

Electronic Supplementary Information

A (μ -Hydrido)diborane(4) Anion and Its Coordination Chemistry with Coinage Metals

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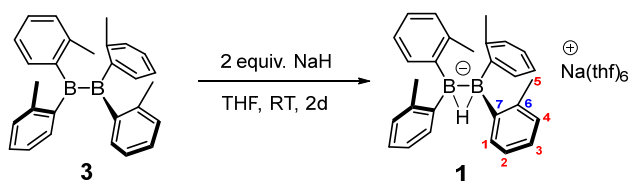
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Experimental Section

General Procedure. All operations were carried out under a dry argon atmosphere using standard Schlenk and glovebox techniques. All organic solvents were dried and distilled by standard methods prior to use. ^1H , ^{13}C and ^{11}B NMR spectra were recorded on Bruker DPX 400/500 spectrometer at 400/500, 101/126 and 128/160 MHz, respectively. All chemical shifts were reported in δ unit with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $\text{BF}_3\cdot\text{OEt}_2$ (0.00 ppm) for boron chemical shifts. Cyclic voltammetry was performed on a PAR Potentiostat / Galvanostat Model 263A Electrochemical Station (Princeton Applied Research). IR spectra were recorded with a Bruker Alpha spectrometer with an apodized resolution of 1 cm^{-1} in the attenuated total reflection (ATR) mode in the region of $4000\text{--}600\text{ cm}^{-1}$ using a setup with a ZnSe crystal. X-ray crystallographic analysis was performed on Bruker D8venture Diffractometer. NMR multiplicities were abbreviated as follows: s = singlet, d = doublet, q = quartet, m = multiplet, br = broad signal. $\text{B}_2(o\text{-tolyl})_4$ (**3**), IPrCuCl , IPrAgCl , and IPrAuCl were synthesized according to the literature methods.¹⁻⁴ All other chemicals were purchased from either Aldrich, J&K or Acros Chemical Co. and used as received unless otherwise specified.

Synthesis of 1



To a THF solution (25mL) of B₂(*o*-tolyl)₄ (100.0 mg, 0.25 mmol) was added NaH (12.4 mg, 0.50 mmol), and the reaction mixture was stirred at room temperature for 2 days. The resulting suspension was filtered through a pad of celite to remove the precipitate. Removal of the solvent from the filtrate under reduced pressure gave **1** as a white powder (176.9 mg, 0.21 mmol, 84% yield). Single crystals suitable for X-ray diffraction analysis were obtained via recrystallization from a THF solution at -30 °C.

¹H NMR (500 MHz, THF-*d*₈): δ = 7.06 (dd, *J* = 6.9, 1.5 Hz, 4H, H1), 6.59 (d, *J* = 6.9 Hz, 4H, H4), 6.51 (m, 8H, H2&H3), 3.61 (m, 4H, THF), 2.00 (s, 12H, H5), 1.79 – 1.75 ppm (m, 4H, THF).

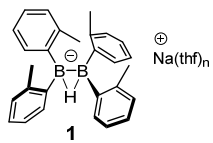
¹³C{¹H} NMR (126 MHz, THF-*d*₈): δ = 156.7 (C7), 140.1 (C6), 135.9 (C1), 127.6 (C4), 123.1, 122.4 (C2, C3), 23.5 (C5) ppm.

¹¹B{¹H} NMR (128 MHz, THF-*d*₈): δ = 30.2 ppm (br s, *h*_{1/2} ≈ 662 Hz).

¹¹B NMR (128 MHz, C₆D₆): δ = 30.2 ppm (br s, *h*_{1/2} ≈ 700 Hz).

mp: 157-159°C (dec.)

Anal. Calcd for C₃₈H₄₉B₂NaO_{2.5} [590.38]: C, 77.30; H, 8.37; Found: C, 77.50; H, 8.24.



^1H NMR (500 MHz, $\text{THF-}d_8$)

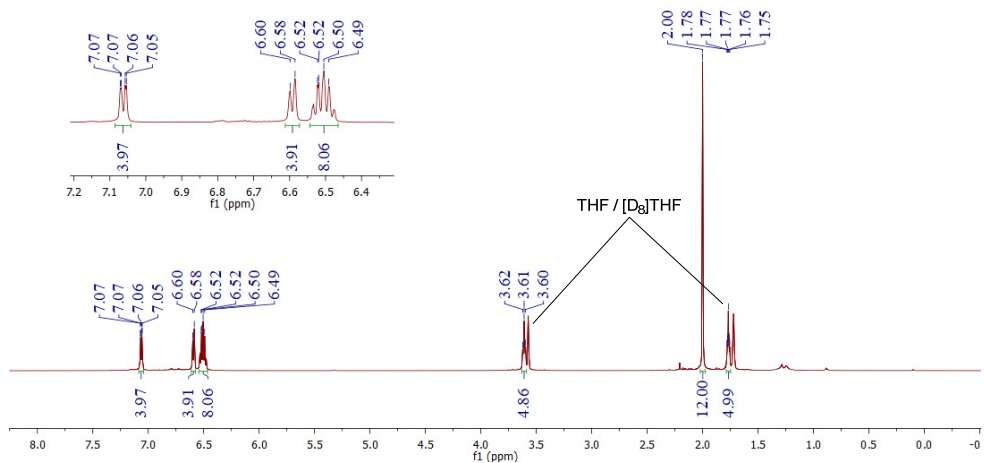
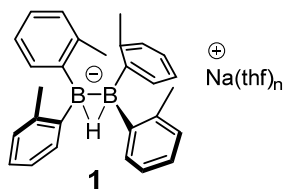


Figure S1. ^1H NMR spectrum of Compound **1** (500 MHz, $\text{THF-}d_8$).



^{11}B NMR (128 MHz, $\text{THF-}d_8$)

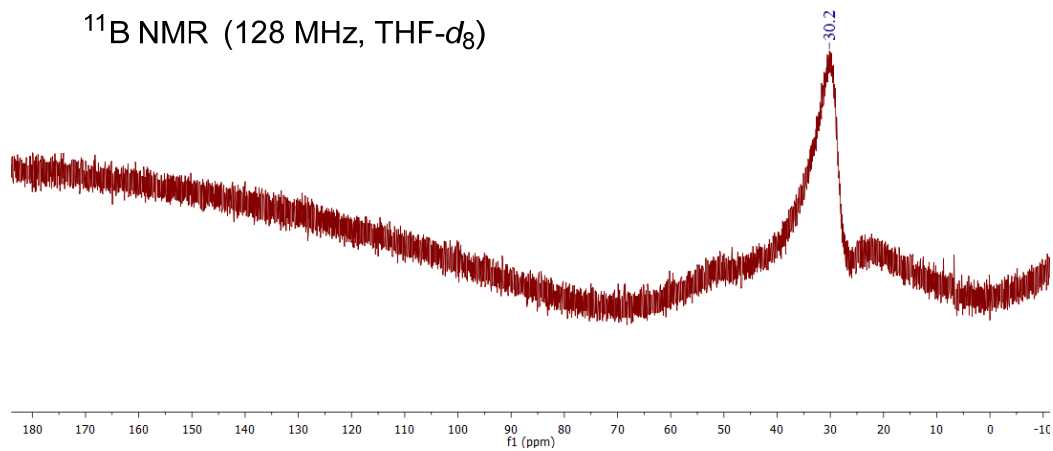


Figure S2. ^{11}B NMR spectrum of Compound **1** (128 MHz, $\text{THF-}d_8$).

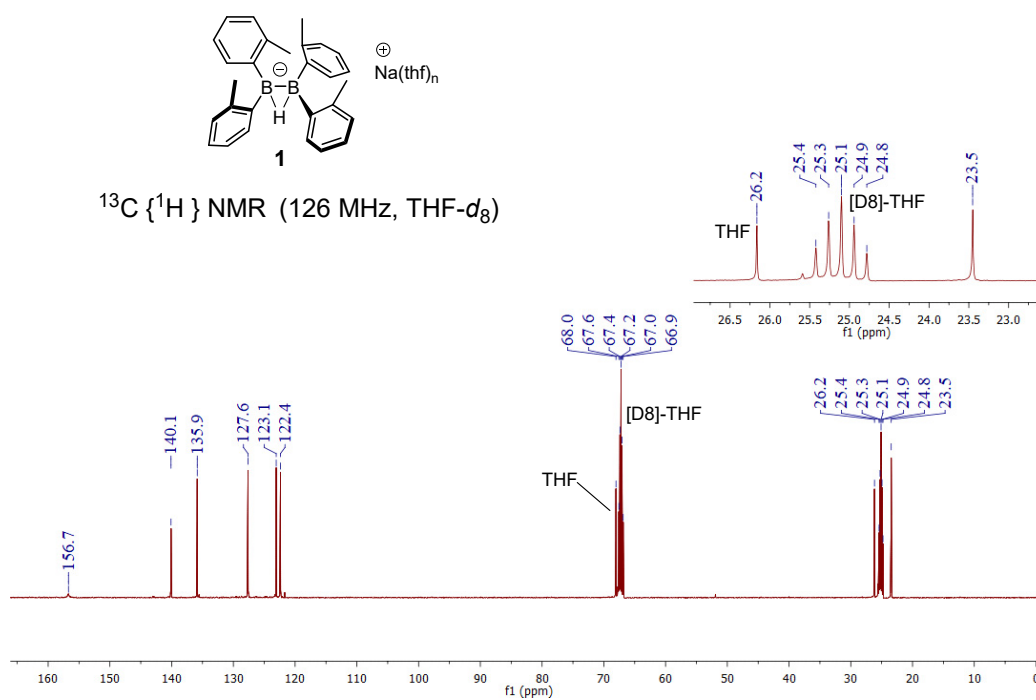


Figure S3. $^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of Compound **1** (126 MHz, THF- d_8).

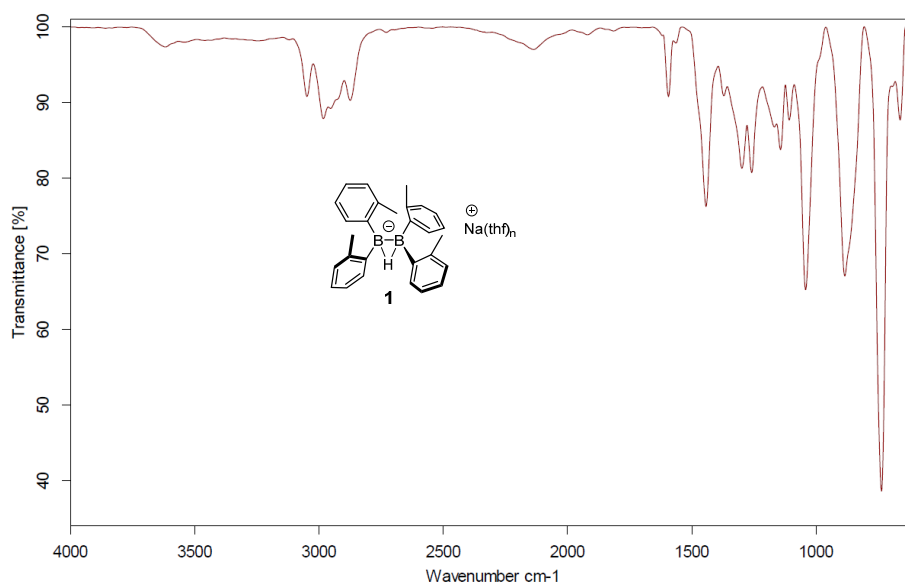


Figure S4. IR spectrum of compound **1**.

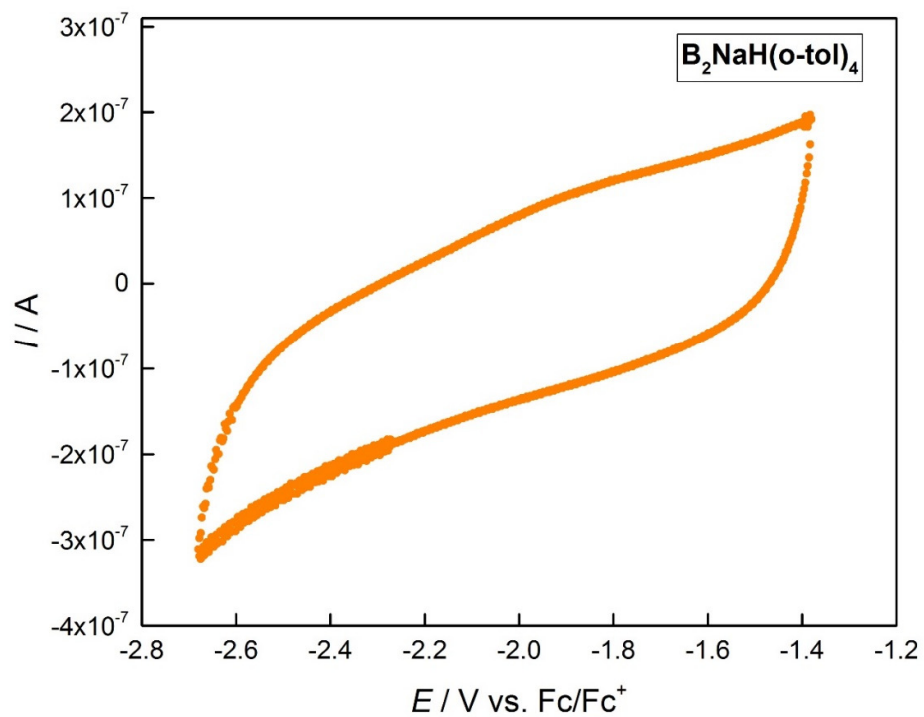
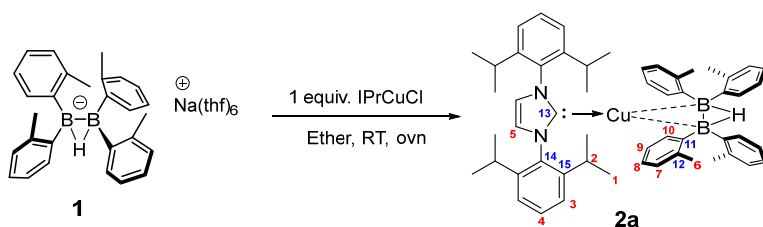


Figure S5. Cyclic voltammogram of **1** (1 mM) in THF (electrolyte: 100 mM $[nBu_4N][PF_6]$, working: platinum carbon, reference: Ag/Ag^+ , counter: Pt wire; Scan rate: 50 mV/s.).

Synthesis of 2a



To a diethyl ether solution (25 mL) of complex **1** (61.8 mg, 0.073 mmol) was added IPrCuCl (35.7 mg, 0.073 mmol), and the reaction mixture was stirred at room temperature for 12 hours. The resulting suspension was filtered through a pad of celite to remove the inorganic salts. Removal of the volatiles from the filtrate under reduced pressure gave **2a** as a white powder (50.0 mg, 0.060 mmol, 81% yield). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a diethyl ether solution at room temperature.

¹H NMR (400 MHz, C₆D₆): δ = 7.24 (t, J = 7.8 Hz, 2H, H₄), 7.14 (d, J = 7.1 Hz, 4H, H₁₀), 7.06 (d, J = 7.8 Hz, 4H, H₃), 7.04 – 6.97 (m, 8H, H₈&H₇), 6.57 (t, J = 6.6 Hz, 4H, H₉), 6.17 (s, 2H, H₅), 2.81 – 2.69 (m, 4H, H₂), 1.98 (s, 12H, H₆), 0.95 (d, J = 6.8 Hz, 12H, H₁) 0.91 ppm (d, J = 6.8 Hz, 12H, H₁).

¹³C{¹H} NMR (101 MHz, C₆D₆): δ = 180.3 (C₁₃), 149.4 (C₁₁), 145.3 (C₁₅), 140.6 (C₁₂), 135.9, 135.8 (C₁₄, C₁₀), 130.7 (C₄), 129.9 (C₇), 125.1, 124.6, 124.4, 124.2 (C₃, C₅, C₈, C₉), 28.5 (C₂), 25.1 (C₆), 22.8 (C₁), 22.6 ppm (C₁).

¹¹B{¹H} NMR (128 MHz, C₆D₆): δ = 24.3 ppm (br s, $h_{1/2} \approx 1697$ Hz).

¹¹B NMR (128 MHz, C₆D₆): δ = 24.3 ppm (br s, $h_{1/2} \approx 1781$ Hz).

mp: 149-151°C (dec.)

HRMS (ESI-MS): calculated for C₅₅H₆₅B₂N₂CuNa [M+Na]⁺: 861.4540. Found: 861.4512.

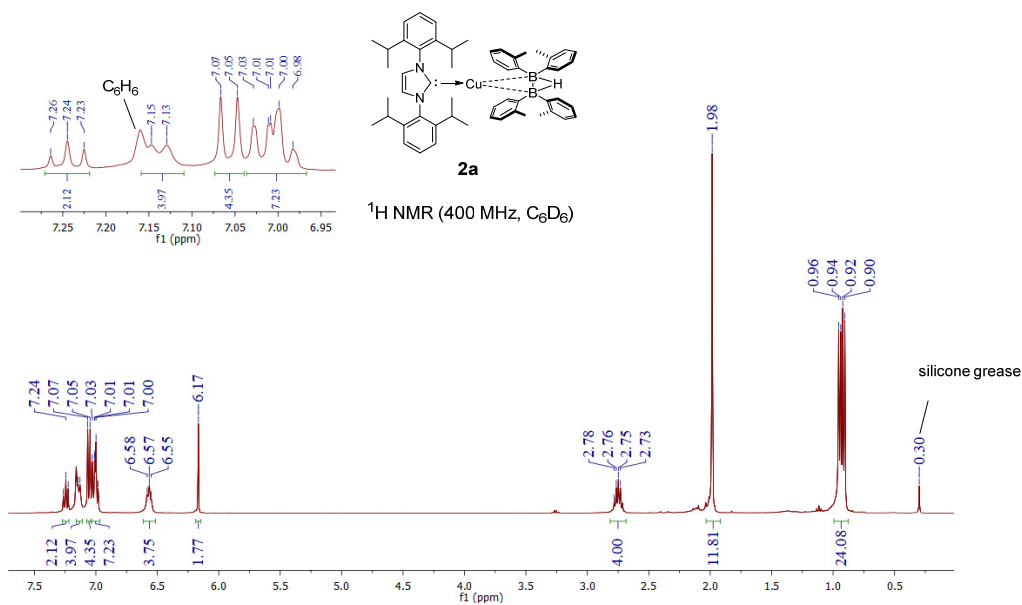


Figure S6. ^1H NMR spectrum of Compound **2a** (400 MHz, C_6D_6).

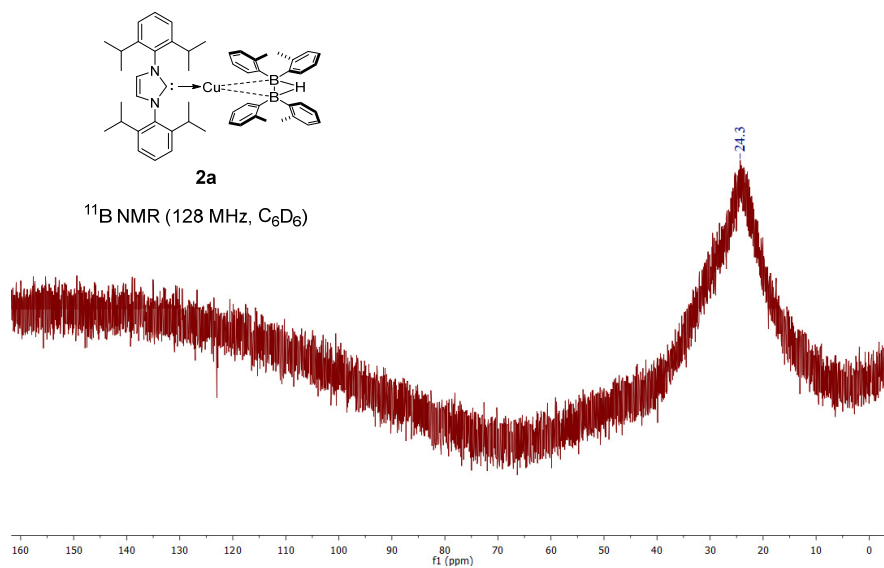


Figure S7. ^{11}B NMR spectrum of Compound **2a** (128 MHz, C_6D_6).

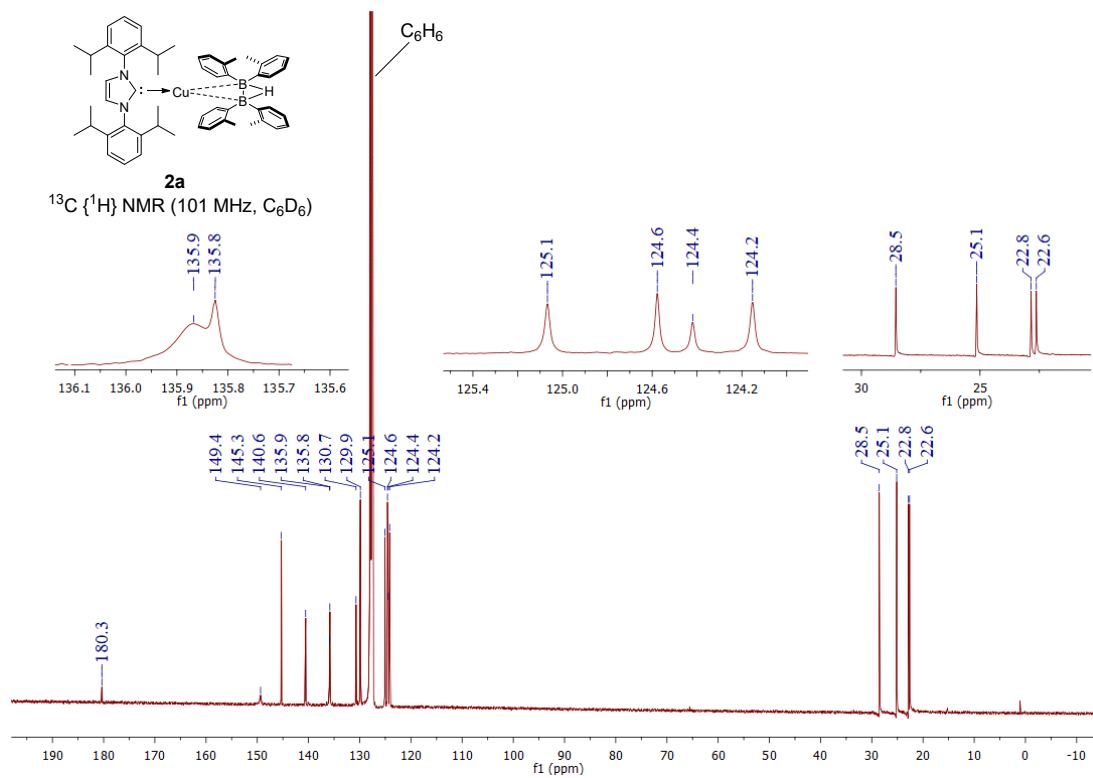


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of Compound **2a** (101 MHz, C_6D_6).

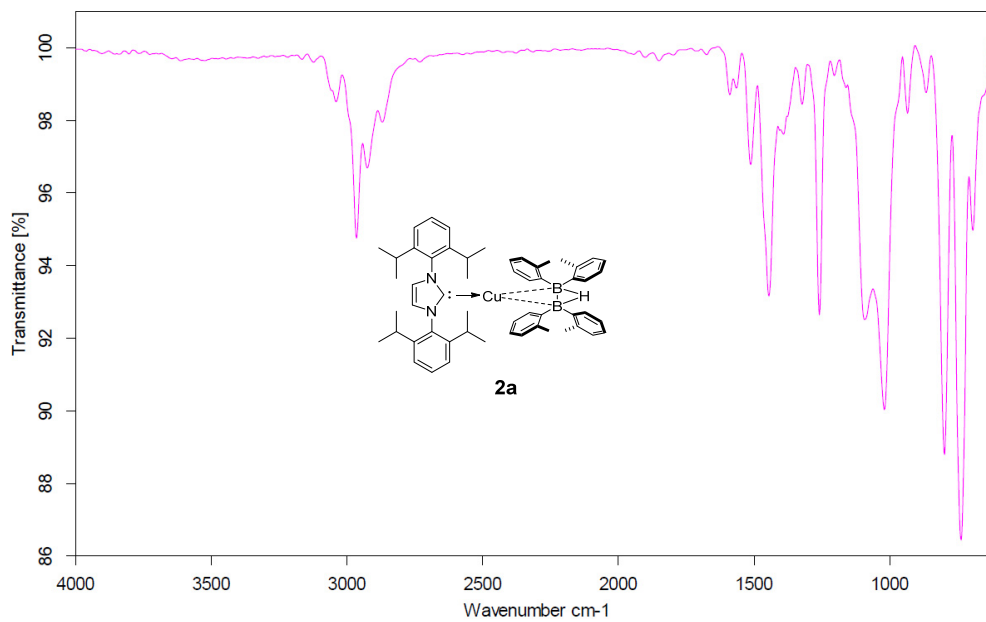


Figure S9. IR spectrum of compound **2a**.

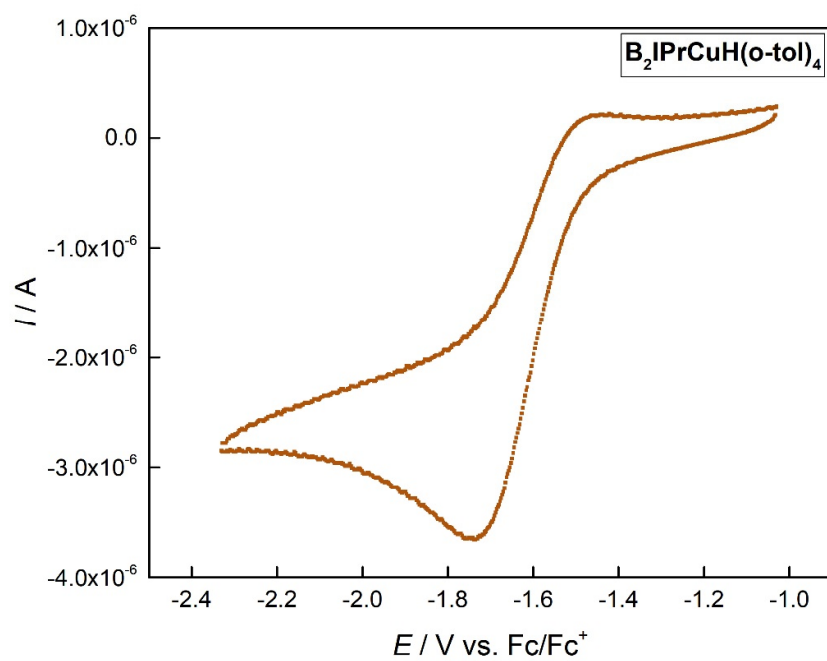
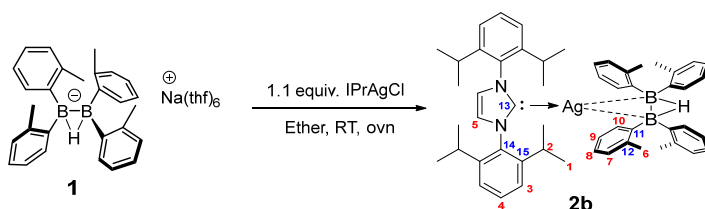


Figure S10. Cyclic voltammogram of **2a** (1 mM) in THF (electrolyte: 100 mM $[nBu_4N][PF_6]$, working: platinum carbon, reference: Ag/Ag^+ , counter: Pt wire; Scan rate: 100mV/s.).

Synthesis of 2b



To a diethyl ether solution (25mL) of complex **1** (138.3 mg, 0.16 mmol) was added IPrAgCl (95.7 mg, 0.18 mmol), and the reaction mixture was stirred at room temperature for 12 hours. The resulting suspension was filtered through a pad of celite to remove the inorganic salts. Removal of the volatiles from the filtrate under reduced pressure gave **2b** as a white powder (128.9 mg, 0.14 mmol, 89% yield). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a diethyl ether solution at room temperature.

¹H NMR (500 MHz, C₆D₆): δ = 7.25 (t, J = 7.8 Hz, 2H, H4), 7.13 (d, J = 7.3 Hz, 4H, H10), 7.05 (m, J = 8.2 Hz, 8H, H3&H8), 6.99 (d, J = 7.3 Hz, 4H, H7), 6.68 (t, J = 7.3 Hz, 4H, H9), 6.28 (s, 2H, H5), 2.70 (m, 4H, H2), 2.04 (s, 12H, H6), 1.00 (d, J = 6.8 Hz, 12H, H1), 0.93 ppm (d, J = 6.8 Hz, 12H, H1).

¹³C{¹H} NMR (126 MHz, C₆D₆): δ = 187.7 (dd, $J_{1(\text{Ag-C})}$ = 179 Hz, $J_{2(\text{Ag-C})}$ = 178 Hz, C13), 149.1 (C11), 145.6 (C15), 140.8 (C12), 136.9 (C10), 135.7 (C14), 131.1 (C4), 130.0 (C7), 125.4, 124.9, 124.7, 124.4 (C3, C5, C8, C9), 28.9 (C2), 25.1 (C6), 24.0, 23.4 ppm (C1).

¹¹B{¹H} NMR (160 MHz, C₆D₆): δ = 27.2 ppm (br s, $h_{1/2} \approx 702$ Hz).

¹¹B NMR (160 MHz, C₆D₆): δ = 27.2 ppm (br s, $h_{1/2} \approx 823$ Hz).

mp: 152-155°C (dec.)

HRMS (ESI-MS): calculated for C₅₅H₆₅B₂N₂AgNa [M+Na]⁺: 907.4299. Found: 907.4290.

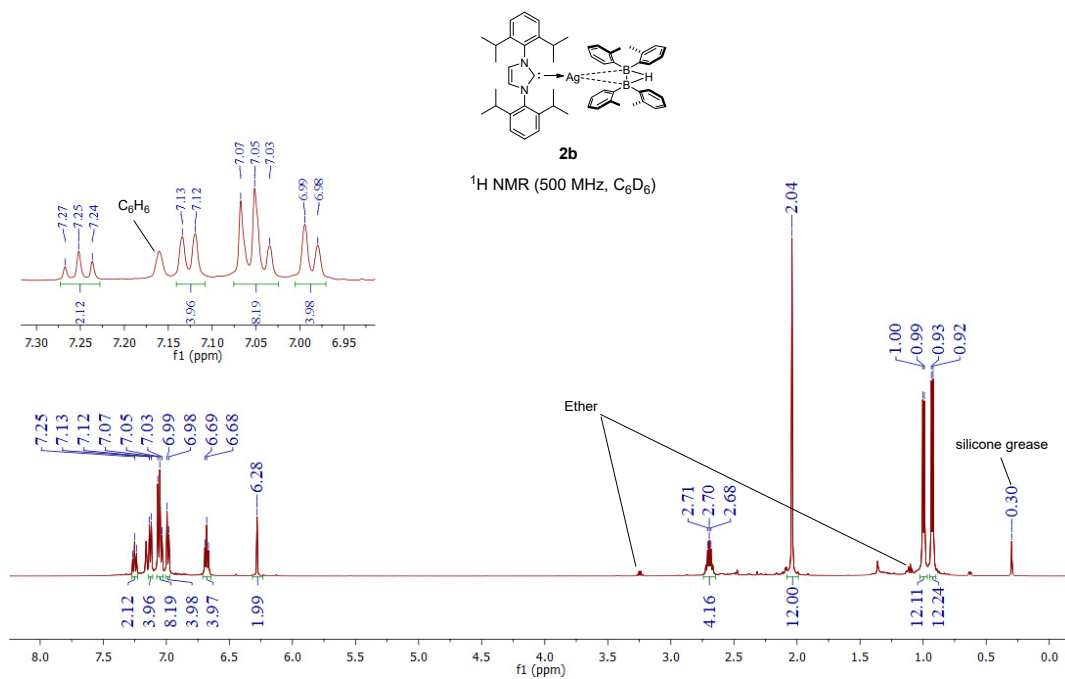


Figure S11. ¹H NMR spectrum of Compound **2b** (500 MHz, C₆D₆).

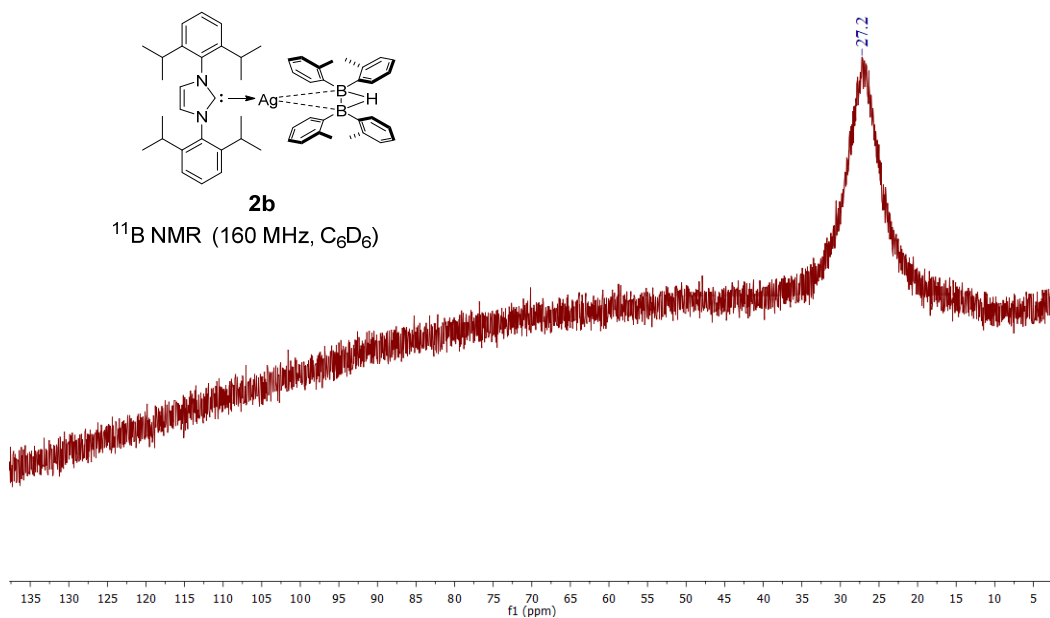


Figure S12. ¹¹B NMR spectrum of Compound **2b** (160 MHz, C₆D₆).

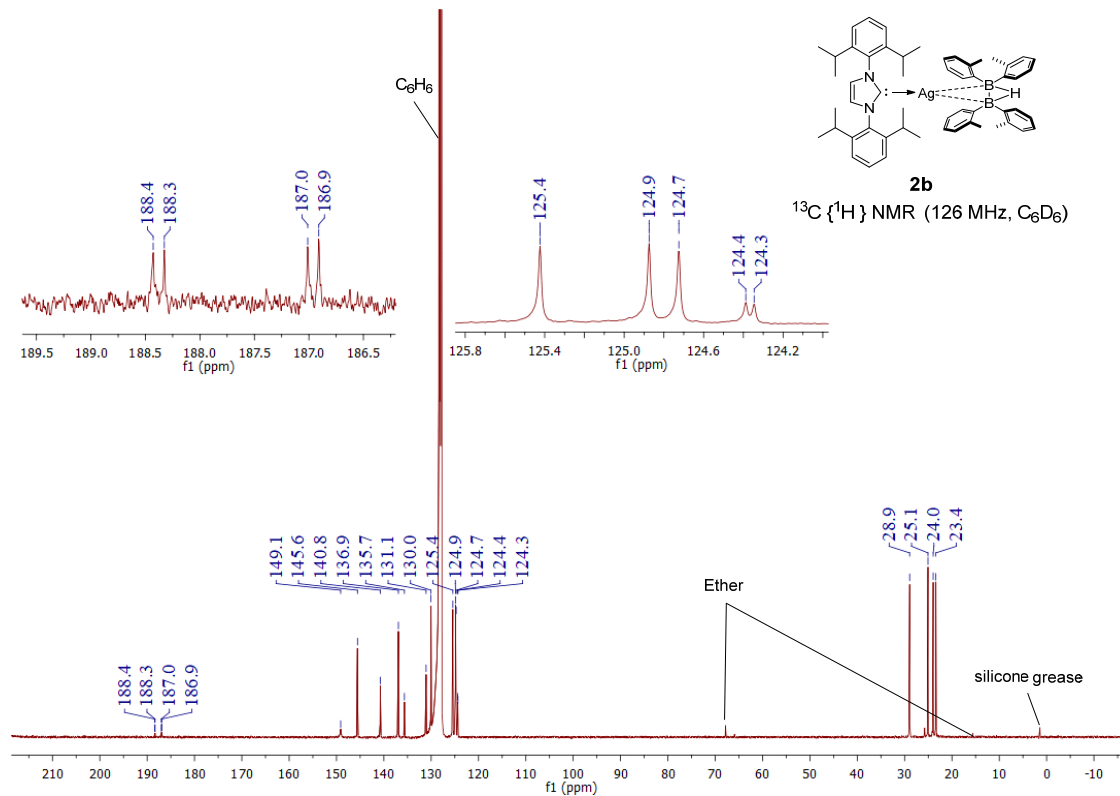


Figure S13. $^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of Compound **2b** (126 MHz, C_6D_6).

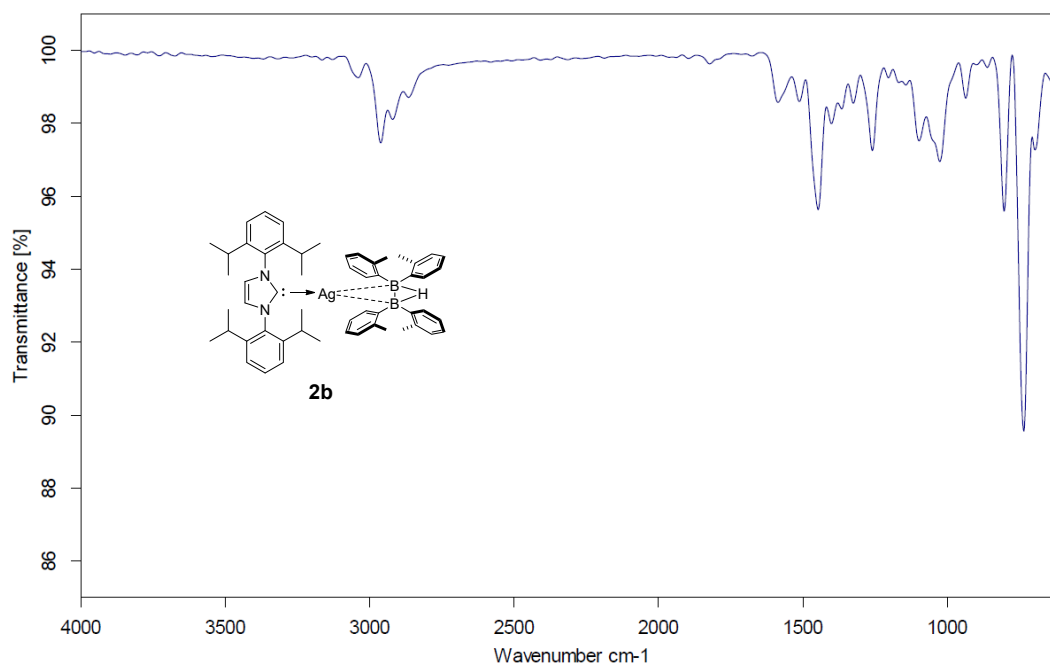


Figure S14. IR spectrum of compound **2b**.

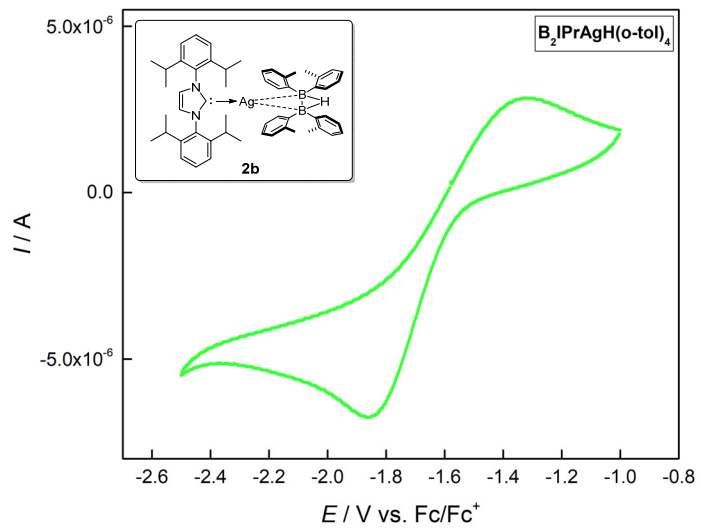
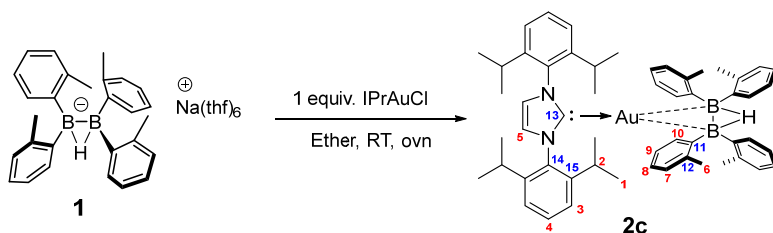


Figure S15. Cyclic voltammogram of **2b** (1 mM) in THF (electrolyte: 100 mM $[nBu_4N][PF_6]$, working: platinum carbon, reference: Ag/Ag^+ , counter: Pt wire; Scan rate: 100mV/s.).

Synthesis of 2c



To a diethyl ether solution (25 mL) of complex **1** (130.1 mg, 0.16 mmol) was added IPrAuCl (99.3 mg, 0.16 mmol), and the reaction mixture was stirred at room temperature for 12 hours. The resulting suspension was filtered through a pad of celite to remove the inorganic salts. Removal of the volatiles from the filtrate under reduced pressure gave **2c** as a white powder (132.9 mg, 0.14 mmol, 88% yield). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a diethyl ether solution at room temperature.

¹H NMR (400 MHz, C₆D₆): δ = 7.26 (t, *J* = 7.8 Hz, 2H, H4), 7.17 (d, *J* = 6.3 Hz, 4H, H10), 7.08 (d, *J* = 7.8 Hz, 4H, H3), 7.04 (dd, *J* = 7.3 Hz, 1.2 Hz, 4H, H8), 6.99 (d, *J* = 7.1 Hz, 4H, H7), 6.71 (t, *J* = 7.3, 6.4 Hz, 4H, H9), 6.31 (s, 2H, H5), 2.82 – 2.72 (m, 4H, H2), 2.12 (s, 12H, H6), 1.00 (d, *J* = 6.8 Hz, 12H, H1), 0.92 ppm (d, *J* = 6.8 Hz, 12H, H1).

¹³C{¹H} NMR (101 MHz, C₆D₆): δ = 201.3 (C13), 148.0 (C11), 145.5 (C15), 141.1 (C12), 137.2 (C10), 135.2 (C14), 131.2 (C4), 130.0 (C7), 125.6, 124.9, 124.4, 124.6 (C3, C5, C8, C9), 29.0 (C2), 25.4 (C6), 24.3 (C1), 23.1 ppm (C1).

¹¹B{¹H} NMR (128 MHz, C₆D₆): δ = 24.2 ppm (br s, *h*_{1/2} ≈ 754 Hz).

¹¹B NMR (128 MHz, C₆D₆): δ = 24.2 ppm (br s, *h*_{1/2} ≈ 1582 Hz).

mp: 154-157°C (dec.).

HRMS (ESI-MS): calculated for C₅₅H₆₅B₂N₂AuNa [M+Na]⁺: 995.4909. Found: 995.4887.

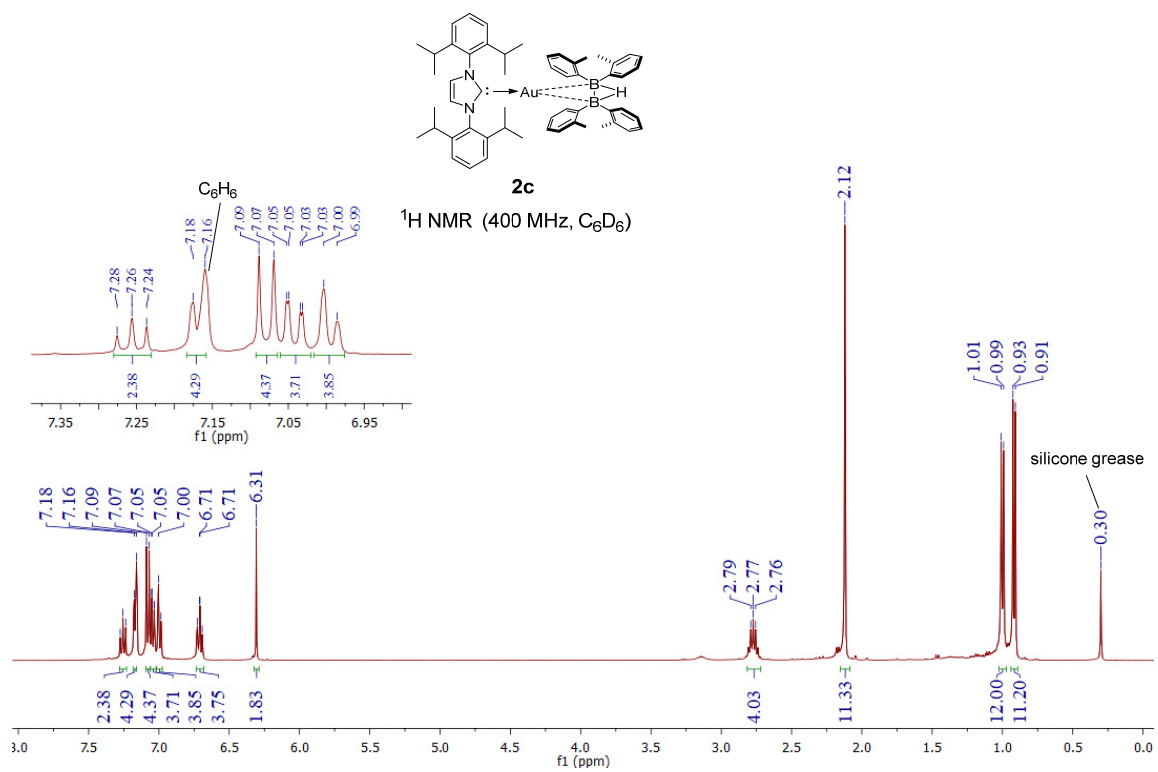


Figure S16. $^1\text{H NMR}$ spectrum of Compound **2c** (400 MHz, C_6D_6).

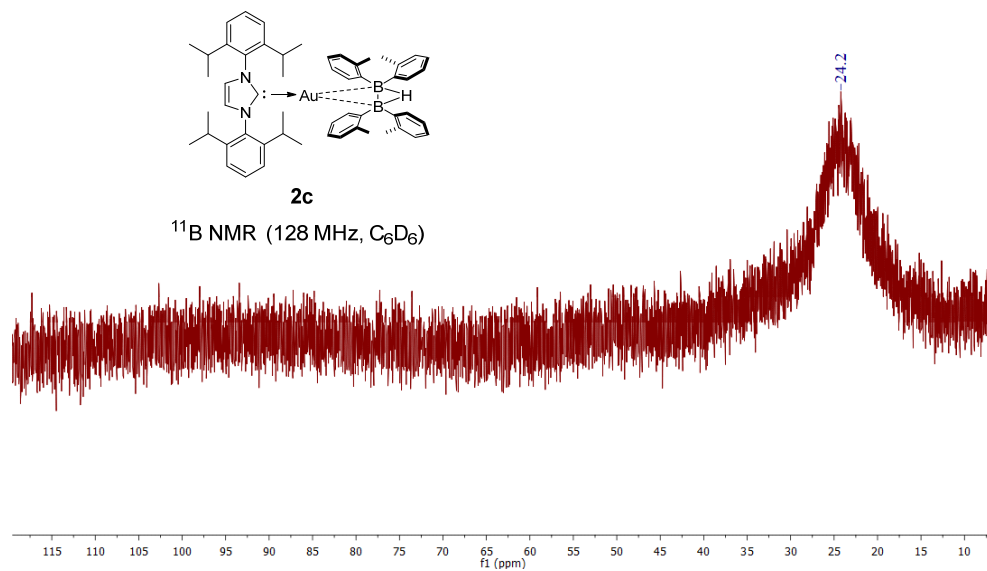


Figure S17. $^{11}\text{B NMR}$ spectrum of Compound **2c** (128 MHz, C_6D_6).

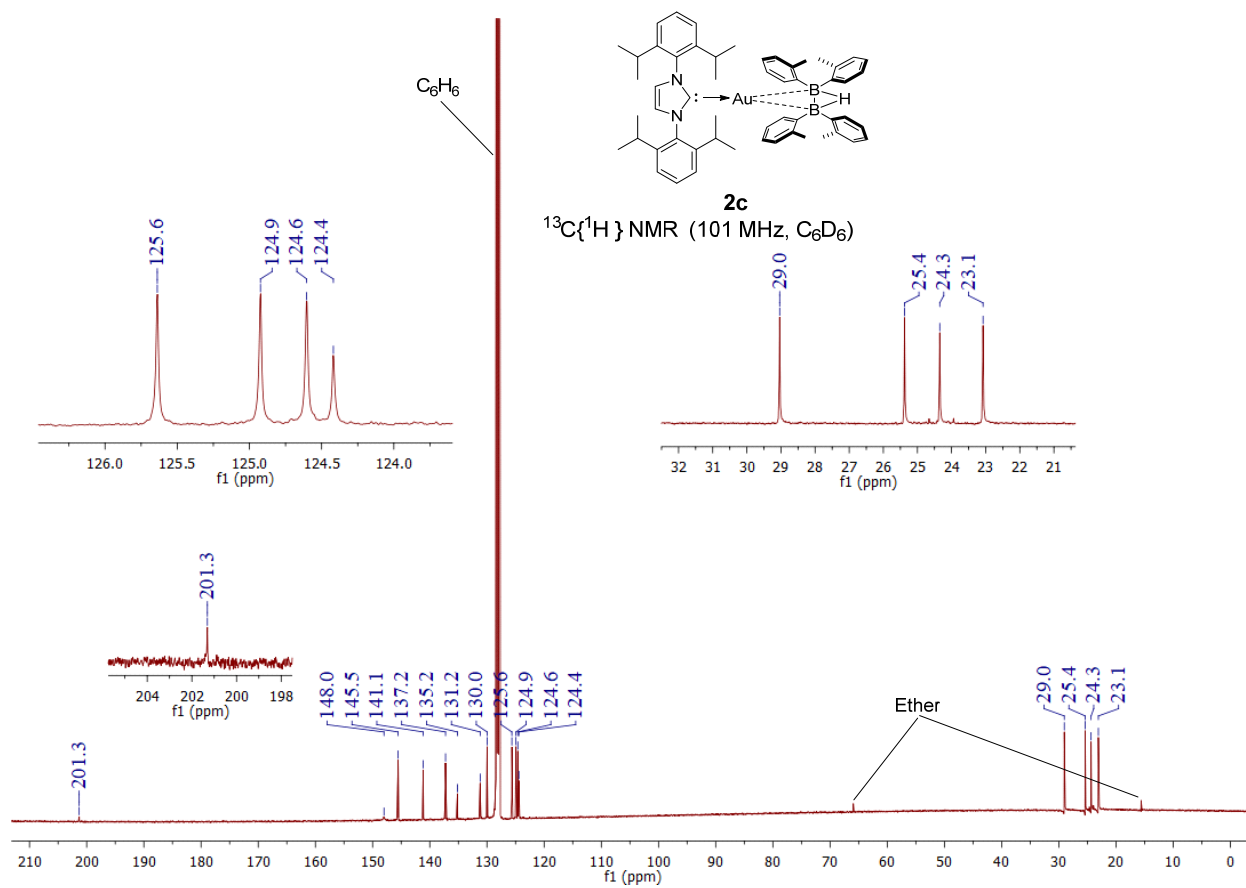


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of Compound **2c** (101 MHz, C_6D_6).

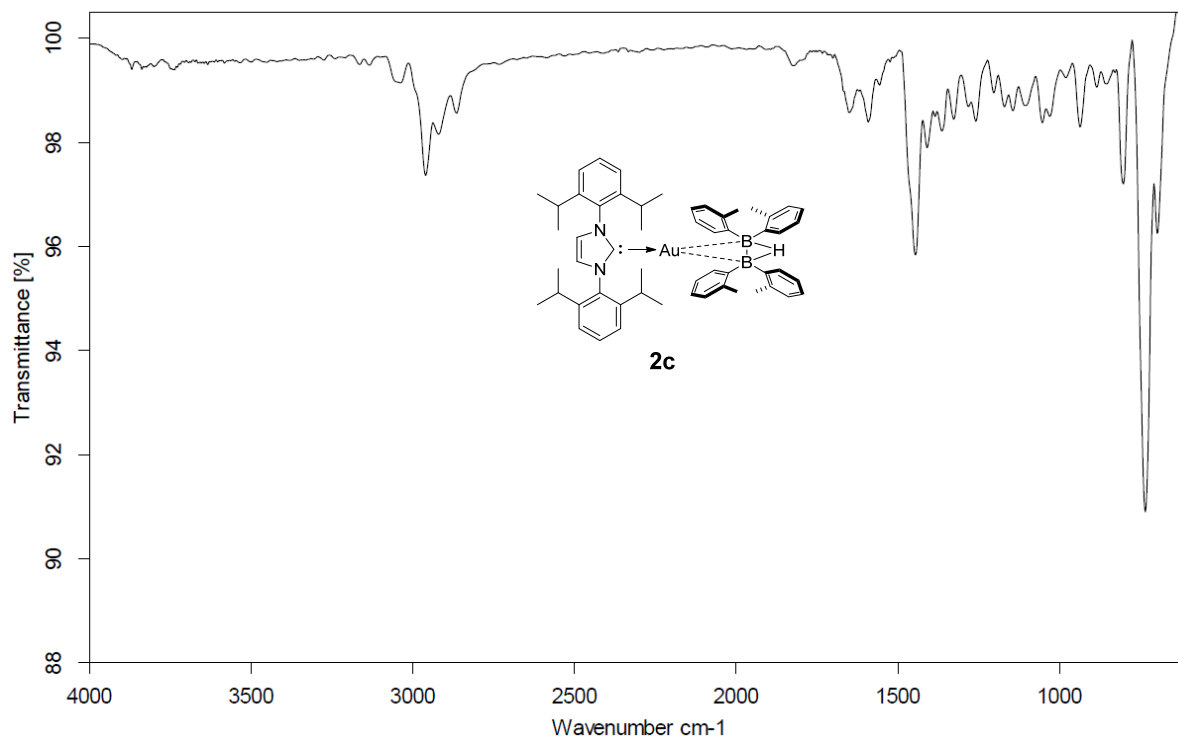


Figure S19. IR spectrum of compound **2c**.

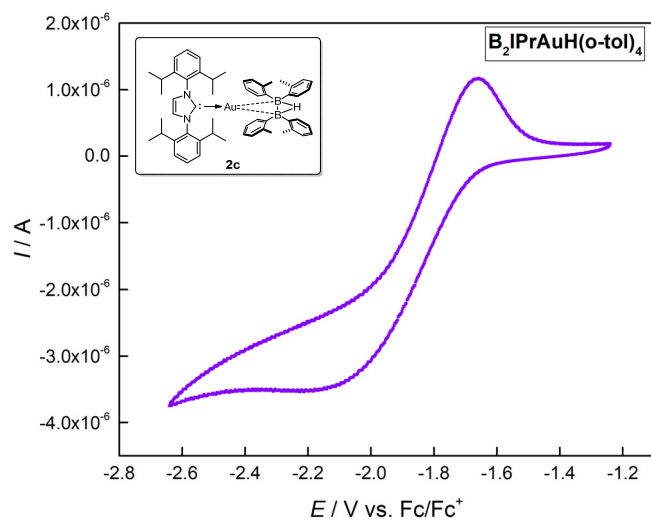


Figure S20. Cyclic voltammogram of **2c** (1 mM) in THF (electrolyte: 100 mM $[\text{nBu}_4\text{N}][\text{PF}_6]$, working: platinum carbon, reference: Ag/Ag^+ , counter: Pt wire; Scan rate: 100mV/s.).

Crystal Data

X-ray Structure Determination. Data were collected at 183(2) K for **1**, 173(2) K for **2a** and **2b**, 177(2) K for **2c** on Bruker D8venture Diffractometer. An empirical absorption correction was applied using the SADABS program.⁵ All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F^2 using the SHELXTL program package.⁶ All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and refinement are given in Table S1. Details of the crystal structures were deposited in the Cambridge Crystallographic Data Centre with CCDC 2133420-2133423 for **1**, **2a**, **2b**, and **2c**, respectively.

Table S1. Crystal Data and Summary of Data Collection and Refinement for **1**, **2a**, **2b**, and **2c**.

Compound	1	2a	2b	2c
Formula	C ₅₂ H ₇₇ B ₂ NaO ₆	C ₅₅ H ₆₅ B ₂ CuN ₂	C ₅₅ H ₆₅ B ₂ AgN ₂	C ₅₅ H ₆₅ B ₂ AuN ₂
Mw	842.74	839.25	883.58	972.67
Wavelength, Å	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space Group	P2 _{1/c}	C2/c	C2/c	Pbca
a, Å	12.5628(10)	13.3120(12)	13.3073(13)	21.161(4)
b, Å	13.3264(11)	19.989(2)	20.5224(19)	17.679(4)
c, Å	15.5838(13)	17.2387(17)	17.1012(15)	25.912(5)
α,deg	90	90	90	90
β,deg	106.231(2)	96.574(3)	96.418(3)	90
γ,deg	90	90	90	90
V, Å ³	2505.0(4)	4557.0(8)	4641.0(7)	9694(3)
Z	2	4	4	8
D _{calcd} , (Mg/m ³)	1.117	1.223	1.265	1.333
F(000)	916	1792	1864	3984
Crystal size, mm ³	0.50 x 0.40 x 0.30	0.40 x 0.30 x 0.20	0.40 x 0.30 x 0.20	0.50 x 0.40 x 0.30
2θ range, deg	4.092 to 50.498	4.758 to 50.488	4.638 to 50.498	4.97 to 50.496
No. of obsd reflns	4500	4126	4204	8764
No. of params refnd	277	274	274	545

Goodness-of-fit on F ²	1.048	1.032	1.066	1.119
R1	0.0711	0.0497	0.0469	0.0346,
wR2	0.2001	0.1254	0.1161	0.0670

Computational details.

Geometry optimizations were carried out with the Gaussian09 program, Revision D.01⁷ at the B3LYP⁸-D3⁹ level of density functional theory. The Los Alamos National Laboratory (LANL) effective core potentials (ECP) with the appropriate valence basis set of double- ζ quality (denoted LANL2DZ)¹⁰ was used for Cu, Ag and Pd while the 6-31G(d,p) basis set was used for all other atoms. Frequency calculations were made to determine the characteristics of all stationary points as energy minimum and obtain thermal corrections. Orbital energies of compound **2** were calculated at the B3LYP/6-311+G(d,p) level of theory. NBO analysis at the B3LYP/6-311+G(d,p) level of theory was carried out using the NBO program implemented in the Gaussian 09 package. LMO (Localized Molecular Orbital) analysis was performed using Multiwfn software.¹¹ The graphics of the molecular orbitals were produced by using the visualizing software VMD.¹²

Table S2. Selected second order perturbation energies $E^{(2)}$ in NBO analysis of **2a**.

donor NBOs	acceptor NBOs	$E^{(2)}_{ij} / \text{kcal mol}^{-1}$
193, $\sigma(\text{B-B})$	246, vacant $s(\text{Cu})$	54.28
61, occupied $p(\text{Cu})$	245, $\sigma^*(\text{B-B})$	1.18
197, occupied $d(\text{Cu})$	245, $\sigma^*(\text{B-B})$	3.46

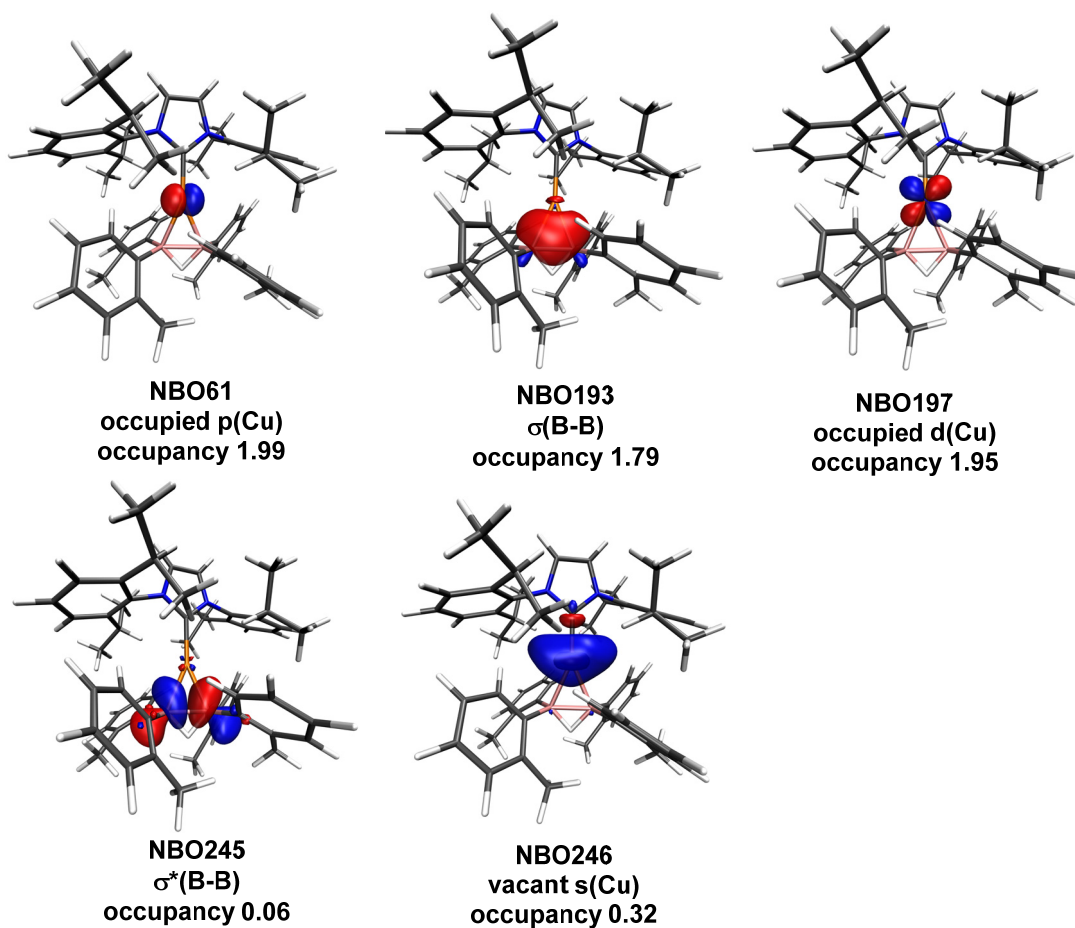
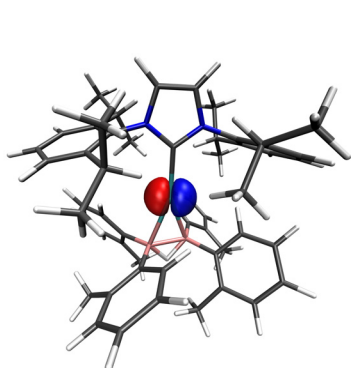
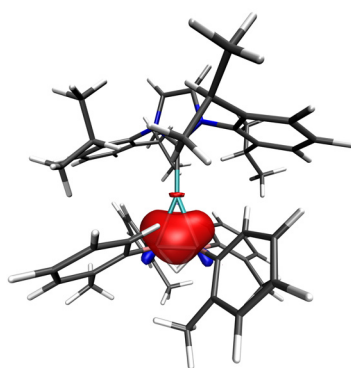


Table S3. Selected second order perturbation energies $E^{(2)}$ in NBO analysis of **2b**.

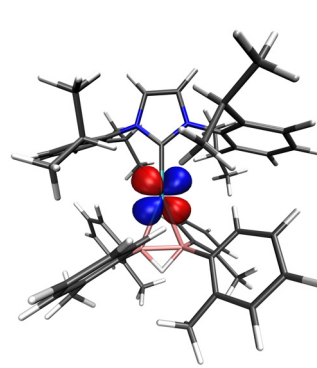
donor NBOs	acceptor NBOs	$E^{(2)}_{ij} / \text{kcal mol}^{-1}$
193, $\sigma(\text{B-B})$	245, vacant $s(\text{Ag})$	60.64
62, occupied $p(\text{Ag})$	246, $\sigma^*(\text{B-B})$	1.50
194, occupied $d(\text{Ag})$	246, $\sigma^*(\text{B-B})$	4.26



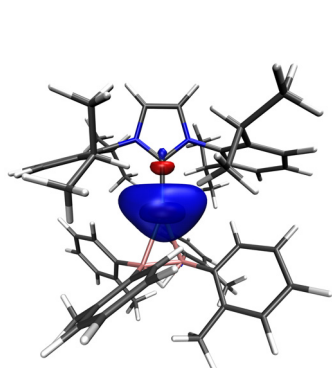
NBO62
occupied $p(\text{Ag})$
occupancy 1.99



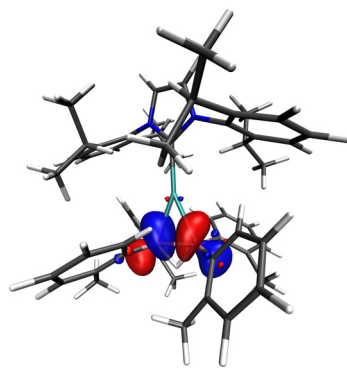
NBO193
 $\sigma(\text{B-B})$
occupancy 1.76



NBO194
occupied $d(\text{Ag})$
occupancy 1.95



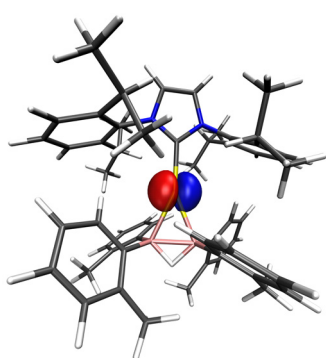
NBO245
vacant $s(\text{Ag})$
occupancy 0.37



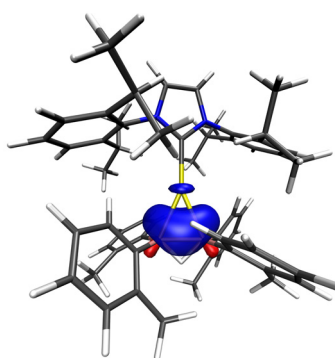
NBO246
 $\sigma^*(\text{B-B})$
occupancy 0.06

Table S4. Selected second order perturbation energies $E^{(2)}$ in NBO analysis of **2c**.

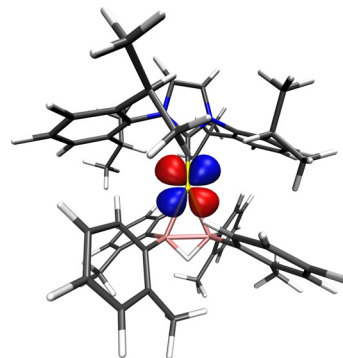
donor NBOs	acceptor NBOs	$E^{(2)}_{ij} / \text{kcal mol}^{-1}$
193, $\sigma(\text{B-B})$	228, vacant $s(\text{Au})$	174.27
62, occupied $p(\text{Au})$	246, $\sigma^*(\text{B-B})$	2.70
196, occupied $d(\text{Au})$	246, $\sigma^*(\text{B-B})$	9.61



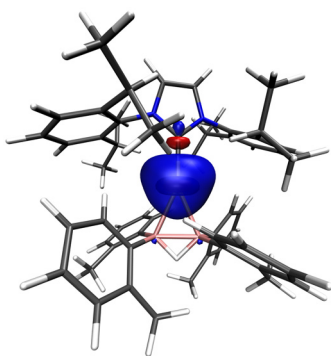
NBO62
occupied $p(\text{Au})$
occupancy 1.99



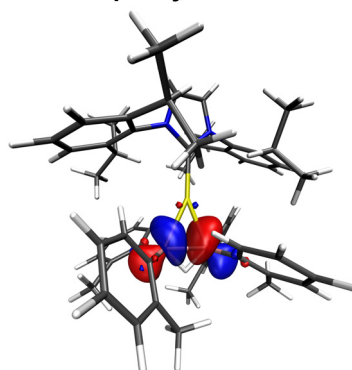
NBO193
 $\sigma(\text{B-B})$
occupancy 1.62



NBO196
occupied $d(\text{Au})$
occupancy 1.91



NBO228
vacant $s(\text{Au})$
occupancy 0.63



NBO246
 $\sigma^*(\text{B-B})$
occupancy 0.08

Table S5. NPA (natural population analysis) charge

	1	2a	2b	2c	$[(o\text{-tol})_2\text{BH}]_2$
B	0.144/0.165	0.123	0.154	0.231	0.416
H	0.102	0.096	0.091	0.057	0.088
M	0.601	0.490	0.456	0.271	--

Figure S6. Calculated Bond lengths of B-H and B-B bonds

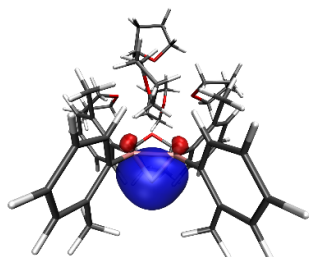
	1	2a	2b	2c	$[(o\text{-tol})_2\text{BH}]_2$
Bond length of B-H/Å	1.38	1.32	1.32	1.31	1.33
Bond length of B-B/Å	1.65	1.77	1.78	1.85	1.82

Figure S7. Experimental Bond lengths of B-H and B-B bonds in $[(o\text{-tol})_2\text{BH}]_2$.¹

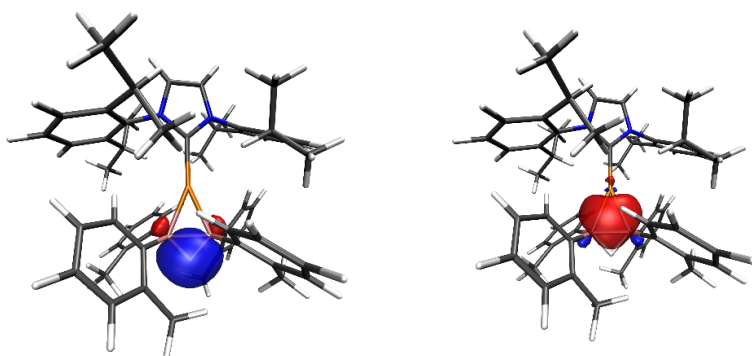
	$[(o\text{-tol})_2\text{BH}]_2$
Bond length of B-H/Å	1.26 / 1.33 / 1.33 / 1.31
Bond length of B-B/Å	1.832

Figure S21. Selected Localized Molecular Orbitals (LMO) of 3c-2e bonds in **1**, **2a-2c** and [(*o*-tol)₂BH]₂

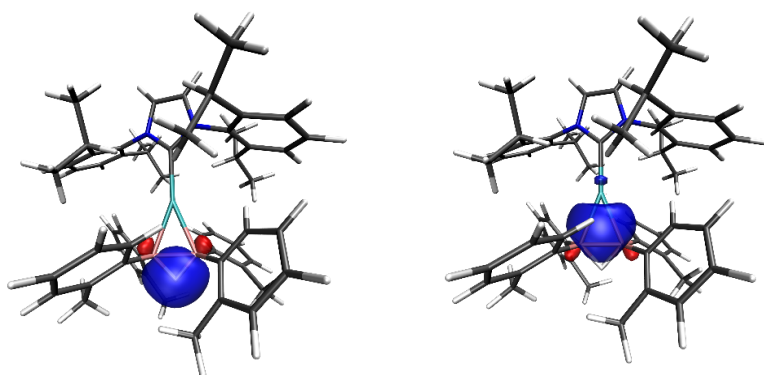
1



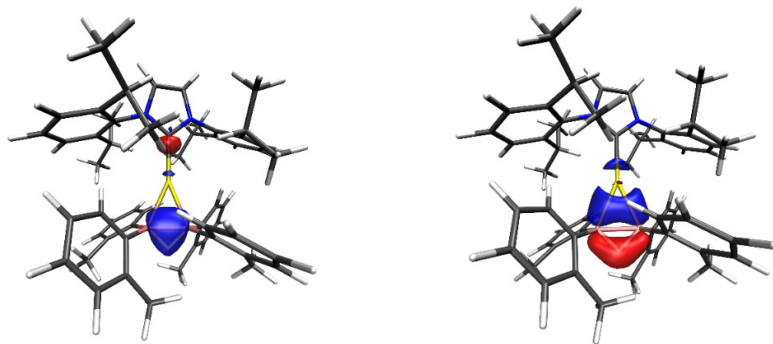
2a



2b



2c



[(*o*-tol)₂BH]₂



Cartesian Coordinates

1

Na	-3.50199500	-0.10921400	-0.00635900
O	-1.53856400	0.25830200	-1.13838200
O	-2.98464200	-2.38633800	-0.08309600
O	-4.80630500	-0.20690600	-1.99538200
C	-0.18825300	0.00642800	-0.63708200
H	-0.22902600	-0.83167400	0.06094700
H	0.16404600	0.89767300	-0.11192000
C	0.65016000	-0.26355000	-1.87767300
H	0.55319900	-1.31035100	-2.18376700
H	1.70535900	-0.05857000	-1.69591000
C	-0.01143000	0.66191900	-2.90640000
H	0.31077300	1.69266100	-2.73777800
H	0.20402200	0.39361200	-3.94431400
C	-1.49198600	0.50901600	-2.55471200
H	-2.09220600	1.40058700	-2.77204600
H	-1.94343600	-0.34366100	-3.08272100
C	-2.11262900	-2.97249400	-1.08233700
H	-1.08537300	-2.66433400	-0.88720300
H	-2.41845800	-2.58565500	-2.05993900
C	-2.30073800	-4.49279100	-0.97781700
H	-2.24960200	-4.98827400	-1.95069900

H	-1.52326600	-4.92541400	-0.33989800
C	-3.67305700	-4.62122000	-0.29707600
H	-3.81607800	-5.57523900	0.21727600
H	-4.48144400	-4.49873900	-1.02793500
C	-3.64141000	-3.42902300	0.65471600
H	-4.62055700	-3.04923600	0.95545100
H	-3.06100800	-3.66613100	1.55903000
C	-5.37449200	0.98478700	-2.58289700
H	-4.70691900	1.81990800	-2.36488300
H	-6.34441800	1.18371300	-2.10438700
C	-5.54229400	0.67041600	-4.06917000
H	-6.33585100	1.25798500	-4.53762900
H	-4.60760100	0.86581800	-4.60646300
C	-5.83180500	-0.83821800	-4.03678200
H	-6.87626600	-1.01952700	-3.75818700
H	-5.64080500	-1.34131700	-4.98793300
C	-4.89018300	-1.30533400	-2.92580200
H	-5.23935500	-2.18977600	-2.38380100
H	-3.88798300	-1.51515400	-3.32020600
O	-5.52877000	-0.70455400	1.15149900
O	-3.83067400	2.25802800	-0.07548500
O	-2.66059200	0.19806300	2.15711400
C	-6.78420900	-0.92549500	0.50007900

H	-6.59082900	-0.95525900	-0.57259700
H	-7.20939000	-1.88868500	0.82510000
C	-7.65956900	0.24763000	0.95528900
H	-7.48808100	1.10776400	0.30099300
H	-8.72640900	0.01140300	0.92578000
C	-7.14238700	0.54019200	2.38924600
H	-7.86300400	0.23410700	3.15209500
H	-6.94885800	1.60636500	2.53027700
C	-5.84120700	-0.29168800	2.49164900
H	-5.99458200	-1.18260900	3.11833700
H	-4.97412700	0.25646200	2.86196800
C	-4.73722000	2.89365400	0.84607000
H	-5.76373700	2.69521300	0.52076600
H	-4.59562100	2.44684400	1.83865900
C	-4.37655700	4.38200500	0.84288700
H	-4.60606700	4.87022100	1.79358600
H	-4.92174500	4.90704900	0.05055400
C	-2.87612000	4.33894200	0.52061300
H	-2.48902700	5.27784000	0.11755500
H	-2.29940500	4.08882000	1.41646000
C	-2.80317600	3.19305300	-0.48520500
H	-1.84749300	2.66733200	-0.50011500
H	-3.02953200	3.54373500	-1.50296200

C	-2.28335700	-0.98767300	2.89492700
H	-3.20257100	-1.51620500	3.16578600
H	-1.67574000	-1.63378000	2.25083200
C	-1.48220700	-0.47060800	4.08539800
H	-0.83140900	-1.23259300	4.52028200
H	-2.15675600	-0.10752600	4.87013100
C	-0.71610700	0.69483100	3.44380800
H	0.13813400	0.32198200	2.87176000
H	-0.34984200	1.42669800	4.16770800
C	-1.76250800	1.28478900	2.49408800
H	-1.32047600	1.68461100	1.57981600
H	-2.35420300	2.07466200	2.97642600
B	4.06164300	-0.77755500	0.14337000
C	2.77941900	-1.64781900	0.54200300
C	2.13929400	-1.50506600	1.79061900
H	2.52131500	-0.76431800	2.48676500
C	1.06997200	-2.30728400	2.19539600
H	0.64412900	-2.18152100	3.18662200
C	0.58421000	-3.29682100	1.34196300
H	-0.23462900	-3.94431800	1.64765000
C	1.19171400	-3.46088000	0.09453600
H	0.83431100	-4.24075500	-0.57647800
C	2.26985800	-2.66582200	-0.31194200

C	2.89260500	-2.92238600	-1.66339300
H	3.10904000	-1.98282900	-2.18124100
H	3.85087200	-3.44115400	-1.56281500
H	2.23794800	-3.52904900	-2.29893500
C	5.43270500	-1.61472200	0.00487100
C	6.10853100	-2.17731300	1.11664700
C	7.28800800	-2.90983900	0.92790600
H	7.79669600	-3.32723400	1.79506900
C	7.82151800	-3.11713300	-0.34403900
H	8.73678100	-3.69104100	-0.46617500
C	7.17002600	-2.57417300	-1.44945500
H	7.57235300	-2.71419700	-2.44997900
C	6.00311000	-1.83258400	-1.26083000
H	5.51191800	-1.40244900	-2.12885100
C	5.58163600	-1.99103600	2.52255600
H	6.22726600	-2.47936500	3.25963100
H	5.51472500	-0.92922400	2.78617100
H	4.57236600	-2.40292500	2.62705900
H	4.23454000	0.17097200	1.13444200
B	4.09513000	0.85530000	-0.05984000
C	5.49708100	1.57811700	-0.38992700
C	6.06471900	1.46883100	-1.67067900
H	5.54772800	0.86913700	-2.41406300

C	7.25998800	2.09499700	-2.02647500
H	7.65859500	1.97995800	-3.03167000
C	7.94387400	2.85296500	-1.07831500
H	8.88120400	3.34253700	-1.33069000
C	7.41353600	2.97234300	0.20622800
H	7.94675800	3.55897000	0.95219200
C	6.20583900	2.35591000	0.55962700
C	5.68421300	2.52513800	1.96973500
H	5.60000300	1.55967600	2.48207000
H	4.68364700	2.97001100	1.97324400
H	6.34354900	3.16385900	2.56632600
C	2.84507900	1.84140800	0.10287000
C	2.35457900	2.61637200	-0.98577900
C	1.29251500	3.50998800	-0.79981300
H	0.94269600	4.09553500	-1.64891100
C	0.69585000	3.69195800	0.45019100
H	-0.08968000	4.42999600	0.58020500
C	1.16161300	2.94457300	1.53133500
H	0.73172800	3.08320300	2.52049800
C	2.20631500	2.03595000	1.34591800
H	2.56862300	1.48219400	2.20680700
C	2.98574500	2.51044000	-2.35419100
H	2.36762000	2.98732200	-3.12219000

H	3.14865600	1.46522300	-2.63787400
H	3.97184700	2.98420500	-2.36725600

2a

Cu	0.00013900	-0.00304700	0.00056300
B	0.80708500	2.02301400	-0.34943700
N	1.06889900	-2.81740300	-0.13018500
C	2.09397200	2.15862500	0.59691800
C	2.34048500	3.24166800	1.48199900
C	1.40693100	4.42824200	1.59051400
H	1.12722400	4.81879900	0.60550100
H	0.47820000	4.16405000	2.10634900
H	1.87622000	5.24457400	2.14750800
C	3.49429200	3.24012600	2.27641100
H	3.66936800	4.07626900	2.95008500
C	4.42805500	2.20566400	2.21631500
H	5.31685300	2.23434500	2.84134500
C	4.21463700	1.15101400	1.33105400
H	4.93491700	0.34452700	1.24660500
C	3.06368300	1.14040300	0.54109700
H	2.91543200	0.31606300	-0.15024500
C	1.00721700	2.08003800	-1.95377100

C	2.02756200	2.82741300	-2.60974100
C	3.06342300	3.64488500	-1.86613500
H	2.60198900	4.31105300	-1.13278900
H	3.76316500	3.01371600	-1.31197800
H	3.63795000	4.26220200	-2.56341800
C	2.07477300	2.85976800	-4.01309700
H	2.85801200	3.44040600	-4.49559800
C	1.13968800	2.19371700	-4.80356500
H	1.20113400	2.25026000	-5.88726200
C	0.12995300	1.46329100	-4.18210500
H	-0.61998900	0.93735000	-4.76721500
C	0.08653500	1.41252700	-2.79055400
H	-0.72849000	0.86664500	-2.33209200
C	0.00304800	-1.97688700	-0.00226600
C	0.67771500	-4.15241500	-0.08687200
H	1.39221300	-4.95464900	-0.17264500
C	2.45353600	-2.43485300	-0.26581700
C	2.92300400	-2.01365400	-1.52504600
C	4.29382600	-1.74640100	-1.63083000
H	4.70233100	-1.40892300	-2.57516800
C	5.14401200	-1.90033700	-0.53927100
H	6.20436000	-1.69217100	-0.64938300
C	4.64206800	-2.29480100	0.69803100

H	5.31685500	-2.38124000	1.54165400
C	3.27913100	-2.55963400	0.86876000
C	1.98500300	-1.84313600	-2.71810500
H	1.06896800	-1.37358200	-2.34294600
C	1.60368900	-3.20227400	-3.33927200
H	0.91242100	-3.05028700	-4.17498500
H	2.49425400	-3.71127100	-3.72478300
H	1.11754300	-3.86688400	-2.62114200
C	2.54515700	-0.90965200	-3.79774300
H	1.78233000	-0.73336700	-4.55840700
H	2.81911200	0.06490600	-3.38593000
H	3.41738200	-1.34473300	-4.29895500
C	2.69776800	-2.89055000	2.24137100
H	1.88378000	-3.61094900	2.10284600
C	2.08502500	-1.62159700	2.86893200
H	1.63544200	-1.85160800	3.84116000
H	2.84644800	-0.84773900	3.00607800
H	1.30851600	-1.20209500	2.22737400
C	3.70760500	-3.53468200	3.20220400
H	3.19339100	-3.86652000	4.10941100
H	4.20198700	-4.40178300	2.75234900
H	4.48075600	-2.82403000	3.51250400
H	-0.00469300	2.99711800	0.00296900

B	-0.81373100	2.01981500	0.35288600
C	-2.10075900	2.15368200	-0.59352600
C	-2.35011200	3.23804100	-1.47621300
C	-1.42001200	4.42759800	-1.58165400
H	-1.14118100	4.81630100	-0.59565800
H	-0.49065600	4.16741900	-2.09840000
H	-1.89175800	5.24407800	-2.13635500
C	-3.50358200	3.23499500	-2.27110500
H	-3.68081900	4.07219000	-2.94290600
C	-4.43438100	2.19773200	-2.21374600
H	-5.32303100	2.22529700	-2.83903500
C	-4.21823200	1.14166400	-1.33083200
H	-4.93621600	0.33290500	-1.24851400
C	-3.06753100	1.13250600	-0.54048100
H	-2.91721300	0.30691200	0.14891200
C	-1.01419700	2.07312400	1.95737600
C	-2.03718500	2.81576100	2.61467200
C	-3.07600800	3.63082400	1.87255300
H	-2.61693000	4.30017100	1.14060100
H	-3.77334300	2.99821200	1.31704600
H	-3.65290000	4.24463500	2.57098000
C	-2.08434700	2.84566400	4.01808500
H	-2.86962200	3.42267100	4.50162700

C	-1.14673600	2.18178700	4.80739100
H	-1.20827100	2.23636600	5.89118400
C	-0.13440900	1.45606300	4.18465800
H	0.61754300	0.93196600	4.76884000
C	-0.09098200	1.40766400	2.79302300
H	0.72614600	0.86569700	2.33361800
N	-1.06069900	-2.82046800	0.12290400
C	-0.66623400	-4.15435300	0.07499600
H	-1.37870100	-4.95864700	0.15834000
C	-2.44609700	-2.44169700	0.26126300
C	-2.91493600	-2.02452200	1.52212500
C	-4.28622900	-1.76067700	1.63024200
H	-4.69433100	-1.42628100	2.57584300
C	-5.13747700	-1.91410200	0.53944700
H	-6.19815200	-1.70861600	0.65141700
C	-4.63627400	-2.30476700	-0.69933400
H	-5.31201400	-2.39102800	-1.54220600
C	-3.27293100	-2.56598700	-0.87246400
C	-1.97592400	-1.85446400	2.71452000
H	-1.06227000	-1.38001700	2.33971200
C	-1.58823000	-3.21412900	3.33056600
H	-0.89666300	-3.06206500	4.16601500
H	-2.47620000	-3.72818300	3.71535500

H	-1.10006600	-3.87423600	2.60966500
C	-2.53815500	-0.92687900	3.79815500
H	-1.77488800	-0.75017100	4.55829400
H	-2.81652900	0.04800600	3.39010600
H	-3.40793600	-1.36706200	4.29917600
C	-2.69265000	-2.89274300	-2.24655900
H	-1.87812900	-3.61305000	-2.11073000
C	-2.08126900	-1.62172400	-2.87131100
H	-1.63265600	-1.84884200	-3.84467000
H	-2.84329400	-0.84795900	-3.00548900
H	-1.30427400	-1.20345700	-2.22951900
C	-3.70299400	-3.53480100	-3.20821700
H	-3.18945700	-3.86376000	-4.11685100
H	-4.19641200	-4.40348300	-2.76035400
H	-4.47685800	-2.82371200	-3.51573800

2b

Ag	-0.00007500	-0.01598500	0.00007900
B	-0.80958800	2.18499800	-0.36672100
N	-1.06838900	-2.99659900	-0.11446100
C	-0.67694200	-4.33221600	-0.07446300
H	-1.39106800	-5.13629200	-0.14609800
C	-2.44267000	-2.56967600	-0.22181200

C	-3.23890100	-2.61937000	0.93764000
C	-4.58878100	-2.27723100	0.80037400
H	-5.23966600	-2.30264400	1.66695000
C	-5.10421500	-1.87914600	-0.43004200
H	-6.15338300	-1.61098000	-0.51423600
C	-4.27786500	-1.79326200	-1.54779800
H	-4.69129900	-1.44832400	-2.48780000
C	-2.92281600	-2.13730500	-1.47352400
C	-2.64174000	-2.93515100	2.30566500
H	-1.77744300	-3.59202700	2.16124500
C	-3.61246100	-3.66934300	3.24348700
H	-3.08519300	-3.98460300	4.14928000
H	-4.03977900	-4.55824200	2.76833500
H	-4.43821900	-3.02433500	3.56112800
C	-2.12641900	-1.63434900	2.95675800
H	-1.69583600	-1.84170100	3.94274300
H	-2.93673300	-0.90761200	3.07261800
H	-1.35599200	-1.16558700	2.34146500
C	-2.01635500	-2.05364700	-2.69789400
H	-1.02732700	-1.73658600	-2.35379400
C	-1.85831100	-3.43642900	-3.36200200
H	-1.45910500	-4.18042900	-2.66662900
H	-1.17400800	-3.37062100	-4.21463300

H	-2.82446800	-3.79999200	-3.72947000
C	-2.47910500	-1.00950700	-3.72301400
H	-1.71536700	-0.88916000	-4.49478500
H	-2.62913600	-0.02947700	-3.26281700
H	-3.40641600	-1.31198100	-4.22244900
C	-2.10850100	2.29622000	0.56811300
C	-3.07118700	1.26965200	0.49119800
H	-2.92410900	0.45880700	-0.21901200
C	-4.21852700	1.25159000	1.28494200
H	-4.93009200	0.43873300	1.18595700
C	-4.44048000	2.28519000	2.19371800
H	-5.32654500	2.29011000	2.82323500
C	-3.51932200	3.32905400	2.27021800
H	-3.70116000	4.14975200	2.96089000
C	-2.36743300	3.35925500	1.47245100
C	-1.44657200	4.55380700	1.60219800
H	-1.16106200	4.95760100	0.62417200
H	-0.52016000	4.29275800	2.12400100
H	-1.92898500	5.35960200	2.16338500
C	-1.00129400	2.22583500	-1.97363300
C	-0.08924100	1.54060100	-2.80782700
H	0.74392000	1.02055200	-2.35011700
C	-0.17422200	1.53073800	-4.19818000

H	0.56658700	0.99100300	-4.78248400
C	-1.21558000	2.21460900	-4.82110800
H	-1.31201200	2.21759500	-5.90374700
C	-2.13203500	2.90926600	-4.03397800
H	-2.93553600	3.46049800	-4.51781400
C	-2.04094200	2.94225400	-2.63269400
C	-3.05770400	3.78870700	-1.89488400
H	-3.61875200	4.41302900	-2.59699000
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H	-3.77171200	3.17758100	-1.33592300
C	-0.00145700	-2.16374100	-0.00027000
B	0.81264600	2.18370800	0.36748400
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C	3.07273500	1.26570000	-0.49156300
H	2.92463600	0.45454700	0.21807800
C	4.21989600	1.24659700	-1.28553700
H	4.93035400	0.43268900	-1.18725900
C	4.44314100	2.28054600	-2.19360400
H	5.32908000	2.28464100	-2.82330600
C	3.52344600	3.32576200	-2.26917600
H	3.70630000	4.14668800	-2.95930700
C	2.37176200	3.35702300	-1.47114200
C	1.45252200	4.55292800	-1.59992300

H	1.16746600	4.95626300	-0.62158600
H	0.52581200	4.29354300	-2.12204900
H	1.93606000	5.35854400	-2.16039800
C	1.00449900	2.22353900	1.97439200
C	0.09140700	1.53936900	2.80832600
H	-0.74248000	1.02066700	2.35039300
C	0.17629200	1.52898600	4.19868000
H	-0.56533000	0.99015800	4.78279000
C	1.21862700	2.21114000	4.82185500
H	1.31501300	2.21366100	5.90449800
C	2.13616700	2.90466100	4.03498000
H	2.94047100	3.45452700	4.51903200
C	2.04520100	2.93819800	2.63370100
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H	2.58732300	4.44610800	1.16908400
H	3.77582700	3.17140400	1.33633300
H	0.00213200	3.15886800	0.00072500
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C	0.67130300	-4.33309500	0.07304400
H	1.38442000	-5.13809600	0.14433000
C	2.43924600	-2.57281300	0.22102600
C	3.23538500	-2.62302100	-0.93847100

C	4.58564100	-2.28241000	-0.80113700
H	5.23646400	-2.30824000	-1.66774900
C	5.10155800	-1.88527400	0.42938200
H	6.15101000	-1.61823600	0.51360100
C	4.27536700	-1.79892900	1.54721700
H	4.68922500	-1.45480800	2.48733200
C	2.91993700	-2.14145500	1.47288100
C	2.63785800	-2.93777700	-2.30657800
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C	3.60777900	-3.67278900	-3.24458800
H	3.08017300	-3.98724300	-4.15046500
H	4.03413900	-4.56227100	-2.76966400
H	4.43423900	-3.02859300	-3.56205400
C	2.12393000	-1.63626600	-2.95734700
H	1.69307900	-1.84292600	-3.94335900
H	2.93503200	-0.91039400	-3.07308300
H	1.35405500	-1.16680500	-2.34190300
C	2.01367600	-2.05737200	2.69736300
H	1.02495300	-1.73910100	2.35351200
C	1.85419500	-3.44029200	3.36084200
H	1.45411600	-4.18352800	2.66515100
H	1.17004100	-3.37415500	4.21356800
H	2.81998300	-3.80509100	3.72805500

C	2.47766600	-1.01422300	3.72293500
H	1.71413300	-0.89338800	4.49483300
H	2.62878900	-0.03415400	3.26318700
H	3.40466800	-1.31798200	4.22216000

2c

B	0.84973100	2.04574500	-0.36770800
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C	1.38527200	4.53576200	1.45212500
H	1.14850400	4.88224100	0.43989800
H	0.43684200	4.28473300	1.93856700
H	1.82278700	5.37890800	1.99457500
C	3.46369100	3.40443300	2.25967400
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C	4.40341300	2.37436700	2.28082800
H	5.27430000	2.44244300	2.92759700
C	4.21815900	1.27049300	1.45046000
H	4.94440100	0.46438700	1.43040300
C	3.08931700	1.20752300	0.63248700
H	2.96661900	0.34364000	-0.01437400
C	1.05577500	2.16031200	-1.97164000

C	2.13810200	2.84201800	-2.60036300
C	3.22383200	3.58129100	-1.84432200
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H	3.88299100	2.90113400	-1.29842700
H	3.83742300	4.16625500	-2.53623900
C	2.22002300	2.87314800	-4.00326900
H	3.05624000	3.39474000	-4.46356200
C	1.26191100	2.27752800	-4.81976400
H	1.35682700	2.32838400	-5.90133600
C	0.18287800	1.62825800	-4.22511100
H	-0.59114700	1.16318000	-4.83003100
C	0.10221400	1.57425900	-2.83639700
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C	2.44170500	-2.53533300	-0.22249900
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C	4.26753700	-1.72516900	-1.53890300
H	4.67891400	-1.37019200	-2.47605300
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H	6.13206400	-1.50212000	-0.49341700
C	4.57557500	-2.20553300	0.81097400

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C	2.01459500	-2.02426800	-2.69869200
H	1.02209000	-1.71614000	-2.35726300
C	1.87496300	-3.41026000	-3.36011800
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H	2.84606800	-3.76316700	-3.72499200
H	1.48316800	-4.15813000	-2.66449300
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H	1.70129900	-0.86592300	-4.49704900
H	2.60166000	0.00564300	-3.26312700
H	3.39752900	-1.26631700	-4.22226300
C	2.63526600	-2.90899600	2.30487100
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C	2.12207000	-1.62012200	2.98052100
H	1.67766300	-1.84962700	3.95543600
H	2.93722300	-0.90454900	3.12669600
H	1.36544700	-1.12681000	2.36726700
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H	3.08166800	-3.98851900	4.13065900
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H	4.43714500	-3.02686600	3.55051600
H	-0.00070500	2.97540800	0.00082100

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C	-2.11586600	2.22253000	-0.60559100
C	-2.33264300	3.35363400	-1.43429600
C	-1.38725500	4.53623500	-1.44908200
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C	-3.46487600	3.40448500	-2.25818900
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H	-5.27475700	2.44204600	-2.92743600
C	-4.21830100	1.26937800	-1.45108700
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C	-3.08961900	1.20633200	-0.63289100
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C	-2.13999500	2.83926900	2.60155700
C	-3.22638200	3.57782400	1.84577300
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C	-2.22194000	2.86984400	4.00447500
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C	-0.10299500	1.57321300	2.83715900
H	0.75463700	1.07567500	2.40382500
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H	-2.60033600	0.00258500	3.26353500
H	-3.39600900	-1.26998700	4.22202000
C	-2.63447900	-2.90908000	-2.30609000
H	-1.76910900	-3.56233500	-2.15267600
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H	-1.67655500	-1.84892700	-3.95596500
H	-2.93592600	-0.90406600	-3.12670000
H	-1.36423600	-1.12712100	-2.36735800
C	-3.60586900	-3.66167300	-3.22885400
H	-3.08125700	-3.98718400	-4.13261200
H	-4.02660500	-4.54575200	-2.73899900
H	-4.43641000	-3.02550000	-3.55176600
Au	0.00004300	-0.05720300	0.00001500

[(*o*-tol)₂BH]₂

B	0.00642800	-0.91674000	0.00270900
C	1.40255300	-1.65828100	-0.06697200
C	2.32396400	-1.34028100	-1.07887500
H	2.08144500	-0.55131000	-1.78633300
C	3.54696100	-1.99661700	-1.19779300

H	4.23597700	-1.72761300	-1.99302200
C	3.87848300	-2.99221700	-0.28030500
H	4.82949300	-3.51240600	-0.35326200
C	2.98509500	-3.31477100	0.74141300
H	3.25115300	-4.08455600	1.46184400
C	1.74946100	-2.66735500	0.86275300
C	0.81551500	-3.05697500	1.98774400
H	0.45757800	-2.18143100	2.54096500
H	-0.07590300	-3.56692200	1.60848200
H	1.31189000	-3.72182700	2.69995100
C	-1.37935200	-1.67813400	0.07084400
C	-1.71441100	-2.68613600	-0.86422900
C	-2.94239100	-3.34853100	-0.74595300
H	-3.20007000	-4.11744800	-1.47031800
C	-3.83921800	-3.04188200	0.27762200
H	-4.78408300	-3.57350000	0.34793200
C	-3.51941200	-2.04710100	1.20020500
H	-4.21158300	-1.78995800	1.99661900
C	-2.30435600	-1.37558500	1.08429800
H	-2.07115900	-0.58669900	1.79488700
C	-0.77625900	-3.05770600	-1.99166000
H	-1.26342600	-3.72711800	-2.70599400
H	-0.43213400	-2.17481000	-2.54199700

H	0.12322300	-3.55571200	-1.61556300
H	-0.00006700	-0.00006600	-0.96339200
B	-0.00629800	0.91651700	0.00265800
C	-1.40245700	1.65805600	-0.06671000
C	-2.32394800	1.33990300	-1.07855200
H	-2.08153100	0.55078200	-1.78585700
C	-3.54692600	1.99624800	-1.19754000
H	-4.23598500	1.72713400	-1.99269200
C	-3.87838100	2.99199100	-0.28017100
H	-4.82938500	3.51219200	-0.35313600
C	-2.98495900	3.31463400	0.74148000
H	-3.25100500	4.08447500	1.46185700
C	-1.74933000	2.66720000	0.86287300
C	-0.81528300	3.05695700	1.98775500
H	0.07543300	3.56815000	1.60844100
H	-0.45613100	2.18141700	2.54014500
H	-1.31205300	3.72076400	2.70066000
C	1.37943900	1.67798300	0.07057300
C	1.71409700	2.68663600	-0.86396000
C	2.94202000	3.34911800	-0.74554500
H	3.19942600	4.11854800	-1.46946100
C	3.83914800	3.04195800	0.27762500
H	4.78394200	3.57368800	0.34804100

C	3.51970400	2.04656300	1.19966900
H	4.21208100	1.78902600	1.99577700
C	2.30471400	1.37494800	1.08361400
H	2.07177300	0.58557900	1.79377500
C	0.77555800	3.05909200	-1.99078600
H	1.26263400	3.72876900	-2.70493200
H	-0.12360400	3.55717800	-1.61403900
H	0.43093800	2.17663000	-2.54151400
H	0.00030400	-0.00012000	0.96879900

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