965537000	-1.023059000	4.381230000
C	0.738252000	-3.412293000	-1.499676000
H	0.635961000	-4.304498000	-0.869475000
H	-0.221355000	-2.877635000	-1.510527000
H	0.959242000	-3.734924000	-2.524130000
C	3.165012000	-3.318160000	-1.000502000
H	3.381102000	-3.600823000	-2.036508000
H	4.013141000	-2.735245000	-0.627695000
H	3.074805000	-4.245205000	-0.421879000
C	-2.088861000	2.984673000	0.067565000
C	-2.932707000	4.235966000	0.268855000
H	-3.575852000	4.444574000	-0.594038000
H	-3.547583000	4.183226000	1.174694000
H	-2.250864000	5.084405000	0.387422000
C	-1.203052000	3.184474000	-1.155144000
H	-0.618867000	4.102567000	-1.018422000
H	-0.501669000	2.355382000	-1.297598000
H	-1.807099000	3.293753000	-2.064497000
C	-1.260315000	2.735345000	1.319554000
H	-1.912951000	2.562886000	2.185461000
H	-0.638664000	3.614591000	1.529564000
H	-1.173749000	-0.092489000	2.226553000
H	-0.600223000	1.868965000	1.190308000
H	-2.923713000	-1.884076000	-1.293965000
H	-1.358690000	0.302420000	-1.988157000
B	2.903634000	-0.125076000	-1.237804000
O	4.048152000	-0.341815000	-0.519706000
O	2.570991000	1.201111000	-1.327683000
C	4.627015000	0.957921000	-0.236236000
C	3.390629000	1.897888000	-0.356398000
C	5.680892000	1.213211000	-1.300399000
C	5.263830000	0.913791000	1.135432000
C	3.684996000	3.290659000	-0.865114000
C	2.572841000	1.965960000	0.924733000
H	6.224283000	2.146444000	-1.112252000
H	6.404706000	0.390571000	-1.288271000
H	5.240262000	1.263408000	-2.303079000
H	6.132426000	0.245442000	1.119007000
H	5.613562000	1.910530000	1.432259000
H	4.567689000	0.544828000	1.895738000
H	2.752432000	3.865405000	-0.918973000
H	4.364813000	3.814800000	-0.181723000
H	4.131843000	3.279336000	-1.863881000
H	3.099204000	2.512206000	1.716003000
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H	2.327585000	0.960127000	1.295318000

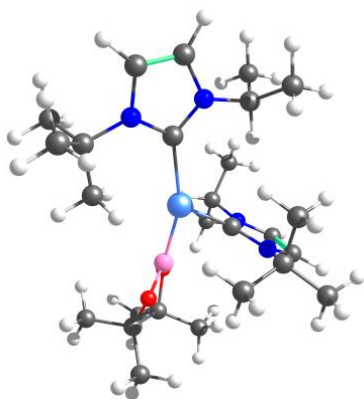
TS4



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N	-0.372379000	-1.225549000	1.779467000
N	-0.375773000	-2.439229000	-0.011474000
C	2.368052000	0.505044000	-0.218648000
C	4.530166000	0.304907000	0.362575000
C	4.287459000	1.623962000	0.158154000
C	-0.210225000	-1.164368000	0.432275000
C	-0.628225000	-3.280354000	1.064827000
C	-0.619110000	-2.523171000	2.183636000
H	5.441244000	-0.210116000	0.634994000
H	4.944451000	2.479357000	0.232593000
H	-0.806956000	-4.339271000	0.948511000
H	-0.770076000	-2.794410000	3.219163000
C	-0.381339000	-2.980282000	-1.415344000
C	0.506433000	-4.221869000	-1.449525000
H	0.108384000	-5.043723000	-0.845234000
H	0.572325000	-4.581133000	-2.482516000
H	1.523187000	-3.993867000	-1.103705000
C	-1.819949000	-3.338357000	-1.771999000
H	-1.843723000	-3.806055000	-2.763584000
H	-2.248767000	-4.049030000	-1.054830000
H	-2.442455000	-2.435693000	-1.798267000
C	3.200282000	-1.834408000	0.130759000
C	2.171800000	2.944059000	-0.486483000
C	0.986730000	2.520890000	-1.368053000
H	1.325744000	2.224312000	-2.368681000
H	0.361735000	3.413120000	-1.503079000
C	3.499494000	-2.414598000	1.499258000
H	4.548967000	-2.258580000	1.779971000
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H	3.313912000	-3.495075000	1.482866000
C	4.071457000	-2.444137000	-0.952723000
H	3.854561000	-2.007057000	-1.934460000
H	5.136895000	-2.294068000	-0.736127000
H	3.893918000	-3.524373000	-1.008358000
C	3.035805000	3.942272000	-1.246003000
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H	3.444528000	3.498180000	-2.161423000
H	2.427244000	4.810182000	-1.523932000
C	1.708610000	3.542541000	0.835895000
H	1.125355000	4.452346000	0.649936000
H	1.079982000	2.835228000	1.391623000

H	2.570602000	3.811096000	1.459393000
C	-0.280476000	-0.072195000	2.699904000
C	-1.416713000	-0.096996000	3.704144000
H	-2.389275000	-0.224350000	3.212648000
H	-1.293296000	-0.898913000	4.443136000
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C	1.079439000	-0.032667000	3.371083000
H	1.247731000	-0.940342000	3.965927000
H	1.135663000	0.828799000	4.046512000
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H	1.887142000	0.058281000	2.632986000
H	-0.473574000	1.933826000	-1.111669000
B	-1.838738000	0.794076000	-0.444757000
O	-2.706425000	0.019006000	-1.173959000
O	-2.485036000	1.578282000	0.480330000
C	-3.989126000	0.076947000	-0.491665000
C	-3.911273000	1.452127000	0.230269000
C	-4.025688000	-1.096594000	0.476777000
C	-5.093793000	-0.053258000	-1.515344000
C	-4.649153000	1.524627000	1.548441000
C	-4.306124000	2.621361000	-0.657005000
H	-4.969418000	-1.127357000	1.033529000
H	-3.935703000	-2.034023000	-0.084351000
H	-3.196669000	-1.048690000	1.196570000
H	-5.050062000	-1.047022000	-1.976745000
H	-6.076948000	0.053456000	-1.040007000
H	-5.006814000	0.693427000	-2.310092000
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H	-5.718538000	1.327469000	1.401730000
H	-4.258762000	0.807610000	2.278215000
H	-5.388220000	2.648149000	-0.829698000
H	-4.019051000	3.555449000	-0.160957000
H	-3.798828000	2.580102000	-1.628385000
H	-0.391188000	0.807130000	2.052408000
C	0.151569000	-1.969813000	-2.415465000
H	-0.457854000	-1.060106000	-2.449544000
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TS5

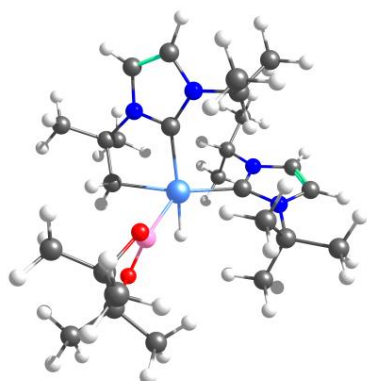


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N	-1.110470000	-2.051878000	-1.138309000

C	2.543372000	0.482132000	-0.071032000
C	4.774037000	0.128463000	-0.128111000
C	4.579395000	1.464698000	-0.057105000
C	-0.668456000	-1.408694000	-0.027517000
C	-1.719923000	-3.241366000	-0.792041000
C	-1.669733000	-3.333824000	0.553729000
H	5.686761000	-0.450222000	-0.168344000
H	5.291704000	2.277507000	-0.032824000
H	-2.132289000	-3.917535000	-1.527415000
H	-2.045954000	-4.109287000	1.201375000
C	-0.891919000	-1.623413000	-2.534716000
C	0.214175000	-2.459013000	-3.152028000
H	-0.084165000	-3.513050000	-3.222883000
H	0.434092000	-2.102633000	-4.164538000
H	1.135078000	-2.400274000	-2.559226000
C	-2.179016000	-1.695829000	-3.332069000
H	-2.004858000	-1.287959000	-4.333897000
H	-2.524979000	-2.729791000	-3.455801000
H	-2.966595000	-1.105930000	-2.852341000
C	3.302032000	-1.905936000	-0.254392000
C	2.603879000	3.026311000	0.031123000
C	1.093996000	2.902765000	0.131931000
H	0.671212000	2.394701000	-0.762927000
H	0.628939000	3.895268000	0.130028000
C	3.977119000	-2.640381000	0.888893000
H	5.069059000	-2.558705000	0.821494000
H	3.661132000	-2.245895000	1.861364000
H	3.723489000	-3.705573000	0.847795000
C	3.783610000	-2.392097000	-1.609801000
H	3.335042000	-1.809829000	-2.423435000
H	4.875040000	-2.313779000	-1.693368000
H	3.515472000	-3.445702000	-1.747432000
C	2.980197000	3.764753000	-1.247233000
H	4.066221000	3.876076000	-1.342543000
H	2.607328000	3.230137000	-2.129557000
H	2.539888000	4.768451000	-1.237274000
C	3.130793000	3.752532000	1.263098000
H	2.652455000	4.735586000	1.341270000
H	2.904697000	3.185443000	2.174223000
H	4.213232000	3.914242000	1.212112000
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C	-1.404058000	-3.018864000	3.326923000
H	-2.489937000	-2.925598000	3.201398000
H	-1.103724000	-4.052372000	3.121503000
H	-1.170995000	-2.817192000	4.377696000
C	-1.019761000	-0.611053000	2.957519000
H	-0.787826000	-0.541731000	4.026777000
H	-0.457814000	0.171582000	2.435871000
H	-2.090041000	-0.412375000	2.822588000
C	0.848341000	-2.251202000	2.595119000
H	1.100324000	-3.259735000	2.241962000
H	1.156632000	-2.166806000	3.644240000
H	2.211693000	-2.026013000	-0.182805000
H	1.415740000	-1.517350000	2.008622000
H	-0.568741000	-0.577901000	-2.457714000
H	0.787307000	2.422233000	1.075107000
B	-1.646151000	0.831700000	-0.082405000

O	-2.544814000	0.601908000	-1.094667000
O	-2.181041000	1.587745000	0.933072000
C	-3.851091000	0.949811000	-0.566679000
C	-3.489204000	2.034901000	0.485218000
C	-4.404882000	-0.326784000	0.051192000
C	-4.739365000	1.427570000	-1.691968000
C	-4.421887000	2.101456000	1.673310000
C	-3.300449000	3.416645000	-0.118716000
H	-5.434350000	-0.199080000	0.404801000
H	-4.396195000	-1.118410000	-0.708570000
H	-3.783657000	-0.665411000	0.891991000
H	-4.963699000	0.599571000	-2.375001000
H	-5.692300000	1.797982000	-1.293093000
H	-4.267675000	2.228998000	-2.268561000
H	-4.101613000	2.897466000	2.355633000
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H	-4.442241000	1.161271000	2.233326000
H	-4.257026000	3.864226000	-0.412076000
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TS A

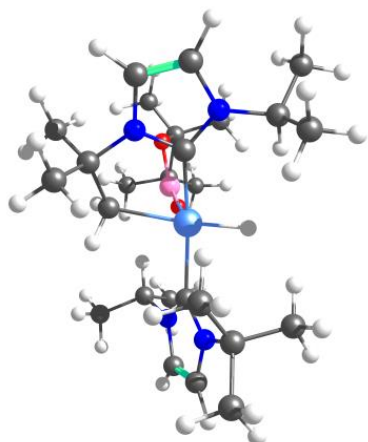


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N	-2.636534000	1.206640000	-1.044964000
C	-1.036486000	-1.403316000	0.816557000
C	-2.332415000	-2.501456000	2.278515000
C	-1.743746000	-3.430168000	1.480084000
C	-1.370050000	1.396270000	-0.591784000
C	-3.382471000	2.361575000	-0.915312000
C	-2.569463000	3.285504000	-0.358767000
H	-3.010165000	-2.617789000	3.113057000
H	-1.822905000	-4.508554000	1.477692000
H	-4.415160000	2.429610000	-1.224888000
H	-2.777514000	4.308769000	-0.089669000
C	-3.113518000	-0.011308000	-1.733823000
C	-4.583916000	-0.261151000	-1.465475000
H	-5.221924000	0.482265000	-1.958709000
H	-4.855767000	-1.241163000	-1.871462000
H	-4.810590000	-0.262581000	-0.393310000
C	-2.815682000	0.085435000	-3.219325000
H	-3.138990000	-0.830184000	-3.727790000
H	-3.358596000	0.930252000	-3.663146000

H	-1.744631000	0.224169000	-3.406756000
C	-2.193703000	0.019845000	2.518714000
C	-0.118570000	-3.229684000	-0.526655000
C	0.957792000	-2.154688000	-0.770782000
H	1.391509000	-2.301157000	-1.767814000
H	1.753752000	-2.326799000	-0.032354000
C	-1.421077000	0.105343000	3.822191000
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H	-0.344234000	-0.009107000	3.648789000
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C	-3.686583000	0.193031000	2.708924000
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H	-3.887611000	1.183605000	3.131099000
C	-1.006714000	-3.423735000	-1.749284000
H	-1.851254000	-4.086124000	-1.519985000
H	-1.397542000	-2.464956000	-2.112427000
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H	1.233609000	-4.850768000	-0.912595000
H	1.071204000	-4.456027000	0.813817000
H	-0.217825000	-5.351799000	-0.033524000
C	-0.129027000	3.410967000	0.370116000
C	-0.532446000	4.811057000	0.813390000
H	-0.878461000	5.430655000	-0.021895000
H	-1.302777000	4.790964000	1.593495000
H	0.353124000	5.297890000	1.235477000
C	0.897678000	3.525112000	-0.749342000
H	1.761942000	4.099958000	-0.395122000
H	1.248449000	2.543909000	-1.088318000
H	0.466494000	4.052759000	-1.609311000
C	0.416307000	2.661198000	1.576810000
H	-0.334077000	2.617641000	2.377116000
H	1.293661000	3.193961000	1.964008000
H	-1.822711000	0.786958000	1.827114000
H	0.726505000	1.641297000	1.330224000
H	-2.538328000	-0.838851000	-1.296807000
H	0.706290000	0.491933000	-1.853642000
B	2.038058000	-0.077587000	-0.354923000
O	3.032290000	0.032914000	-1.282183000
O	2.483873000	-0.028432000	0.937716000
C	4.236365000	0.414970000	-0.555420000
C	3.938937000	-0.116545000	0.879152000
C	4.324491000	1.929871000	-0.616323000
C	5.432790000	-0.211388000	-1.234056000
C	4.516984000	0.711653000	2.004309000
C	4.304655000	-1.579049000	1.067819000
H	5.258991000	2.292566000	-0.172794000
H	4.297273000	2.249022000	-1.664641000
H	3.484560000	2.402863000	-0.092794000
H	5.559880000	0.222662000	-2.232453000
H	6.346619000	-0.008124000	-0.662021000
H	5.322686000	-1.294317000	-1.344493000
H	4.252804000	0.259309000	2.967257000
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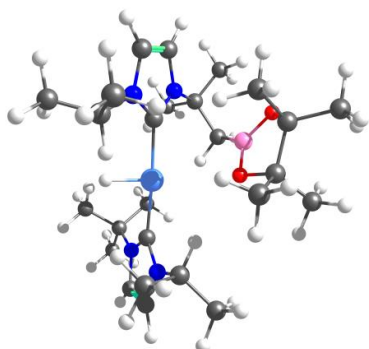
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C	2.617962000	-2.508710000	1.771977000
H	3.150170000	-2.644906000	2.703367000
C	1.118628000	-0.580595000	2.611850000
C	0.270654000	-1.342365000	3.624011000
H	-0.594837000	-1.810195000	3.137302000
H	-0.097358000	-0.655301000	4.394819000
H	0.854467000	-2.128935000	4.118501000
C	0.266330000	0.469082000	1.869427000
H	0.735007000	1.462079000	1.948161000
H	-0.713064000	0.583133000	2.351877000
C	1.572391000	-3.033784000	-1.672234000
H	1.110797000	-2.167308000	-2.161803000
C	2.873583000	-3.376535000	-2.368109000
H	3.598482000	-2.557573000	-2.303642000
H	2.672182000	-3.572503000	-3.426311000
H	3.330828000	-4.282023000	-1.949976000
C	0.598116000	-4.197393000	-1.671392000
H	1.021009000	-5.052636000	-1.128144000
H	0.390797000	-4.514720000	-2.699359000
H	-0.351920000	-3.920221000	-1.198793000
C	-2.302272000	0.608530000	-0.184308000
C	-3.977009000	2.122503000	-0.191072000
H	-4.427408000	3.103563000	-0.140319000
C	-4.534814000	0.906063000	-0.355529000
H	-5.572494000	0.638584000	-0.471557000
C	-3.781551000	-1.504194000	-0.416493000
C	-2.935725000	-2.239054000	0.616126000
H	-1.858157000	-2.204823000	0.401842000
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H	-3.110162000	-1.835280000	1.621062000
C	-3.527433000	-1.989679000	-1.837722000
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C	-2.118112000	3.733459000	1.515719000
H	-3.076710000	4.257208000	1.411851000
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O	2.488483000	0.660414000	0.056337000
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C	2.285197000	3.712652000	0.327784000
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H	1.431995000	4.400437000	0.284460000
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H	3.305185000	4.035243000	-2.268326000
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TS C

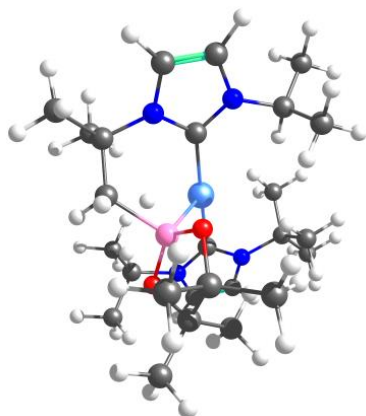


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H	-0.867663000	-4.255308000	-1.599661000
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H	-1.110460000	-0.882803000	-3.388402000
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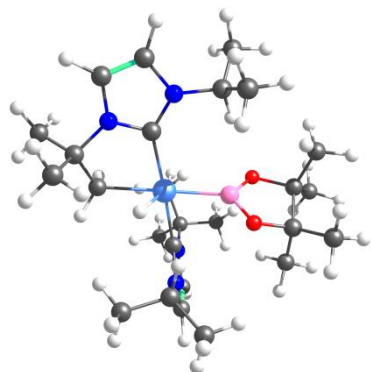


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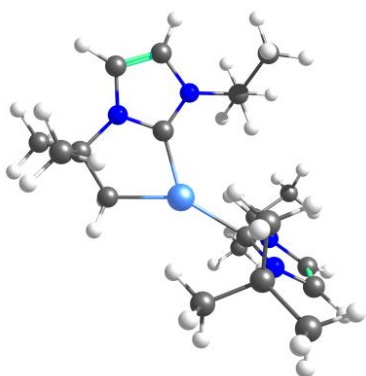
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H	-2.903725000	-1.540791000	2.240799000
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H	-2.054157000	-2.205951000	-1.421606000
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H	3.027265000	-2.443991000	3.586252000
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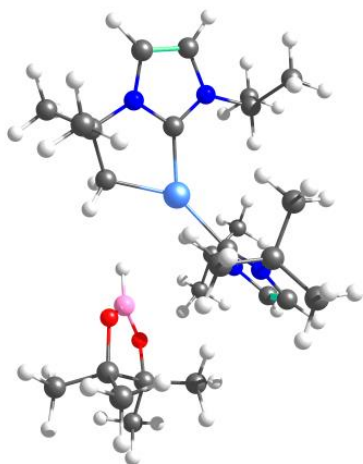
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C	1.896765000	-0.041511000	-0.161804000
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H	3.440271000	3.678343000	-0.772925000
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H	1.991164000	2.873857000	-3.405989000
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H	-0.344283000	3.176029000	3.379528000
C	-1.125301000	3.627461000	0.735785000
H	-0.990070000	3.437152000	-0.335977000
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H	-4.043937000	-2.635839000	0.736676000
C	2.512535000	-2.121555000	1.157526000

C	3.805608000	-2.733737000	1.675205000
H	4.514832000	-2.941195000	0.865058000
H	4.291769000	-2.098823000	2.425095000
H	3.564272000	-3.686437000	2.158071000
C	1.874982000	-3.081797000	0.160789000
H	1.706617000	-4.049068000	0.648774000
H	0.902670000	-2.712776000	-0.196528000
H	2.530682000	-3.240317000	-0.703942000
C	1.580411000	-1.839093000	2.329939000
H	2.037974000	-1.126706000	3.027718000
H	1.384854000	-2.772525000	2.871031000
H	-0.101383000	1.829910000	1.334274000
H	0.619736000	-1.430871000	1.989875000
H	0.931402000	1.984921000	-1.324597000

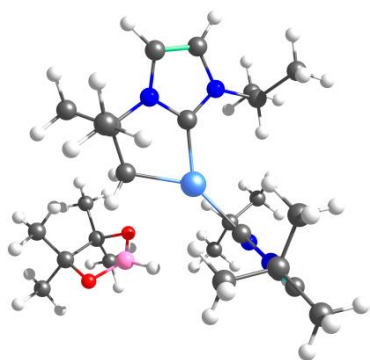
TS isom'



Pt	0.865728000	0.252192000	-0.244488000
N	3.848193000	-0.174105000	-0.020935000
N	3.269834000	1.902326000	-0.130669000
N	-0.961055000	-1.948442000	1.226487000
N	-1.009461000	-2.196651000	-0.916201000
C	2.780700000	0.645521000	-0.152891000
C	5.001833000	0.586312000	0.089234000
C	4.637705000	1.893399000	0.031205000
C	-0.494876000	-1.408895000	0.063088000
C	-1.760382000	-3.216582000	-0.386951000
C	-1.729465000	-3.061852000	0.962229000
H	5.975976000	0.129152000	0.194341000
H	5.227890000	2.797994000	0.079558000
H	-2.258525000	-3.959169000	-0.994982000
H	-2.209419000	-3.649275000	1.729759000
C	-0.712147000	-2.051630000	-2.356814000
C	0.312195000	-3.090682000	-2.773017000
H	-0.094047000	-4.104856000	-2.667238000
H	0.585436000	-2.944194000	-3.823799000
H	1.222151000	-3.018114000	-2.165597000
C	-1.985084000	-2.131982000	-3.175901000
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H	-2.740047000	-1.433102000	-2.800213000
C	3.805365000	-1.648357000	-0.012472000
C	2.275905000	2.983391000	-0.156509000
C	1.022528000	2.273780000	-0.686084000

H	0.982997000	2.324846000	-1.784058000
H	0.109947000	2.721850000	-0.267669000
C	4.461369000	-2.184512000	1.245313000
H	5.535792000	-1.961639000	1.260196000
H	4.007163000	-1.757559000	2.147129000
H	4.346609000	-3.273221000	1.283424000
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H	3.960549000	-1.762199000	-2.172483000
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H	4.326243000	-3.279151000	-1.318305000
C	2.731143000	4.097903000	-1.083340000
H	3.619772000	4.607696000	-0.689923000
H	2.960600000	3.709368000	-2.082599000
H	1.932296000	4.842702000	-1.175917000
C	2.076018000	3.499226000	1.261502000
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H	1.723358000	2.697428000	1.922721000
H	3.013652000	3.899390000	1.667249000
C	-0.613805000	-1.461984000	2.605346000
C	-1.449172000	-2.220540000	3.626792000
H	-2.524572000	-2.086685000	3.452645000
H	-1.217515000	-3.291893000	3.643233000
H	-1.220246000	-1.820680000	4.620034000
C	-0.921697000	0.025054000	2.725078000
H	-0.731597000	0.342060000	3.757397000
H	-0.289810000	0.630275000	2.062212000
H	-1.971937000	0.235103000	2.487485000
C	0.867015000	-1.734609000	2.845378000
H	1.100440000	-2.795571000	2.686487000
H	1.128372000	-1.474551000	3.878258000
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H	1.487933000	-1.132148000	2.169538000
H	-0.274141000	-1.048151000	-2.446537000
H	-1.474193000	1.182984000	-1.623149000
B	-2.514827000	1.159571000	-1.042325000
O	-3.573519000	0.413235000	-1.464561000
O	-2.758979000	1.887224000	0.083833000
C	-4.570538000	0.478369000	-0.408513000
C	-4.194558000	1.805010000	0.316105000
C	-4.367600000	-0.757309000	0.453437000
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H	-3.374801000	-0.764244000	0.924253000
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H	-6.720586000	0.593965000	-0.268981000
H	-6.065641000	1.238131000	-1.793452000
H	-4.133938000	2.769172000	2.231110000
H	-5.538947000	1.714542000	1.994865000
H	-3.943620000	1.007468000	2.328540000
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TS isom''



Pt	0.655761000	-0.204308000	-0.254943000
N	2.427639000	-2.209039000	1.124875000
N	1.011202000	-3.102573000	-0.238832000
N	1.627575000	2.796107000	-0.917888000
N	0.626814000	2.669565000	0.988035000
C	1.420660000	-1.924367000	0.271829000
C	2.646275000	-3.578318000	1.135709000
C	1.761131000	-4.140363000	0.271014000
C	1.008430000	1.920814000	-0.076998000
C	1.003070000	3.980879000	0.829636000
C	1.630466000	4.061849000	-0.372814000
H	3.407806000	-4.028394000	1.757696000
H	1.604997000	-5.172605000	-0.010631000
H	0.804808000	4.742854000	1.570844000
H	2.064459000	4.919783000	-0.862780000
C	-0.052114000	2.140594000	2.188840000
C	0.908705000	2.143499000	3.363203000
H	1.187851000	3.167113000	3.644287000
H	0.437219000	1.671656000	4.232492000
H	1.824275000	1.587564000	3.123948000
C	-1.322982000	2.918657000	2.464206000
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H	-1.994598000	2.899028000	1.597990000
C	3.171020000	-1.214362000	1.920604000
C	-0.035310000	-3.021444000	-1.268925000
C	-0.639058000	-1.634385000	-1.012781000
H	-1.434600000	-1.694179000	-0.254937000
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H	5.048448000	-2.301291000	2.007357000
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C	2.812714000	-1.349682000	3.387447000
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C	2.765834000	3.678282000	-2.918025000
H	1.974340000	4.414816000	-3.101202000
H	3.568748000	4.150988000	-2.340045000
H	3.183081000	3.390924000	-3.888836000
C	1.151726000	1.807716000	-3.122078000
H	1.567686000	1.609559000	-4.116977000
H	0.782505000	0.857046000	-2.713391000
H	0.302924000	2.494010000	-3.233305000
C	3.381452000	1.453426000	-1.997416000
H	4.132888000	1.900420000	-1.334184000
H	3.864725000	1.214024000	-2.952118000
H	2.814087000	-0.243220000	1.547973000
H	3.028596000	0.517120000	-1.545448000
H	-0.307544000	1.105083000	1.924007000
H	-1.805086000	1.407698000	-0.934630000
B	-2.804581000	0.894344000	-0.534796000
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C	-4.335108000	0.068781000	0.906587000
C	-4.830105000	-0.102670000	-0.564687000
C	-4.976478000	1.245265000	1.623583000
C	-4.435856000	-1.178491000	1.756639000
C	-6.244931000	0.368625000	-0.818332000
C	-4.644287000	-1.510242000	-1.105022000
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H	-4.460434000	1.409981000	2.576422000
H	-4.907610000	2.167795000	1.034133000
H	-4.072432000	-0.966622000	2.768836000
H	-5.479887000	-1.506485000	1.836114000
H	-3.841997000	-2.002049000	1.346943000
H	-6.504055000	0.207430000	-1.871042000
H	-6.953945000	-0.202017000	-0.205789000
H	-6.367990000	1.432556000	-0.596484000
H	-5.352276000	-2.212306000	-0.650189000
H	-4.820033000	-1.500644000	-2.186561000
H	-3.625989000	-1.877511000	-0.927149000

15. Crystallographic details

Low-temperature diffraction data were collected on a Bruker D8 Quest APEX-III single crystal diffractometer with a Photon III detector and a μ S 3.0 microfocus X-ray source at the Centro de Investigación, Tecnología e Innovación de la Universidad de Sevilla. Data were collected by means of ω and ϕ scans using monochromatic radiation $\lambda(\text{Ag K}\alpha 1) = 0.56086 \text{ \AA}$. The diffraction images collected were processed and scaled using APEX-III v2018.7-2 software. The structures were solved with SHELXT and was refined against F² on all data by full-matrix least squares with SHELXL,^[24] using Olex2 as graphical interface.^[25] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model, unless otherwise noted. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups). C-F and F-F distances in BAr^{F} counterions were restricted with SADI instructions.

The x-ray crystallographic coordinates for structures **2c**, **3c**, **4a** and **5** have been deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition numbers 2033931-2033934, respectively. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

The hydride ligand in structure (**4a**) was found from different Fourier maps and included in a refinement with isotropic parameters. BPin fragment were refined according to positional disorder of C atoms in 3:1 occupancy ratio. The H atom in PtHB in structure (**3c**) was found from difference Fourier maps and included in a refinement with isotropic parameters. The unit cell contains two dichloromethane molecules which were treated as a diffuse contribution to the overall scattering without specific atom positions by BYPASS.^[26] High residual electronic density can be found near Pt in structure (**2c**), probably due to absorption problems in the sample.

The hydride ligand in structure (**5**) was found from different Fourier maps and included in a refinement with isotropic parameters.

Crystal Data for $C_{58}H_{54}B_2F_{24}N_6Pt$ (**2c**) ($M=1507.78$ g/mol): triclinic, space group P-1 (no. 2), $a = 17.7840(10)$ Å, $b = 19.3314(12)$ Å, $c = 19.4985(12)$ Å, $\alpha = 77.056(3)^\circ$, $\beta = 83.793(3)^\circ$, $\gamma = 71.134(3)^\circ$, $V = 6177.4(7)$ Å³, $Z = 4$, $T = 99.99$ K, $\mu(AgK\alpha) = 1.302$ mm⁻¹, $D_{calc} = 1.621$ g/cm³, 140866 reflections measured ($3.298^\circ \leq 2\theta \leq 48.21^\circ$), 39747 unique ($R_{int} = 0.0671$, $R_{sigma} = 0.0875$) which were used in all calculations. The final R_1 was 0.0600 ($I > 2\sigma(I)$) and wR_2 was 0.1624 (all data).

Crystal Data for $C_{58}H_{54}B_2F_{24}N_6Pt$ (**3c**) ($M=1507.78$ g/mol): triclinic, space group P-1 (no. 2), $a = 12.8046(7)$ Å, $b = 13.6804(7)$ Å, $c = 18.4265(10)$ Å, $\alpha = 96.145(3)^\circ$, $\beta = 98.035(3)^\circ$, $\gamma = 91.631(3)^\circ$, $V = 3174.7(3)$ Å³, $Z = 2$, $T = 173.15$ K, $\mu(AgK\alpha) = 1.267$ mm⁻¹, $D_{calc} = 1.577$ g/cm³, 89536 reflections measured ($3.392^\circ \leq 2\theta \leq 51.602^\circ$), 24625 unique ($R_{int} = 0.0653$, $R_{sigma} = 0.0827$) which were used in all calculations. The final R_1 was 0.0438 ($I > 2\sigma(I)$) and wR_2 was 0.0888 (all data).

Crystal Data for $C_{58}H_{60}B_2F_{24}N_4O_2Pt$ (**4a**) ($M=1517.81$ g/mol): monoclinic, space group P2₁/c (no. 14), $a = 13.9627(11)$ Å, $b = 24.4797(19)$ Å, $c = 20.1924(16)$ Å, $\beta = 109.711(4)^\circ$, $V = 6497.4(9)$ Å³, $Z = 4$, $T = 173.15$ K, $\mu(AgK\alpha) = 1.239$ mm⁻¹, $D_{calc} = 1.552$ g/cm³, 134022 reflections measured ($3.628^\circ \leq 2\theta \leq 45.08^\circ$), 17211 unique ($R_{int} = 0.0699$, $R_{sigma} = 0.0450$) which were used in all calculations. The final R_1 was 0.0358 ($I > 2\sigma(I)$) and wR_2 was 0.0813 (all data).

Crystal Data for $C_{63}H_{69}B_2F_{24}N_5O_2Pt$ (**5**) ($M=1517.81$ g/mol): monoclinic, space group P2₁/c (no. 14), $a = 13.0010(7)$ Å, $b = 26.3167(13)$ Å, $c = 21.0636(10)$ Å, $\beta = 101.229(2)^\circ$, $V = 7068.8(6)$ Å³, $Z = 4$, $T = 273.15$ K, $\mu(AgK\alpha) = 1.239$ mm⁻¹, $D_{calc} = 1.505$ g/cm³, 83935 reflections measured ($3.342^\circ \leq 2\theta \leq 47.814^\circ$), 21793 unique ($R_{int} = 0.0574$, $R_{sigma} = 0.0644$) which were used in all calculations. The final R_1 was 0.0506 ($I > 2\sigma(I)$) and wR_2 was 0.1148 (all data).

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